QUANTUM INFORMATION THEORETIC APPROACH TO EXPLORE NON-CLASSICAL CORRELATIONS AND UNCERTAINTY

A Thesis

Submitted for the Degree of

Doctor of Philosophy

to the **Jawaharlal Nehru University**

by

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DEDICATED TO

My Parents

&

to those who doubted me and didn't

Swagruhe Poojyathe Pithara:
Swagraame Poojyathe Prabhu:
Swadeshe Poojyathe Raja:
Vidwan Sarvathra Poojyathe!!!

Swagruhe (In his own house) Parents are respected and adored.
Swagraame(In his own village) A landlord or a rich man is respected and adored.
Swadeshe (In his own kingdom) The King is respected and adored.
But a Vidwan (a Scholar) is respected and adored all over the world.

Subhashita

DECLARATION

I, hereby, declare that this thesis is composed independently by me at Raman Research Institute, Bengaluru, India, under the supervision of Prof. Andal Narayanan. The subject matter presented in this thesis has not previously formed the basis of the award of any degree, diploma, associateship, fellowship or any other similar title in any other university. I also declare that I have run it through the **Turnitin** plagiarism software.

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CERTIFICATE

This is to certify that the thesis entitled "**Quantum information theoretic approach to explore non-classical correlations and uncertainty**" submitted by *Karthik H S* for the award of the degree of Doctor of Philosophy of Jawaharlal Nehru University is his original work. This has not been submitted to any other University for any other degree or diploma.

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First of all, I can't believe that five years have been completed since the day I set foot on this journey to get my doctorate. It is all like a dream. Some parts of this journey very vivid in memory yet the details like the starting and the ending of a dream, obscure. At first, the mere thought of joining the institute and to be amongst the scientific community was as scary and intimidating as confronting my own fears. This was the result of the naivety of being an university student. However, all these inhibitions were put to rest once I started to interact with the student as well as the academic members of the institute.

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SYNOPSIS

Non-classical features like non-locality, contextuality, temporal correlations, uncertainty draw attention both from the conceptual point of view and also in view of their impact on applications in quantum information technology. They offer insights into why/how quantum information protocols outperform their classical counterparts. Bringing forth new and distinct information theoretic signatures of non-classicality has attained renewed interest from this perspective. The importance of understanding the quantum-classical similarities/distinctions goes beyond the realm of foundational aspects and investigations in this direction are found to be significant in the new arena of quantum information technology. Entanglement, coherence and uncertainties are central features in the development of future quantum information technology. It is from this view that information theoretic approach to explore foundational notions is expected to throw light on aspects that are not envisioned so far.

Chapter 1 **is basically a brief introduction of the background needed to develop the content of the thesis.** It covers the essentials of the counter intuitive and puzzling features of quantum theory in brief.

In Chapter 2, we discuss the notion of uncertainties in the classical realm. More specifically, we address the question: how would the uncertainty product of canonical observables in the quantum realm compares itself with the corresponding dispersions in the classical realm? In this chapter, parallels between the uncertainty product of position and momentum in stationary states of quantum systems and the corresponding fluctuations of these observables in the associated classical ensemble are explored. Connection with area preservation in the underlying symplectic geometry of the classical phase space has also been identified. [1, 2, 3]

Macrorealism is a feature in the classical world that is at variance with the quantum description. In 1985, Leggett and Garg (LG) designed an inequality (which places bounds on certain linear combinations of temporal correlations of a dichotomic dynamical observable) to test whether a single macroscopic object exhibits classicality [4]. **In chapter 3, we discuss possible extensions of LG inequality to observables, which are not necessarily dichotomic. This is based on information entropies in contrast to second order correlations considered originally by LG. The entropic Leggett-Garg inequalities enlarges the platform for investigating the role of non-classicality (but not limited to) in biological processes** [5].

Quantum description being intrinsically statistical (probabilistic) in nature paves the way to seek how different is the nature of probabilities arising in the quantum world (in various physical situations) in comparison with that of its classical counterpart. Exploring the underlying nature of probabilities in the two domains helps to understand the physical context when classicality emerges from quantum world. It becomes highly pertinent to explore and contrast the attributes that form the characteristic features of both classical and quantum physics. If one believes in the notion that the latter theory subsumes the former, a relevant question would be to ask how does the correspondence set in. One of the ways to do that is through seeking the structure of probabilities arising under both the classical and the corresponding quantum scenario of the same physical situation. This forms the basis of various no-go theorems on non-locality, contextuality and absence of macro realism. **Chapters 4, 5, 6 focus on three distinct ways (sketched in the following) to probe the contrasting nature of quantum probabilities compared to their classical statistical counterparts.**

A. A sequence of moments obtained from statistical trials encodes a classical probability distribution. We discuss how moments realized in the context of quantum sequential measurements on a single quantum system encode the signature of quantum probabilities. This is based on a well-known issue of "moment inversion" (to determine the probabilities from the moments) in classical statistics. **We show that quantum moment inversion in connection with the sequential measurement of three observables brings out a clear distinction between quantum and classical scenario**.

B. Continuing further, we investigate whether a given set of moments, arising from correlation measurements of three dichotomic observables in the quantum scenario, corresponds to a legitimate grand joint probability distribution. A valid sequence of moments requires that the corresponding moment matrix be positive. **We**

bring out an interesting link between moment matrix and the structure of admissible joint probability distribution: positivity of the moment matrix necessarily enforces that the associated joint probabilities are of the hidden variable form. We discuss our results with the help of illustrative physical examples of spatial and temporal correlations arising within the quantum framework.

C. The uncertainty principle brings out intrinsic quantum bounds on the precision of measuring non-commuting observables. Statistical outcomes in the measurement of incompatible observables reveal a trade-off on the sum of their corresponding entropies. Maassen-Uffink entropic uncertainty relation [6] constrains the sum of entropies associated with the measurements of two non-commuting observables. However, a deterministic prediction is ensured when the system is entangled maximally with another party. Berta et al., [7] brought out the subtle interplay between uncertainty and entanglement by extending the entropic uncertainty principle in the presence of quantum side information (memory). Taking lead from our investigations on non-classical correlations in a single quantum system, we discuss an analogue of Berta et al. inequality by conditioning the measurements of a pair of discrete non-commuting observables in terms of the outcomes of a prior measurement. **We bring out the interesting association between non-classical temporal correlations and uncertainty. Our extended entropic uncertainty relation reflects that the presence of side information in a single quantum system too plays a significant role in beating the uncertainty bound. These results offer a unified view**

that prior quantum knowledge, achieved with the help of suitable spatially/temporally separated observations, reduces the intrinsic trade-off in the measurement outcomes of non-commuting observables, thus empowering their deterministic prediction.

The notion of incompatibility of measurements in quantum theory is in stark contrast with the corresponding classical perspective, where all physical observables are jointly measurable (JM). It is of interest to examine if the results of two or more measurements in the quantum scenario can be perceived from a classical point of view. Clearly, commuting observables can be measured jointly using projective valued measurements (PVM) and their statistical outcomes be discerned classically. However, compatibility of measurements with commutativity turns out to be limited in an extended framework, where the notion of sharp PVMs of self adjoint observables gets broadened to include unsharp measurements of generalized observables constituting Positive Operator Valued Measures (POVM). There is a surge of research activity recently [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19] towards gaining new physical insights on the emergence of classical behavior via joint measurability of unsharp observables.

Here, **we explore the entropic uncertainty relation for a pair of discrete observables (of Alice's system) when an entangled quantum memory of Bob is restricted to record outcomes of jointly measurable POVMs only. Within the joint measurability regime, the sum of entropies associated with Alice's measurement outcomes conditioned by the results registered at Bob's end are constrained to obey an entropic steering inequality. In this case, Bob's non-steerability reflects itself as his inability in predicting the outcomes of Alice's pair of non-**

commuting observables with better precision, even when they share an entangled state. The final chapter explains these observations in detail.

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PUBLICATIONS

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1. A.R. Usha Devi and **Karthik H. S.**.
   "Uncertainty relations in the realm of classical dynamics".
   Am. J. Phys. 80, 708 (2012).

2. A. R. Usha Devi, **Karthik H. S.**, Sudha, A. K. Rajagopal.
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   "Joint Measurability , Steering and Entropic Uncertainty".
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Other publications not included in this thesis:

8. A R Usha Devi, A K Rajagopal, Sudha, **Karthik H. S.**, J Prabhu Tej. *"Equivalence of classicality and separability based on P phase-space representation of symmetric multiqubit states"*. Quantum Inf Process, 12, 3717 (2013).

9. J. Prabhu Tej, A. R. Usha Devi, **Karthik H. S.**, Sudha, A. K. Rajagopal. *"Quantum which-way information and fringe visibility when the detector is entangled with an ancilla"*. Physical Review A, 89, 062116 (2014).

Contents

"Understand this: things are now in motion it cannot be undone"

Gandalf in THE RETURN OF THE KING

Chapter 1

An Introduction to Quantum Foundations

Quantum Theory has been the crowning jewel of twenty first century modern physics. Ever since its conception, it has been both the conservatives nightmare and turncoats delight! Its enigmatic features have captured the attention and imagination of researchers. Topics ranging from the meaning and interpretation of quantum theory to correspondence to our classical world have ever since occupied the discussions at conferences and dinner tables alike.

The advent of quantum theory was less of a smooth transition in itself. Newtonian (classical) mechanics was considered as *the* theory which explained all the phenomena observed in nature. Ranging from the most modest happenings around like the falling of an apple from the tree to the occurrences of the eclipses and the comets to the workings of a steam engine to the deflection of a magnetic needle when a flux of charges sprint across a rod of iron fell as the pieces into the structured markings of a grand puzzle, which was the *Universe.* Up until the end of the 18th century, the workings of the physical universe was thought to be completely understood as the mathematical machinery of classical mechanics provided the necessary apparatus to predict and perceive the happenings around us. Only when the murky dealings of the microscopic world (world of "smaller" dimension than the one which we, as human beings, are used to) started to befall the edifice of the established theory, did the purists give away to revisionists! As such the period from 1900s to 1930s saw one of the most tumultuous period in the history of physics. A new theory sprang to supersede the existing one. *Quantum theory was born.*

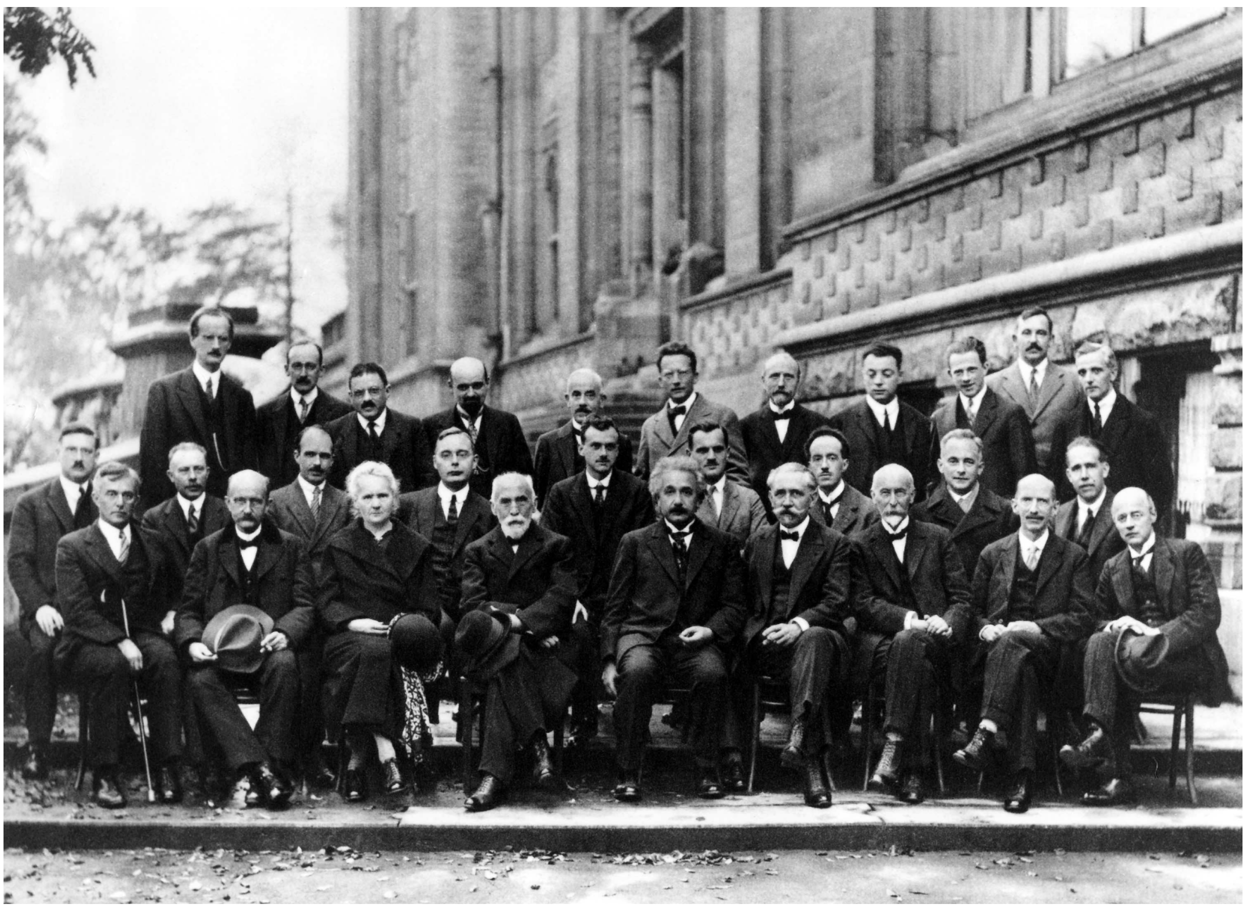

Figure 1.1: The fifth Solvay meeting of 1927 had all the stalwarts of modern physics participating. 17 of the 29 were/became Nobel laureates. Pic credit: Wikipedia

The chief architects of Quantum theory were Max Planck,Louis de Broglie Albert Einstein, Neils Bohr, Erwin Schrödinger, Werner Heisenberg, P A M Dirac. The fifth Solvay meeting of 1927 was an earmarked event on *Electrons* *and Photons.* The meeting was arranged to discuss the newly formulated quantum theory. Einstein was discontented with the outcome of the meeting and famously rebuked against the Heisenberg's uncertainty principle that *"God does not play dice"* to which Neils Bohr responded saying *"Einstein,stop telling God what to do"*.

> *"Einstein was unable to accept as final the wholly unorthodox mathematical formulation of Planck's quantum theory,...,since it did not correspond to his philosophical conceptions of the task of the exact sciences. He felt it disturbing that natural laws should have to relate not to objective processes but to the possibility or probability of such processes."*
>
> –Werner Heisenberg
> in Planck's Discovery and Atomic Theory

So, disenchanted was Einstein towards quantum theory that he would propose *gedanken* experiments (thought experiments) to bring out "flaws" in the logic of the theory to which Neils Bohr would respond in his own erudite manner. Bohr would first carefully study the problem and would try to convince Einstein that the apparent flaw arises due to the classical way of thinking. He would then try to resolve the "flaw" by using quantum mechanics. In one of such resolutions, he had used Einstein's own theory of relativity in explaining the apparent flaw in the proposed thought experiment.

Notwithstanding, Einstein came back with his full prowess in the form of his 1935 paper, famously known as the *EPR* paper. This work highlighted the incompleteness and the non local aspect of quantum theory.[1] Neils Bohr re-

[1] It is said that Einstein was not completely satisfied with the exposition of the ideas in the EPR paper. Apparently it was Nathan Rosen who drafted the final version. For more on what Einstein had in mind to say see [20, 21, 22]

sponded with a draft of his own but physicists found it to be too terse to comprehend the meaning of the content [20]. Erwin schrödinger followed suit with his own inspired version of the puzzling features of quantum theory [23]. It was he who caged the proverbial cat and gave it the famed status. Schrödinger's cat became the quintessential identity of the mysterious nature of quantum theory.

While all these developments seemed as if the quantum physicists were taking the question at hand seriously, the real issue of the interpretation of quantum mechanics took a back seat as the framework of quantum mechanics offered an excellent arena to resolve problems which had been nagging for a long period of time. Also, this offered a new perspective to physicists who were ready to accept the theory at face value and march ahead in applying the theory to understand the phenomena which sprang out as a result of the enigmatic operations of the microscopic constituents. Though some people kept their curiosity at bay with respect to the interpretations, John von Neumann [24, 25], David Bohm [26, 27] and others pursued it with complete zeal even when the said notion of investing time on foundational aspects were considered the work of a second rate mind. *Shut up and calculate* was the dictum!! [28]

It was around the 1960's that John Bell focused his attention in realizing the lifelong pursuits of Albert Einstein. It was he who, contrary to the reason, disproved the existence of a *hidden variable* description of quantum theory. He was inspired by the work of David Bohm who propounded the Non-local hidden variable distribution [29]. Once the results were established, experiments were performed to check the robustness of these results, in particular and quantum theory, in general. The verifications in terms of these observed results further strengthened the notion that nature is *inherently random*. That is, the physical world is inherently quantum mechanical. This important realization had to wait another two decades for physicists to pick up interest again and to learn the mind boggling implications of the theory. With this, *Quantum Information Science was born.*

Quantum information science is the study of quantum theory as seen through the eyes of an information theorist. Rolf Landauer, famously said that *Information is physical*. As such, quantum theory when studied in the language of information theory brought forth a whole new dimension in the way we see the world around us. Many queer aspects such as the Uncertainty relation, Superposition/Coherence, Entanglement were seen as resources through which real time applications in the security of communication, simulation of microscopic happenings etc could be envisioned. Foundational aspects looked in the language of information theory ushered in the development as well as the application of Quantum Information theory in a rapid manner. All of a sudden foundational aspects of quantum theory gained much importance and *Shut up and contemplate* became the new dictum!![30]

In the rest of this chapter, on the introductory and the necessary aspects needed for the development of this thesis, we give a brief glimpse into the rudiments of quantum mechanics, information theory, EPR argument, Local Realism and the Bell's Inequality, Uncertainty Principle, Macro Realism and the Leggett-Garg inequality.

1.1 Principles of Quantum Mechanics

Any physical theory necessitates the integration of physical notions, a mathematical framework and a set of conforming rules. Translation of the observed phenomena into the mathematical language requires the mapping of the physical notions to mathematical objects. This mapping requires the set of conforming rules mentioned earlier. Once a physical problem is translated in such a way to mathematical language, it is solved completely in mathematical terms without the botheration of what the physical interpretation might mean. This solution is then reverted back into the vocabulary of the physical world and interpreted accordingly. This is the whole essence of what is termed as the working of a theory. Quantum Theory is formulated in more or less the same way.

1.1.1 Physical notions of Quantum Theory

The main physical notions of quantum theory are the concept of the *state* of the system, *attributes* (observable properties) of the system, it's *evolution* and the *measurement* of the attributes. Akin to the idea of a classical phase space description of the systems wherein the "state" refers to the prescription of the coordinates and the conjugate momenta (which is the *complete* characterization of the system), the notion of the "state" of a quantum mechanical system is an identification of the probability distributions for the attributes of the system under study. These attributes or in other words, the observable properties of the system are recognized through the observables characterizing them.[1] Evolution of the system takes place due to the factors affecting the system such as its surrounding or an external interaction. A scheme to represent this is known as the *"equation of motion"* or the *"evolution equation"*. With the known initial conditions, once this is solved, the state of the system at all times is known in principle.

[1]For example, an object could be located through the observable "x"characterizing its position.

The final notion is that of measurement and modeling the process of measuring an observable is one of the quintessential problems of quantum theory. The root cause of this is due to the intrinsic randomness inherent in the workings of the microscopic world. This is tacitly expressed mathematically in the form of the *Uncertainty Principle* which inhibits the measurement of any two conjugate observables to arbitrary precision.

The state of any quantum mechanical system is denoted by ρ. As mentioned earlier, by "state" we mean the collection of all possible knowledge pertaining to the system, which is obtained by the identification of the probability distribution for the outcomes of measurements on observables of the system. In this sense, ρ denotes the complete specification of the state.

The conforming rules, which provide the mapping between the physical world to the mathematical framework of quantum theory are the postulates of the theory. These have been framed after a lot of rigmarole and physicists still continue to ponder about the motivation behind the origination of these postulates. For our purpose, it suffices to mention these postulates in the passing so that the functioning of the theory is grasped in terms of the working of these postulates.

Postulate 1: Every dynamical or physical system is described by a *State Operator or Density Operator ρ.*
This is also called as a Density Matrix when ρ is expanded with a complete orthonormal basis: $\rho = \sum_i \rho_i |\phi_i\rangle \langle\phi_i|$ (Orthonormality implies that $\langle\phi_i|\phi_j\rangle = \delta_{ij}$ for any $|\phi_i\rangle$ and completeness requires that $\sum_i |\phi_i\rangle\langle\phi_i| = \mathbb{I}$ where $\mathbb{I}$ is the identity operator.)
The Density matrix has the following properties:

$$\begin{aligned} \rho^{\dagger} &= \rho \;\text{(Hermiticity)} \\ Tr(\rho) &= 1 \;\text{(Normalization)} \\ \rho &\geq 0 \;\text{(Positive semi-definiteness)} \end{aligned} \tag{1.1}$$

The term "***density matrix***" refers to the collection of all the observable properties of the ***ensemble***.

A PURE state has to satisfy one more property that $\rho^2 = \rho \Rightarrow Tr(\rho^2) = 1$. In all those scenarios wherein the complete specification of the state is not possible, the concept of a MIXED state is introduced. Here, the total state of the system is represented as a weighted sum of the individual pure states constituting the system.
As an example, in an ensemble of N systems, N_1 of them could be in state ρ_1 , N_2 of them in ρ_2 and so on. Here, the total state is written as $\rho_{mix} = \sum_i p_i\, \rho_i^{pure} = \sum_i p_i\, |\psi_i\rangle\langle\psi_i|$ in contrast to a pure state where all the systems of the ensemble are specified by a single state $\rho_{pure} = |\Psi\rangle\langle\Psi|$.

For a pure state, the complete specification of the state can also be represented by the ket $|\Psi\rangle$ [1]. This is a vector in the Hilbert space which is a linear vector space with an inner product [2].

[1] The symbol $|\cdot\rangle$ is called *ket* and the corresponding $\langle\cdot|$ is known as *bra*. The existence of a bra corresponding to a ket is established by the Reisz theorem [31].

[2] A **Linear Vector Space (LVS)** $\mathcal{V}$ is a collection of objects **v**, called **vectors** that is closed under addition and multiplication by scalars. i.e, if $|\phi\rangle$ and $|\psi\rangle$ are two vectors belonging to $\mathcal{V}$ then so is a$|\phi\rangle$ + b$|\psi\rangle$. Here a and b are arbitrary scalars. If they are complex(real), then we have a complex(real) linear vector space. An inner product associates a scalar $\langle\phi|\phi\rangle$ with the ordered pair of vectors $|\phi\rangle$ and $|\psi\rangle$. $|\Phi_n\rangle$ is a Cauchy sequence if $\lim ||\psi_n - \psi_m|| \to 0$ as n,m tends to ∞. When $\lim_{n\to 0} |\psi_n\rangle = |\psi\rangle$ then $|\psi\rangle$ is called the Cauchy sequence limit point. However there is no guarantee that all Cauchy sequence limit points are inside the vector space. If the limit point of every Cauchy sequence in a LVS $\mathcal{V}$ is also in $\mathcal{V}$, then $\mathcal{V}$ is a *Complete* LVS. A complete LVS with

Any pure state $|\Psi\rangle$ can be expressed as a linear combination of the basis vectors as

$$|\Psi\rangle = \sum_i C_i \, |\phi_i\rangle$$

where $C_i = \langle\phi_i|\Psi\rangle$, the interpretation of which is to learn how much of $|\Psi\rangle$ points along $|\phi_i\rangle$. The summation index i runs through the dimension of the system. If the basis set is denumerable, then the expansion is as shown above, else we need continuous basis to express the state of the system. See any text book on quantum mechanics for more details [32, 33, 34].

Attributes of the system are represented by the ***Operators*** in Hilbert space.

Postulate 2: Physical observables or dynamical variables are represented by *Hermitian* operators.

An operator, say $\mathbf{A}$, is said to be hermitian if $\mathbf{A}^\dagger = \mathbf{A}$. Here, $\mathbf{A}^\dagger$ is the hermitian conjugate of $\mathbf{A}$. One might wonder as to how to associate values for an operator. A natural way to do it is to look at the *eigen*values of the operator. If $\mathbf{A}|\Psi\rangle = \lambda|\Psi\rangle$ then λ is an eigenvalue of $\mathbf{A}$ and $|\Psi\rangle$ it's eigen vector .The reason hermitian operators find their way in representing physical observables is due to the fact that their eigenvalues are real.
Position and Momentum of a particle are, for example, physical observables represented by hermitian operators $\mathbf{r}$ and $-i\hbar\nabla$.

Let $\mathbf{A}$ be an observable with $|\phi_i\rangle$ as it's orthonormal eigenstates. Then

$$\mathbf{A} = \sum_i \lambda_i \, |\phi_i\rangle\langle\phi_i| \qquad \text{(Spectral decomposition)}$$

an inner product is called Hilbert Space. For more on the math please refer [31].

This is the operator analog of expressing the state as linear combination of it's basis vectors. Consider,

$$\begin{aligned}\langle\Psi|\mathbf{A}|\Psi\rangle &= \langle\Psi|(\sum_i \lambda_i\,|\phi_i\rangle\langle\phi_i)|\Psi\rangle \\ &= \sum_i \lambda_i\,|\langle\phi_i|\Psi\rangle|^2 \\ &= \sum_i \lambda_i\,p(\lambda_i) \end{aligned} \tag{1.2}$$

This is observed as the ***average value*** or ***expectation value*** of the observable (operator) $\mathbf{A}$ in the state $|\Psi\rangle$. The λ_i's occur with probability $p(\lambda_i) = |\langle\phi_i|\Psi\rangle|^2$.

In terms of the density matrix, the ***expectation value*** of the observable $\mathbf{A}$ in the state $\rho = |\Psi\rangle\langle\Psi|$ is given by

$$\langle\mathbf{A}\rangle = Tr(\rho\,\mathbf{A}) = Tr(|\Psi\rangle\langle\Psi|\,\mathbf{A}) = \langle\Psi|\,\mathbf{A}\,|\Psi\rangle \tag{1.3}$$

An example of a state

A two dimensional state in quantum mechanics is known as a **Qubit**. The state of the qubit is usually represented as the linear ***superposition*** of the basis states $|0\rangle$ and $|1\rangle$.

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \tag{1.4}$$

with the constraint that $|\alpha^2| + |\beta^2| = 1$. The kets $|0\rangle$ and $|1\rangle$ are called as *Computational basis states*. These are the eigenstates of one of the *Pauli sigma* matrices $\boldsymbol{\sigma}_z$ and form an orthonormal basis set in the two dimensional Hilbert space.

The Pauli sigma matrices are

$$\boldsymbol{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \qquad \boldsymbol{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \qquad \boldsymbol{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The two states $|0\rangle$ and $|1\rangle$ are analogous to the classical bits 0 and 1 but the difference between a bit and a qubit is that a qubit can take states other than $|0\rangle$ and $|1\rangle$ as *superposition* is allowed in quantum theory. A bit can be identified to be in a state 0 or 1 whereas a qubit cannot be identified as to which state it is in, that is, to know the values of α and β in (1.4). The coefficients α and β are the *probability amplitudes* whose modulus square gives the probability of the qubit being in $|0\rangle$ and $|1\rangle$ respectively. The constraint $|\alpha^2| + |\beta^2| = 1$ is known as the *normalization* condition and it implies that the state of the qubit is a unit vector in the two dimensional Hilbert space.
In terms of the density matrix, the state of the qubit can be represented as

$$\rho = \frac{1}{2}\left[\mathbb{I} + \boldsymbol{\sigma} \cdot \mathbf{a}\right]$$

where $\mathbf{a}$ is the vector which characterizes the qubit. That is, the specification of the three parameters a_x, a_y, and a_z is required for determining the state of the qubit.

Postulate 3: The evolution equation for the state $|\Psi\rangle$ is given by the time dependent Schrödinger's equation;

$$-i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle \ \xrightarrow{\dagger}\ i\hbar\frac{\partial}{\partial t}\langle\Psi| = \langle\Psi|H \tag{1.5}$$

The solution of the equation is

$$|\Psi(t)\rangle = \mathbf{U}(t)|\Psi(0)\rangle$$

where $\mathbf{U}(t) = \exp^{\frac{-i\mathbf{H}t}{\hbar}}$ where $\mathbf{H}$ is the **Hamiltonian** of the system and $\mathbf{U}$(t) is the ***Unitary*** operator which transforms the system from time 0 to t. (An operator $\mathbf{U}$ is called as Unitary if it satisfies the equation $\mathbf{U}^\dagger = \mathbf{U}^{-1}$).

From this we can get the evolution equation for the density matrices which is known as the ***von Neumann*** equation which is the quantum analogue of the classical ***Liouville*** equation.

$$-i\hbar\frac{\partial}{\partial t}\rho = [\mathbf{H}, \rho] \tag{1.6}$$

The solution of the evolution equation is

$$\rho(t) = \mathbf{U}(t)\rho(0)\mathbf{U}^\dagger(t)$$

The last physical notion which we discuss in brief is that of ***measurement*** in quantum theory.

Postulate 4: The result of the measurement of any physical observable is always one of the eigenvalues of the corresponding hermitian operator.

Before moving ahead, let's ask the question: *what constitutes a measurement in quantum theory and what is expected out it?*
Looking at *measurement* as an *operation*, we expect the result at the end of this operation to be the probability distribution for the various eigenvalues accompanied by the eigenstates the original state reduces to.

$$|\Psi\rangle\langle\Psi| \xrightarrow{\quad Measurement \quad} \sum_i p_i\,|\phi_i\rangle\langle\phi_i|$$

where $p_i = |\langle\phi_i|\Psi\rangle|^2$ is the probability that the state $|\Psi\rangle$is indeed $|\phi_i\rangle$.

As an operator equation wherein the measurement of a state is seen as a transformation from one state to another, we introduce ***Projection Operator*** $\mathbf{\Pi}_i$. This operator $\mathbf{\Pi}_i = |\phi_i\rangle\langle\phi_i|$ projects any state on which it acts to $|\phi_i\rangle$ i.e, if we express any state $|\Psi\rangle$ as

$$|\Psi\rangle = \sum_i C_i|\phi_i\rangle,$$

then

$$\mathbf{\Pi}_j|\Psi\rangle = |\phi_j\rangle\langle\phi_j|\Psi\rangle$$

and the probability of getting the corresponding eigenvalue is

$$\begin{aligned} p_i &= |\langle\phi_i|\Psi\rangle|^2 = \langle\Psi|\,\mathbf{\Pi}_i\,|\Psi\rangle \\ &= Tr(\mathbf{\Pi}_i\,\rho) \end{aligned} \tag{1.7}$$

Note that this operation is not *Unitary*. The final state is not normalized. Thus, measurement has a separate status in quantum theory as it cannot be represented as a Unitary transformation.

The Projection operator satisfies the properties:

$$\begin{aligned} \mathbf{\Pi}_i &\geq 0 \\ \mathbf{\Pi}_i\mathbf{\Pi}_j &= \delta_{ij}\mathbf{\Pi}_j \\ \sum_i \mathbf{\Pi}_i &= \mathbb{I} \end{aligned} \tag{1.8}$$

Remark

Though the reduction of the original state to that of the projected one occurs in a single projective measurement ($\mathbf{\Pi}_j|\Psi\rangle = |\phi_j\rangle\langle\phi_j|\Psi\rangle$), it is not considered as a complete characterization of the measurement process. For a full characterization the following is the requirement:

$$|\Psi\rangle\langle\Psi| \xrightarrow{Measurement} \sum_i \mathbf{\Pi}_i|\Psi\rangle\langle\Psi|\mathbf{\Pi}_i$$

and in terms of the density matrix ρ,

$$\rho_{in} \xrightarrow{Measurement} \rho_{aft} = \sum_i \mathbf{\Pi}_i \, \rho_{in} \, \mathbf{\Pi}_i$$

1.1.2 The Uncertainty Principle

In classical mechanics, two conjugate observables can be measured simultaneously without affecting the state of the particle (system) or its subsequent evolution. However, in quantum theory, such a measurement is not possible unless the two operators representing the observables ***commute***. **Heisenberg's Uncertainty Principle** is a testament to this fact. This principle is one of the fundamental principles of quantum theory. It was enunciated by Werner Heisenberg.

> *"Here I am in an environment that is diametrically opposed [to our view], and I dont know whether I am just too stupid to understand mathematics. Gottingen is splitting into two camps. Some people, like Hilbert, talk of the great success achieved through the introduction of matrix calculus into physics, and others, like [James] Frank [the noted experimentalist], say that these matrices can never be understood. I am always angry when I hear the theory called nothing but matrix physics. ..'Matrix' is certainly one of the most stupid mathematical words in existence."*

–**Werner Heisenberg**
writing to Pauli

To dispel the smugness of the mathematicians and the bafflement of the physicists, Heisenberg had to discover a physical meaning for his matrices.The hardest facts to reconcile were the photographs taken of cloud chambers in which water droplets revealed the passage of an electron.

The recollection of a discussion with Einstein gave him the nudge to frame his Uncertainty relation. Einstein would have remarked "It is always the theory which decides what can be observed" and as such, would have asserted that its NOT advisable to ask "How can *we* represent the path of the electron in the cloud chamber?"

Heisenberg, realizing the profound insight, turns the question around and asks "Is it not perhaps true that, in nature, only such situations occur as can be represented in quantum mechanics or wave mechanics?" Once he understood the overwhelming nature of his insight he came to a conclusion that "There was not a real path of the electron in the cloud chamber".

His conclusions came in the form of his famous march 1927 paper [35]. The colloquial statement of the Heisenberg's Uncertainty Principle reads as follows:

"*The more precisely the position is determined, the less precisely the momentum is known in this instant, and vice versa.*"

In that paper, Heisenberg presented the physical intuition underlying the uncertainty principle (based on the discussion of his gamma ray microscope gedanken experiment for measuring the position $\mathbf{x}$ and momentum $\mathbf{p}$ of an electron).
Measurement of position of the particle with an "error" $\epsilon(\mathbf{x}) \approx \Delta\lambda$ (where λ corresponds to the wavelength of the photon) causes disturbance $\eta(\mathbf{p})$ of the

momentum by an amount $\eta(\mathbf{p}) \approx \frac{\hbar}{\Delta\lambda}$.

The product of the "noise" in a position measurement $\epsilon(\mathbf{x})$ and the momentum disturbance $\eta(\mathbf{p})$ caused by that measurement turns out to be $\epsilon(\mathbf{x})\eta(\mathbf{p}) \approx \hbar$.

While Heisenberg states that he would prove the error-disturbance relation on a firmer mathematical ground in terms of the canonical commutation relations $[\mathbf{x},\ \mathbf{p}] = \mathrm{i}\hbar$, the paper does not discuss it. Moreover, there was no rigorous mathematical definition of neither error nor disturbance in it. Heisenberg only gives a *rough discussion* of variances in the position measurement and the resulting momentum disturbance in the case of Gaussian wave packets.

The commutator of two operators **A** and **B** representing the observables **A** and **B** respectively is defined as

$$[\mathbf{A}, \mathbf{B}] = \mathbf{A}\,\mathbf{B} - \mathbf{B}\,\mathbf{A}$$

Commutativity of operators representing the observables helps in their simultaneous/joint measurement. In classical physics, physical observables commute, which means that they are jointly measurable. Commuting observables are also called as ***compatible*** observables. In quantum physics, two operators representing physical observables don't commute, in general. If they do, then they share a common set of eigenstates and are thus compatible. They can be jointly measured. It is in this sense that Projective Measurements (PM) are known as ***sharp measurements*** as it assigns sharp values for the measurement of compatible observables in contrast to the measurement of two non-commuting observables. (See Appendix A)

The uncertainty relation captures the essence of Non-Commutativity inherent in quantum theory. Physically, the meaning of the uncertainty relation is that if one performs the measurement of two non-commuting observables **A** and **B** on an ensemble prepared in $|\Psi\rangle$, then the product of the uncertainties of the observables is bounded by their commutator evaluated in $|\Psi\rangle$.

The example of Heisenberg's gedanken experiment subsequently initiated a mathematically formal version of "preparation uncertainty" relation proved by Kennard [36] and Hermann Weyl [37]:

$$\Delta \mathbf{x}\, \Delta \mathbf{p} \;\geq\; \hbar/2 \tag{1.9}$$

This inequality is obeyed by the standard deviations [1] $\Delta \mathbf{x}$, $\Delta \mathbf{p}$ evaluated using the position and momentum probability distributions of the same *preparation* [2] but in two separate experiments.

A proof of the *preparation uncertainty* relation for any two non-commuting observables **A** and **B** i.e.,

$$\Delta \mathbf{A}\, \Delta \mathbf{B} \;\geq\; |\,\langle[\mathbf{A}, \mathbf{B}]\rangle\,|/2 \tag{1.10}$$

was given by Robertson (who was inspired by an argument given in Weyl's book) [38, 37].

It is clear that Kennard, Weyl and Robertson formalized measurement error in terms of standard deviation $\Delta \mathbf{A}$ based on the identification that in general, an observable does not have a definite value in a quantum state.[3]

[1] The standard deviation of an observable **X** is defined as $\Delta \mathbf{X} = \sqrt{\langle \mathbf{X}^2\rangle - \langle \mathbf{X}\rangle^2}$ where the averages are calculated on any state $|\Psi\rangle$

[2] ***von Neumann projection hypothesis*** asserts that the *complete* measurement of an observable **A** with eigenstates $|a_i\rangle$ corresponds to the weighted sum of the eigenstates with the weights identified as the probabilities of obtaining the eigenvalues a_i corresponding to the eigenstates $|a_i\rangle$. If a single projective measurement pertaining to the eigenstate $|a_i\rangle$ is made on an arbitrary state $|\Psi\rangle$ then the state $|\Psi\rangle$ *collapses* to $|a_i\rangle$ and thus a state is *prepared*. This is known as a state preparation procedure.

[3] Textbooks on quantum mechanics exclusively discuss the preparation uncertainty relation. But the error-

1.1.3 Composite systems

The consideration of having a bipartite separation of a system or the interaction amongst two distant systems forces us to look into the concept of composition of states representing the total system. Let the states of system $\mathcal{A}$ and system $\mathcal{B}$ be associated with the Hilbert spaces $\mathbb{H}_{\mathcal{A}}$ and $\mathbb{H}_{\mathcal{B}}$ respectively.

The possible composition of the systems is in terms of a *Product*, *Separable* or an *Entangled* state.

Consider a bipartite *pure* state $|\Psi_{\mathcal{AB}}\rangle$. If $|\Psi_{\mathcal{AB}}\rangle = |\phi_{\mathcal{A}}\rangle \otimes |\chi_{\mathcal{B}}\rangle$, then $|\Psi_{\mathcal{AB}}\rangle$ is considered as a (tensor) *Product* state. Else it is called an *Entangled* state. Superposition in the tensor product space or the composite space leads to the concept of *Entanglement*. Product states do not carry any correlation between them whereas entangled states do as we see in the following sections.

In the case of *mixed* bipartite states, $\rho_{\mathcal{AB}} = \rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}}$ is considered as a product state. These states do not carry any correlation. However, there is a general construction of a bipartite state which is classically correlated. These states are called as *Separable* states.

$$\rho_{\mathcal{AB}} = \sum_i q_i \, \rho_{\mathcal{A}i} \otimes \rho_{\mathcal{B}i} \tag{1.11}$$

disturbance arguments of Heisenberg were not translated into rigorous mathematical formulation. This facet of the uncertainty principle has invoked recent debates on how Heisenberg's original intuition should be interpreted and generalized [39, 40, 41, 42].

with the constraint that $\sum_i q_i = 1$ and the $q_i \geq 0$. This form of the separable state is called as the convex sum of the product form of the constituent states. The states $\rho_{\mathcal{A}}$ and $\rho_{\mathcal{B}}$ are called as *reduced* density matrices or *reduced* states. They are obtained by taking the *partial trace* over the total state $\rho_{\mathcal{AB}}$

$$\rho_{\mathcal{A}} = Tr_{\mathcal{B}}\left(\rho_{\mathcal{AB}}\right)$$

$$\rho_{\mathcal{B}} = Tr_{\mathcal{A}}\left(\rho_{\mathcal{AB}}\right)$$

Any state which is not separable is an *entangled* state.

But how different are these **Entangled states** from other kind of states? Let us consider the states $|\beta_{00}\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right)$ and $|\beta_{11}\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right)$. In these states, the *spin* values of each component are correlated as well as anti-correlated. Each component system of this entangled state doesn't have a definite state. This is what it means to say that the superposition cannot be written as a product of the constituent systems.
Furthermore, the meaning of the terms *correlation and anti-correlation* is that, if we separate the constituents and send one component each to Alice and Bob [1](who are spatially separated)and ask them to measure the Z component of the spin angular momentum **S**,[2] they find that the probability of obtaining the values $\pm 1/2$ is the same for each constituent state. Also, if Alice finds the measured value to be $+1/2$ on the state $|\beta_{00}\rangle$, then the state on her part would have collapsed to $|0\rangle$ and that this is possible only if the total state would have collapsed to $|00\rangle$. Thus, the state of Bob would have reduced to $|0\rangle$ even without him making a measurement at his end. If he makes a measurement of the

[1] The eternal pair!!

[2] The spin angular momentum **S** is defined as a triplet $(\mathbf{S}_x, \mathbf{S}_y, \mathbf{S}_z)$ which satisfies the commutation relation $[\mathbf{S}_x, \mathbf{S}_y] = i\hbar\epsilon_{xyz}\mathbf{S}_z$. The spin angular momentum eigenstates are denoted as $|sm_z\rangle$ where the eigenvalues of the operator are s = 0, ±1/2 ,±3/2 ,±5/2 .... For the case of s = 1/2 , the spin angular momentum **S** is denoted as $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$

Z component of **S**, he finds the value +1/2. This is meant by *correlation* in the measured values and this is a reflection of the inherent correlation in the state $|\beta_{00}\rangle$. The same analysis would imply that the measured values of the spin angular momentum in the state $|\beta_{11}\rangle$ are *anti-correlated.*

In contrast to this, the state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$ is not correlated as it is evident that the state $|\Psi\rangle$ can be decomposed into a product form,$|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle$.

Classical correlations are ubiquitous in nature. However, what differentiates the nature of correlations between the classical and quantum worlds is in the understanding of the origin of these correlations. In classical physics, probabilities arise primarily due to the lack of knowledge of the attributes of the systems and hence when correlations are observed, they can be explained as emerging from an underlying probability distribution characterizing the outcomes of measurement of the observables of the system. However,in quantum physics, due to the notion of non-commutativity of the observables, the complete description of the outcomes of the measurement of observables in terms of specifying the probability distribution is not possible as in the classical case. As such, the correlations arising in the quantum scenario are found to be strikingly different compared to their classical counterpart. It is this deviation from the classical rules of *probability logic* that characterizes the distinctive nature of the probability distributions arising in the quantum scenario.

1.1.4 Generalized Measurements and Evolution

Evolution

We have seen before that the evolution equation for a state ρ of a single system is given by the Schrödinger equation (master equation). A natural question to ask is the applicability of the said equation to the case of a composite system where the constituent parts are interacting with each other. The interest in developing this sort of a mathematical framework for evolution of the composite system is towards modeling the "*system + environment*" interaction and then examining the structure of the evolved state of the system.

Consider the state $\rho_{\mathcal{A}\mathcal{E}}$ to be initially in a product state $\rho_{\mathcal{A}\mathcal{E}}(0) = \rho_{\mathcal{A}} \otimes \rho_{\mathcal{E}}$ and allow it to evolve under a unitary transformation $\mathbf{U}(\mathrm{t})$ in the combined space $\mathbb{H}_{\mathcal{A}}$ and $\mathbb{H}_{\mathcal{E}}$.
Let $|e_i\rangle$ be an orthonormal basis in the state (Hilbert) space of $\mathcal{E}$ and let the state of the environment $\mathcal{E}$ be initialized to $|e_0\rangle\langle e_0|$. The state $\rho_{\mathcal{A}\mathcal{E}}$ at a later time t is given by

$$\rho_{\mathcal{A}\mathcal{E}}(t) = \mathbf{U}(t)\,\rho_{\mathcal{A}} \otimes \rho_{\mathcal{E}}\,\mathbf{U}^{\dagger}(t)$$

and the state of the system after the interaction is obtained by tracing out the state of the environment.

$$\rho_{\mathcal{A}}(t) = \sum_i \langle e_i|\,\mathbf{U}(t)\,[\rho_{\mathcal{A}} \otimes |e_0\rangle\langle e_0|]\,\mathbf{U}^{\dagger}(t)\,|e_i\rangle \tag{1.12}$$

$$= \sum_i \mathcal{K}_i \rho \mathcal{K}_i^{\dagger} \tag{1.13}$$

where $\mathcal{K}_i \equiv \langle e_i|\,\mathrm{U}\,|e_0\rangle$ are called as Krauss operators. These operators act on the state space of the system taking it from the initial state $\rho_{\mathcal{A}}(0)$ to the final state $\rho_{\mathcal{A}}(t)$ and the equation (1.13) is known as *operator sum representation* or *Krauss representation* for the state of the system after the interaction (operation).

The *set* of Krauss operators satisfy the *completeness relation* arising from the constraint that the state of the system be normalized after the interaction.

$$\sum_i \mathcal{K}_i^\dagger \mathcal{K}_i = \mathbb{I}$$

Remark

Schrödinger equation is only for the combined system comprising the system and the environment. As there is no direct Schrödinger equation for the evolution of the reduced density matrix $\rho_{\mathcal{E}}$, the master equation corresponding to *one of the forms* of the solution given by the operator sum representation (1.13) is simply

$$\frac{d\rho}{dt} = \mathcal{L}\rho$$

whose actual solution is $\rho(t) = e^{\mathcal{L}t}\,\rho(0)$. The operator $\mathcal{L}$ is known as the *Lindbladian* for the system.
Note that the special case of the unitary evolution, $\rho' = \mathbf{U}\rho\mathbf{U}^\dagger$ is also an operator sum with only one element in the set of operators $\mathcal{K}_i$ which is equal to $\mathbf{U}$ itself.

Example: Amplitude Damping channel

The amplitude damping channel is a schematic model representing the spontaneous emission of a photon due to the decay of an excited state of a two level atom. The Krauss operators characterizing the channel are

$$\mathcal{K}_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix} \quad ; \qquad \mathcal{K}_1 = \begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix}$$

The Krauss operator $\mathcal{K}_1$ aids in de-exciting the atom to it's ground state ($|1\rangle$ to $|0\rangle$) whereas the operator $\mathcal{K}_0$ describes the evolution when there is no de-excitation. The state of the two level atom after the evolution is given by

$$\rho' = \mathcal{K}_0 \rho \mathcal{K}_0^\dagger + \mathcal{K}_1 \rho \mathcal{K}_1^\dagger$$

where ρ' is the final state after the channel acts on the initial state ρ.

Measurement

The schematic model of a measurement is described as a transformation of a state to another wherein the three properties given by (1.1) has to be satisfied by the state after the measurement. Note that the act of measurement is an *irreversible* operation in contrast to the unitary evolution of the system. Conventional ***von Neumann*** projection measurements expresses the observable in it's spectral form using the projection operators Π.

$$\mathbf{M} = \sum_m m\, \mathbf{\Pi}_m \tag{1.14}$$

Here $\mathbf{\Pi}_m = |m\rangle\langle m|$ and the eigenvalue equation for the observable $\mathbf{M}$ reads as $\mathbf{M}\,|m\rangle = \mathrm{m}\,|m\rangle$. The operators $\mathbf{\Pi}_m$ are called as Projection Operators. The state of the system after the measurement is given by

$$\rho \xrightarrow{\quad Measurement \quad} \rho' = \frac{\mathbf{\Pi}_m\, \rho\, \mathbf{\Pi}_m}{p(m)}$$

where $p(m) = Tr(\rho\, \mathbf{\Pi}_m)$, the probability to find the state in $|m\rangle$. Also, these operators $\mathbf{\Pi}_m$ obey the two properties given by (1.8).

Let us now consider a set of operators $\mathbb{E}_m = \mathbb{M}_m^\dagger \, \mathbb{M}_m$ such that they form the resolution of identity but are non-orthogonal. That is, consider operators which are *not* projection operators but which form a non-orthogonal decomposition of identity:

$$\begin{aligned} \mathbb{E}_m &\geq 0 \\ \sum_m \mathbb{E}_m &= \mathbb{I} \end{aligned} \tag{1.15}$$

In this case, the probability of the results of measurements of $\mathbb{E}_m$ is given by $p(m) = Tr(\rho \, \mathbb{E}_m)$. The set of operators $\mathbb{E}_m$ are called as POVM elements or operators. (The acronym POVM stands for ***Positive Operator Valued Measure***.)

POVM's arise as measurements on a system $\mathcal{A}$, as a result of orthogonal projective measurement done on a composite system $\rho_{\mathcal{AB}}$ in an extended space $\mathbb{H}_{\mathcal{A}} \otimes \mathbb{H}_{\mathcal{A}}$. Consider the initial composite system to be in a product state $\rho_{\mathcal{AB}} = \rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}}$. A *complete* projective measurement on this state is given by

$$\rho'_{\mathcal{AB}} = \sum_m \mathbf{\Pi}_m \, \rho_{\mathcal{AB}} \, \mathbf{\Pi}_m \tag{1.16}$$

Taking the trace over the system $\mathcal{B}$, the state of the system $\mathcal{A}$ is given by

$$\begin{aligned} \rho'_{\mathcal{A}} &= \mathrm{Tr}_{\mathcal{B}} \left(\sum_m \mathbf{\Pi}_m \, \rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}} \, \mathbf{\Pi}_m \right) \\ &= \sum_m \left(\mathrm{Tr}_{\mathcal{B}} \left(\mathbf{\Pi}_m \, \rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}} \right) \right) \end{aligned}$$

$$= \sum_{\Gamma} \mathbb{M}_{\Gamma}\, \rho_{\mathcal{A}}\, \mathbb{M}_{\Gamma}^{\dagger} \tag{1.17}$$

This is the content of the theorem due to Neumark [43].

Example

The projective measurement operators $\mathbf{\Pi}_m$ which satisfy the properties given by (1.8) are POVM elements themselves as $\mathbb{E}_m \equiv \mathbf{\Pi}_m^{\dagger}\mathbf{\Pi}_m = \mathbf{\Pi}_m$.

In this section, we have briefly mentioned the rudiments of standard quantum mechanics which form the physical edifice on which quantum information theory is built. In the ensuing section, we provide an elementary introduction to information theory as needed for developing the contents of this thesis.

1.2 Information and Ignorance

The meaning of information in common parlance is to gather facts or learn about something or someone. The common day to day activities such as watching the news on a television channel and reading a book make us better informed about the worldly affairs and the contents in the book respectively. However, for a scientific understanding of what ***information*** means, we need to model the system (physical process) responsible for the generation of the same in such a way that we appreciate the learning of something "new" through the acts of observation or measurement on the system.

It was through the remarkable work of ***Claude Shannon*** [44, 45] that *Information Theory* as we understand it came into being. This was developed to quantify the information content in a physical system or communication channel. For an efficient communication process, the schematic involved three components. The ***Source***, the ***Channel*** and the ***Destination***. The Source produces *Events* to which information is associated and these are encoded before transmitting through a channel (which could be *noisy*) to the destination where the events are decoded back to it's original form and the information gathered. We now develop a measure for the information content of an event in terms of the probability of the occurrence of that particular event.

The key idea of Shannon was to model the communication process as a *stochastic process* wherein the source produces events modeled as a *random variable* $\mathrm{X} = (x_1, x_2, x_3, \cdots, x_n)$ with the source producing the events x_k with the probability $p_k \equiv p(x_k)$. These appear to be mere *data* from which *information* needs to be extracted out.
In order to bring out a measure of information, some basic assumptions on the part of the measure were carved out. These are as follows:

1. Information is a function of the probabilities of the events, $I(p)$.
2. $I(p)$ is a monotonically increasing continuous function of the probabilities of the events.
3. $I(p)$ is an additive function. The information content of two events occurring with the probabilities p_1 and p_2 is the sum of the information contents of each event occurring independently. i.e, $I(p_1 p_2) = I(p_1) + I(p_2)$.
4. The certainty of an event corresponds to information content being *zero*.

With these assumptions, Shannon says that there is an unique measure of information up to an additive and multiple constant [46], the result of which is that $I(p_k)$ is defined to be

$$I(p_k) = -\log_2(p_k). \tag{1.18}$$

The **Average Information** or **Classical Shannon Information** or **Shannon Entropy** is defined as the weighted sum of the probabilities of the events comprising a *message*. This is given by

$$H(X) = -\sum_x p_x \log_2(p_x). \tag{1.19}$$

Note that $H(X) \geq 0$.

Example

Consider X $= 0, 1$ to be a binary event. Let the event 0 occur with the probability p and 1 with $1 - p$ with $0 \leq p \geq 1$. The Shannon entropy for this binary event is

$$H(X) = -p\log_2(p) - (1-p)\,\log_2(1-p)\,.$$

The maximum information occurs for the value of p $= 1/2$. Also, one bit of data can carry a maximum of 1 bit of information. When we have a source producing a set of $n = 2^x$ symbols with a uniform distribution i.e, $p_x = 1/n$, we obtain x bits of information:

$$\begin{aligned} H(X) &= -\sum_{x=1}^{n} p_x \log_2(p_x) \\ &= -\frac{n}{n}\log_2(1/n) \\ &= -\log_2(1/n) \\ &= x. \end{aligned} \tag{1.20}$$

Thus, Shannon entropy quantifies the total information produced in a collection of events in terms of the sum of the weighted probabilities of occurrence of each event.

Equivalently, Shannon entropy $H(X)$ can also be understood as quantifying the amount of *uncertainty* about an event (modeled as X) before the occurrence of that particular event. Suppose we have two observables **A** and **B**. Let us label the values taken by them to be a and b. A *joint* probability distribution $p(a, b)$ can be assigned if one has knowledge about the values of both a and b. In order to talk in terms of the probabilities, the values a and b are treated as the values of the ***random variables*** **A** and **B** respectively.
Bayes's theorem [47, 48] is an important theorem in the theory of probability which relates the joint probability distribution to the conditional probability distribution.

$$p(a, b) = p(a|b)\, p(b) = p(b|a)\, p(a) \tag{1.21}$$

The information equivalent of Bayes's theorem is

$$I(a, b) = I(a|b) + I(b) = I(b|a) + I(a)$$

. The joint Shannon entropy is defined as

$$H(A, B) = \sum_{a,b} p(a, b)\, I(a, b) = -\sum_{a,b} p(a, b) \log_2 p(a, b) \tag{1.22}$$

The conditional entropy $H(A|B)$ is defined using Bayes's theorem

$$H(A|B) = -\sum_{a,b} p(a|b)p(b) \log_2 p(a|b) \tag{1.23}$$

$$= H(A, B) - H(B) \tag{1.24}$$

Note that $H(A|B) \geq 0$ by definition. The entropic equivalent of Bayes's theorem is

$$H(A, B) = H(A|B) + H(B) = H(B|A) + H(A)$$

The Shannon entropies obey the inequality [49]:

$$H(A|B) \leq H(A) \leq H(A, B) \tag{1.25}$$

left side of which implies that removing a condition never decreases the information – while right side inequality means that two variables never carry less information than that carried by one of them.

Quantum (von-Neumann) Entropy

The Shannon entropy quantifies the amount of *uncertainty* or *ignorance* associated with a classical probability distribution. Analogous to the classical probability distributions are the density matrices representing the states of a quantum system. These density matrices correspond to the quantum probability distributions. A measure of the uncertainty associated with these quantum probability distributions is the *Quantum (von Neumann) Entropy* $S(\rho)$.
The von Neumann entropy is defined as [1]

$$S(\rho) = -Tr(\rho \log \rho) \tag{1.26}$$

For a pure state $\rho = |\Psi\rangle\langle\Psi|$, the von Neumann entropy turns out to be zero. Furthermore, for a mixed state $\rho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|$, the von Neumann entropy is found to be

$$S(\rho) = -Tr(\rho \log \rho)$$

[1]The base to the logarithm is 2.

$$= -\sum_j \langle \Psi_j | \rho \log \rho | \Psi_j \rangle$$
$$= -\sum_i p_j \log p_j$$

which resembles the structure of classical Shannon entropy. Note that the von Neumann entropy $S(\rho) \geq 0$ by definition.

Remark

Measurement always increases the entropy of the system as the classical Shannon entropy is found to be greater or equal to the von Neumann entropy after the act is performed. That is, if we are measuring an observable **A** on a system in a state represented by the density matrix ρ, then the probability distribution

$$p(a) = Tr(\rho \mathbf{\Pi}_a)$$

where $\mathbf{\Pi}_a$ is the projector corresponding to an eigenstate $|a\rangle$ of the observable **A**. After the measurement, we find that

$$H(A) \geq S(\rho)$$

the equality arising only when $[\mathbf{A}, \rho]$ commutes [50].

Given a bi-partite density matrix $\rho_{\mathcal{AB}}$, the entropy for the whole system is defined as $S(\mathcal{AB})_\rho = S(\rho_{\mathcal{AB}})$. To this end, the entropy of the sub system density matrix is denoted as

$$S(A)_\rho = S(\rho_{\mathcal{A}}) = S(Tr_{\mathcal{B}}(\rho_{\mathcal{AB}}))$$

By analogy with the classical (Shannon) conditional entropy, one defines the conditional quantum entropy as

$$S(A|B)_\rho = S(AB)_\rho - S(B)_\rho$$

The subscript ρ is only to remind that we are dealing with quantum states.
For a pure state, the von Neumann entropy $S(\rho)_{pure} = 0$ as all p_i's are zero except one whereas for a completely mixed state of n qubits, $S(\rho)_{mix} = n$ as all the p_i are equal to $1/2^n$.
Furthermore, the von Neumann entropy is utilized to characterize the entanglement of a pure bi-partite state $\rho_{\mathcal{AB}}$. It is done by computing the von Neumann entropy of the subsystem density matrix. If $S(\rho_{\mathcal{A}}) = 0$, then we know that $\rho_{\mathcal{A}}$ is pure and hence $\rho_{\mathcal{AB}}$ is a product state. If not, $\rho_{\mathcal{AB}}$ is an entangled state. The von Neumann entropy $S(\rho_{\mathcal{A}})$ is used as a measure of entanglement of pure bi-partite states.

Entropic Uncertainty Relation

From an information-theoretic perspective, it is natural to capture the "ignorance" associated with a probability distribution in terms of the Shannon entropies rather than variances as was given by (1.10). As such, the Entropic Uncertainty Relation (EUR) was originally formulated by David Deutsch [51] and was subsequently improved [52, 53, 54]. The conjecture put forth by Kraus [54] was proved by Maassen and Uffink [6]. The Entropic Uncertainty Relation has broadened and strengthened the original notion of uncertainty principle first conceived by Heisenberg.
Consider $\mathbf{A} = \sum_a a\,|a\rangle\,\langle a|$ and $\mathbf{B} = \sum_b b\,|b\rangle\,\langle b|$ to be the spectral decomposition of the two observables $\mathbf{A}$ and $\mathbf{B}$. Let *p(a)* and *p(b)* denote the probability distribution for the outcomes of the measurements made on a system prepared initially in the state represented by the density matrix ρ. Let $H(\mathbf{A})$ and $H(\mathbf{B})$

represent the Shannon entropies associated with the probability distributions *p(a)* and *p(b)* respectively. The Entropic Uncertainty Relation (EUR) is stated as

$$H_\rho(\mathbf{A}) + H_\rho(\mathbf{B}) \geq -2\log C(\mathbf{A},\mathbf{B}) \tag{1.27}$$

where $C(\mathbf{A},\mathbf{B}) = \max_{a,b}|\langle a|b\rangle|$. The lower bound limiting the sum of entropies is independent of the state ρ. The term $C(\mathbf{A},\mathbf{B})$ can assume a maximum value $1/\sqrt{d}$ resulting in the maximum entropic bound of $\log d$, where d denotes the dimension of the system.

Example

Consider a qubit prepared in a completely random mixture given by $\rho = \mathbb{I}/2$ ($\mathbb{I}$ denotes the 2×2 identity matrix). Measurements of the observables $\mathbf{A} = \boldsymbol{\sigma}_x$ and $\mathbf{B} = \boldsymbol{\sigma}_z$ in this state leads to Shannon entropies of measurement $H_\rho(\mathbf{A}) = H_\rho(\mathbf{B}) = 1; C(\mathbf{A},\mathbf{B}) = 1/\sqrt{2}$ and the uncertainty bound is $-2\log C(\mathbf{A},\mathbf{B}) = 1$; Thus, the Maassen-Uffink relation (1.27) is satisfied.

In contrast to the original version of the uncertainty relation given in (1.10) whose right hand side is dependent on the *state* of the system on which the measurements are made, the entropic uncertainty relation does not suffer from any such drawback. The lower bound on the right hand side of (1.27) is state independent. Another aspect of the entropic uncertainty relation which differs from (1.27) is that, even if one of the observables has a vanishing entropy in a particular state, the entropy of the other observable is still bounded by the r.h.s of (1.27). This is unlike the case of the uncertainty relation expressed in terms of the variance, wherein if one of the variance vanishes in a state, the commutator too vanishes providing us a null relation.

Till now, we have developed the rudiments of both the mathematical as well as the quantum information theory aspects required for the basic understanding of the contents of this thesis. In the last section of this introductory chapter, we focus on outlining a basic awareness towards the foundational aspects of quantum theory. The main topics include the description of the EPR *paradox*, Bell's inequality and finally the notion of macrorealism as brought out through the Leggett-Garg inequality.

1.3 EPR, Local Realism, macrorealism, Joint Measurability & all that.

The statistical nature of the predictions pertaining to the measurement of the attributes of the quantum system arising from the mathematical framework of quantum theory brought in much dissatisfaction to one of the early proponents of the theory, Albert Einstein. Along with other founding fathers of the theory, he was highly skeptical of the interpretation of the theory as set out by Heisenberg, Bohr and others during the emergence of the theory. He thought that the ***theory was correct*** and successful in explaining the atomic transitions, energy levels of the atom, the structure of the atomic nucleus etc. However, Einstein felt that the ***theory was incomplete*** in the sense that it didn't offer a plausible explanation for the superposition of quantum mechanical states.

Einstein and his supporters believed that the predictions of quantum theory pertaining to experimental scenarios could still be explained in terms of an underlying classical theory whose presence could be non-viable to yield to experiments yet. They believed that an *electron* is a particle (with a *mass*) with a well defined position and momentum [55]. Einstein argued that the mere

Figure 1.2: **Albert Einstein, Boris Podolsky and Nathan Rosen**. Pic credit: Timecomm's Blog

unknowing of the values of these two attributes of the electron would not imply the non-existence of the definiteness of the values of these attributes. In other words, *objective definiteness of the attributes of the system was held by the* ***realists***[33]. However, this was in stark contrast to the ideology of the ***Copenhagen interpretation***, which purported to the view that *objective definiteness should be abandoned and that the values of the attributes take an objective existence only when a measurement is performed wherein the reduction or collapse of the state takes place.* This notion of the *wave function collapse* initiated Erwin Schrödinger to come up with the famous Schrödinger's cat paradox [23].

The essence of the famous paper by **Einstein**, **Podolosky** and **Rosen** (EPR in short)[56] was to enunciate in a lucid manner the *incompleteness* of quantum theory and in order to do so, they came up with a thought experiment wherein the objective definiteness of the attributes of the quantum system is established through the upholding of the principle of ***local causality*** [57, 29, 58] or ***locality*** [59].

The argument of the EPR is as follows: For the success of a physical theory, we must ask:

1. Is the theory correct?

2. Is the theory complete?

It is the second question that EPR tries to consider as applied to Quantum Mechanics.
In order to indicate the requirement for a complete theory, they identify only a necessary condition that
"Every element of the physical reality must have a counterpart in the physical theory"
As a criterion for recognizing the *elements of physical reality*, they proposed only a sufficient condition:
If, without in any way disturbing a system, we can predict with certainty the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity.
Note that this should not be taken as a definition of an element of physical reality.
If $|\Psi\rangle$ is an eigenfunction of the observable $\mathbf{A}$, that is, if

$$|\Psi\rangle' \equiv \mathbf{A}\,|\Psi\rangle = a\,|\Psi\rangle$$

where a is a number, then $\mathbf{A}$ has with certainty the value a whenever the particle is in the state $|\Psi\rangle$.
This is in accordance with our criterion of reality for the particle in state $|\Psi\rangle$ where we can see that a is an element of reality corresponding to the physical quantity represented by the observable $\mathbf{A}$.

Suppose $\mathbf{A}\,|a\rangle = a\,|a\rangle$ and $\mathbf{B}\,|a\rangle \neq b\,|a\rangle$ because $\mathbf{A}$ and $\mathbf{B}$ don't commute: i.e., both $\mathbf{A}$ and $\mathbf{B}$ do not represent realities for the system in state $|a\rangle$.
This leaves us with two possibilities:

1. Quantum Theory is incomplete

2. Quantum Theory is fine but no simultaneous realities for two non-commuting observables is allowed in the theory.

In order to elucidate the essence in a more appealing way, let us use Bohm's version of the paradox [60]. Consider a pair of spin 1/2 particles, $\mathcal{A}$ and $\mathcal{B}$, with spin vectors $\boldsymbol{\sigma}_{\mathcal{A}}$ and $\boldsymbol{\sigma}_{\mathcal{B}}$, which are formed by decay in a spin singlet state, so that their spins are perfectly anti-correlated. Let the spins be spatially separated.

Now, measure $\boldsymbol{\sigma}_z$ at $\mathcal{A}$'s end and next measure $\boldsymbol{\sigma}_x$ at $\mathcal{B}$'s end. These measurements yield us the results at $\mathcal{B}$'s end though nothing was done at $\mathcal{B}$; that is, after the initial state was formed, measurement on particle $\mathcal{A}$ cannot affect the condition of the spatially separated particle $\mathcal{B}$, since there is *NO interaction* between them.

Thus, we have predicted the values of measurements at $\mathcal{B}$'s end though

$$[\boldsymbol{\sigma}_{\mathcal{B}z}, \boldsymbol{\sigma}_{\mathcal{B}x}] \neq 0$$

The implication of this being that there are realities hidden at $\mathcal{B}$'s end which is **not** accounted by the wave function/state. Thus, Quantum Mechanics is an incomplete description of reality that must be extended in some way to describe all these objective properties.

The major importance of the EPR work apart from presenting the incompleteness of quantum theory was that it first confronted quantum theory with the principle of local causality or locality which Einstein remarked as

"The Real factual situation of particle $\mathcal{B}$ is independent of what is done at $\mathcal{A}$, which is spatially separated from $\mathcal{B}$."

EPR did not doubt that quantum theory is correct. They only questioned the completeness of the theory. The conclusion of the EPR is that some other

"hidden variable" is needed to completely specify the state of the system. The hidden variable could be a single number or a whole collection of numbers. It doesn't matter [34].

The idea that the wave function or the state of the system is merely a tool to acquire knowledge of the quantum system was a norm to be followed than to seek about it's meaning and interpretation. Every possibility to explain the statistical predictions of quantum mechanics with an underlying classical description was probed. One of the approaches was the ***Hidden Variable Theory*** with a philosophical manifesto [61] called ***Local Realism***. From the point of view of EPR, local realism is the edifice on which every physical theory is proposed.

The 1935 paper by Einstein, Podolosky and Rosen motivated physicists to construct hidden variable theories [62]. In order to understand the motivation behind the construction of a hidden variable theory, let us look at an example: *Measurement of the spin of a particle*: The spin of a particle is to be measured in a particular direction. Let us suppose that the direction is along the "y" axis. If the spin is measured along the "y" axis, and the value "+1" ("up" in the y direction) is observed, then a hidden variable theory contends that the measured value was *unwrapped* by the act of measurement. This is in stark contrast to the standard notion held in quantum theory that the value of the spin was *created* by the act of measurement [43, 63].
All these programmes of constructing hidden variable theories for explaining the outcomes of experiments will not hold ground unless experimentally testable propositions are offered. Thus, in order to arbitrate between the hidden variable theory and quantum theory, both the theories need to be transformed into a platform where they can be subjected to experimentally testable propositions.

One such lucid proposition was the formulation of **Bell's Inequality** in the year 1964 by *John Bell*.

1.3.1 Bell's Inequality–Test of Local Realism

In 1964, J S Bell brought out a clear mathematical description of what is known as local realism and put forth a test to check whether quantum theory adheres to it. The basis behind such a rigmarole was the inkling that the quantum mechanical state or wave function was just an *object* used to acquire knowledge about the physical world than be a *real* entity. What Bell considered, as EPR wanted to, was an *ontological* framework for explaining the predictions of quantum theory. By an *ontological* framework, they meant the existence of *"ontic"* variables in addition to the parameters already considered such as the settings of the measurements, preparation procedures etc. These variables are also termed as *"hidden"* variables as they are not part of the set of controllable parameters. Usually the symbol λ is used to denote the *"hidden"* variables. The expectation of a hidden variable model for quantum theory is the explanation of the emergence of probabilities of the outcomes of measurements (done on a quantum system) in terms of a distribution over the *"hidden"* variables designated as $\rho(\lambda)$, i.e,

$$P(A, B|a, b) = \int d\lambda \rho(\lambda) P(A, B|a, b, \lambda)$$

where $P(A, B|a, b)$ is the probability for the occurrence of the measurement outcomes A,B due to the settings a,b respectively. $\rho(\lambda)$ is the hidden variable probability distribution. The Hidden variable Probability distribution adheres to $\int \rho(\lambda) d\lambda = 1$ along with $\rho(\lambda) \geq 0$.

The conception of local realism stands on the framing of two tenets, **Locality** and **Realism** as the name itself suggests.

Realism is a conception "according to which external reality is assumed to exist and have definite properties, whether or not they are observed by someone."[64]

and

Locality demands that "if two measurements are made at places remote from one another the (setting of one measurement device) does not influence the result obtained with the other."[57]

The joint assumption of Local Realism (LR) or "local causality" is mathematically put in the form

$$P(A, B|a, b) = \int d\lambda \rho(\lambda) P(A|a, \lambda) P(B|b, \lambda) \tag{1.28}$$

Let us now consider a concrete example and see how the conditions of *locality* and *realism* when manifested mathematically lead us to correlation inequalities which can be tested experimentally. To this end, in full glory, quantum mechanics violates the inequalities and is found to be not adhering to *local realism*.

Let us consider observables denoted as $A(\mathbf{a}, \lambda)$ and $B(\mathbf{b}, \lambda)$ which take values ± 1 respectively. The locality constraint is expressed as

$$P(A|\mathbf{a}, \mathbf{b}, \lambda) = P(A|\mathbf{a}, \lambda) \tag{1.29}$$

and realism as the existence of definite values for $A(\mathbf{a}, \lambda)$ and $B(\mathbf{b}, \lambda)$ which is ± 1. Here $\mathbf{a}$ and $\mathbf{b}$ are unit vectors in the three dimensional space. The correlation observables are denoted as $C(\mathbf{a}, \mathbf{b})$ which is defined by

$$C(\mathbf{a}, \mathbf{b}) = \int d\lambda \rho(\lambda) A(\mathbf{a}, \lambda) B(\mathbf{b}, \lambda) \tag{1.30}$$

The correlation amongst the values of the observables $A(\mathbf{a}, \lambda)$ and $B(\mathbf{b}, \lambda)$ is assumed to stem from the form of the probability distribution given by (1.28).

Consider four directions $\mathbf{a}$, $\mathbf{a}'$, $\mathbf{b}$, $\mathbf{b}'$ to obtain the two inequalities

$$\begin{aligned}
|C(\mathbf{a},\mathbf{b}) - C(\mathbf{a},\mathbf{b}')| &= |\int d\lambda \rho(\lambda) A(\mathbf{a},\lambda)(B(\mathbf{b},\lambda) - B(\mathbf{b}',\lambda))| \\
&\leq \int d\lambda \rho(\lambda) |B(\mathbf{b},\lambda) - B(\mathbf{b}',\lambda)|; \\
|C(\mathbf{a}',\mathbf{b}) + C(\mathbf{a}',\mathbf{b}')| &= |\int d\lambda \rho(\lambda) A(\mathbf{a}',\lambda)(B(\mathbf{b},\lambda) + B(\mathbf{b}',\lambda))| \\
&\leq \int d\lambda \rho(\lambda) |B(\mathbf{b},\lambda) + B(\mathbf{b}',\lambda)|. \qquad (1.31)
\end{aligned}$$

adding which we get the famous **BELL INEQUALITY**:

$$\begin{aligned}
E_{lhv} &= |C(\mathbf{a},\mathbf{b}) - C(\mathbf{a},\mathbf{b}')| + |C(\mathbf{a}',\mathbf{b}) + C(\mathbf{a}',\mathbf{b}')| \\
&\leq \int d\lambda \rho(\lambda) \times (|B(\mathbf{b},\lambda) - B(\mathbf{b}',\lambda)| + |B(\mathbf{b},\lambda) + B(\mathbf{b}',\lambda)|) = 2. \qquad (1.32)
\end{aligned}$$

Thus, local realism, manifested mathematically leads to the condition:

$$E_{lhv} = |C(\mathbf{a},\mathbf{b}) - C(\mathbf{a},\mathbf{b}')| + |C(\mathbf{a}',\mathbf{b}) + C(\mathbf{a}',\mathbf{b}')| \leq 2 \qquad (1.33)$$

This form of Bell's Inequality is known as the Closer-Horne-Shimony-Holt (CHSH) inequality [65]. Notice that both the presumptions of local realism leads to the constraint on the correlations as given above. In order to test whether quantum mechanics is consistent with the inequality, we need to calculate the correlations amongst the results of measurements of observables done on spatially separated quantum systems.

As an example, consider the spin *singlet* state, which is an ***entangled*** state

Figure 1.3: **John Stewart Bell**. Pic credit: Learn-math.info

given by

$$|\Psi_{AB}\rangle = \frac{|0_A\rangle\,|1_B\rangle - |1_A\rangle\,|0_B\rangle}{\sqrt{2}}$$

The finding of the quantum correlation entails the calculation of the expectation value of the quantum observables $\boldsymbol{\sigma}^A \cdot \mathbf{a}$ and $\boldsymbol{\sigma}^B \cdot \mathbf{b}$ on the singlet state. That is, $\langle\Psi_{AB}|\,\boldsymbol{\sigma}^A \cdot \mathbf{a} \otimes \boldsymbol{\sigma}^B \cdot \mathbf{b}\,|\Psi_{AB}\rangle$. To this end, the calculation of this expectation value yields the result

$$\langle\Psi_{AB}|\,\boldsymbol{\sigma}^A \cdot \mathbf{a} \otimes \boldsymbol{\sigma}^B \cdot \mathbf{b}\,|\Psi_{AB}\rangle = -\cos(\theta_{ab}) \tag{1.34}$$

where θ_{ab} is the angle between directions $\mathbf{a}$ and $\mathbf{b}$. Choosing the four directions $\mathbf{a}$, $\mathbf{a}'$, $\mathbf{b}$, $\mathbf{b}'$ to be co-planar with relative directions $ab = \pi/4$; $a'b = \pi/4$; $b'a' = \pi/4$, the left hand side of the inequality (1.33) leads us to $E_{QM} = 2\sqrt{2}$ which is in violation of the CHSH(Bell) inequality. Thus, quantum mechanics violates the presumptions of local realism.

The genius of John Bell was that he was able to frame an experimental proposition to test the idea about the existence of an underlying theory (Hidden Variable Theory) explaining the emergence of statistical distributions of quantum mechanics, akin to the explanation of the theory of Thermodynamics from the postulates of Equilibrium Statistical Mechanics. Thus the answer to the question "Can the Spooky, Action-at-a-distance Predictions (Entanglement) of Quantum Mechanics be Replaced by Some Sort of Local, Statistical, Classical (Hidden Variable) Theory?" was given by Bell in the following way that "The physical predictions of quantum theory disagree with those of any local (classical) hidden-variable theory!" Several experiments, with increasing robustness and precision have been performed over the years to check whether quantum theory adheres to local realism. These have led to the conclusion that quantum theory departs from the lines of thought characteristic to the intuition behind classical mechanics and that in general, ***nature does not respect local realism***. The first experiments were done by Freedman and Clauser in 1972 [66] and more comprehensive experiments were later carried out by Alain Aspect et. al, [67, 68, 69]. Other and recent experiments include (but not limited to) [70, 71, 72]. Thus, violation of Bell inequalities implies that both locality as well as realism is untenable in the quantum domain [73, 74]. Also, see [75] for a review on the historical introduction to the hidden variable theory and the experimental progress towards the elucidation of conclusive Bell tests (experiments).

The outcome of all these experiments was a reinforcement of the worldview that Quantum Theory is a non-local theory and that *Entanglement* is a correlation which is remarkably different in nature to that of it's classical counterpart. This identification has helped us in using entanglement as a unique resource for secure communication protocols [quantum cryptography] and other information theory purposes.

1.3.2 Leggett-Garg Inequality–Test of macrorealism

The construction of Bell's inequality and the proposition and verification of experiments pertaining to the validation of quantum theory being non-local in nature has all the more certified that non-classicality is a feature of the microscopic (quantum) world. Till now, we have focused on the problem of EPR, and the emergence of the non-classical correlation named *entanglement* in composite quantum systems. However, an interesting question would be to seek the characterization of the non-classicality of single quantum systems themselves. To this end, it becomes even more interesting if this is posed in the macroscopic regime where one mostly observes classical behavior. This is interesting in the sense of identifying the boundary between the microscopic and the macroscopic, if any. Furthermore, one may seek to know about the persistence of quantum features like *superposition* in the macroscopic regime. Quantum mechanics answers in the affirmative to this question if one manages to defy *decoherence* [76]. In other words, we ask: When and how do physical systems stop behaving quantum mechanically and begin to behave classically?

All these questions get addressed in the worldview known as macrorealism due to Leggett and Garg [4].

The notion of *macrorealism* rests on the classical world view that

(i) macrorealism per se: Physical properties of a macroscopic object exist independent of the act of observation and

(ii) Non-Invasive Measurability (NIM): The measurements are non-invasive i.e., the measurement of an observable at any instant of time does not influence its subsequent evolution.

Quantum predictions differ at a foundational level from these two contentions. In 1985, Leggett and Garg (LG) [4] designed an inequality (which places bounds on certain linear combinations of temporal correlations of a dynamical observable) to test whether a single macroscopic object exhibits macrorealism or not. The Leggett-Garg correlation inequality is satisfied by all macro realistic theories and is violated if quantum law governs. Debates on the emergence of macroscopic classical realm from the corresponding quantum domain continue and it is a topic of current experimental and theoretical research [77, 78, 79, 80, 81].

Derivation of the Leggett-Garg Inequality (LGI)

Consider a single system **S** and a macroscopic observable **Q** measured at different instants of time t. Let the macroscopic observable Q take values ±1 at any instant of time it is measured.
The joint assumption of macrorealism is mathematically put in the form

$$P(m_i, m_j|t_i, t_j) = \sum_{\lambda} \rho(\lambda) P(m_i|t_i, \lambda) P(m_j|t_j, \lambda) \tag{1.35}$$

where m_i, m_j are the values of the measurements made at time instants t_i and t_j respectively.
The conditions of *macrorealism per se* and *NIM* manifested mathematically provides us the correlation inequality which can be tested experimentally. However, in full glory, quantum mechanics violates the inequality and is found to be not adhering to the tenets of *macrorealism*.

Let us consider a dichotomic observable $Q(t_i) = Q_i$ which take values ±1 at any instant of time t_i. For any set of experimental measurements on given initial state, the NIM constraint is prescribed as the equality of the value of the observable Q_i irrespective of the combination Q_iQ_j along which it occurs. The tenet *macrorealism per se* is expressed as the existence of definite values for $Q_i$which is ± 1.

The correlation observables are denoted as $C_{t_it_j}$ which is defined by

$$C_{t_it_j} \equiv \langle Q_iQ_j \rangle \tag{1.36}$$

The correlation amongst the values of the observables Q_i and Q_j is assumed to stem from the form of the probability distribution given by (1.35).

The derivation of the LGI follows on the footsteps laid out in deriving the Bell's inequality in that the instants denoted as "t_i" plays the role of the measurement settings **a** and **b** in the spatial case. Following the procedure, we arrive at the celebrated **Leggett Garg Inequality** for the case of four measurements done sequentially:

$$\begin{aligned} K_4 &= C_{t_1t_2} + C_{t_2t_3} + C_{t_3t_4} - C_{t_1t_4} \\ &= \langle Q_1Q_2 \rangle + \langle Q_2Q_3 \rangle + \langle Q_3Q_4 \rangle - \langle Q_1Q_4 \rangle \leq 2 \end{aligned} \tag{1.37}$$

The above inequality is known as a LG string with 4 measurements. On the other hand, LG string with 3 measurements is given by

$$\begin{aligned} K_3 &= C_{t_1t_2} + C_{t_2t_3} - C_{t_1t_3} \\ &= \langle Q_1Q_2 \rangle + \langle Q_2Q_3 \rangle - \langle Q_1Q_3 \rangle \leq 1 \end{aligned} \tag{1.38}$$

Note that the lower bound and the upper bound of LG string with 3 measurements are -3 and 1 respectively,i.e, $-3 \leq K_3 \leq 1$ whereas for the 4 measurements it is $-2 \leq K_4 \leq 2$.

As an example, let us consider a spin-1/2 particle (of course! it's not a macroscopic system which the framework of macrorealism wants to address but this simple system suffices for our illustrative purpose) precessing about z-axis – characterized by the Hamiltonian $\mathbf{H} = \frac{\hbar\omega}{2}\boldsymbol{\sigma}_z$. Choosing initial state to be $\rho(0) = \frac{1}{2}[I + \boldsymbol{\sigma}_x]$ and the dichotomic observables

$$\begin{aligned} \mathbf{Q}_i &\equiv \boldsymbol{\sigma}_x((i-1)\,\Delta\, t) = e^{i\,H\,(i-1)\,\Delta\, t/\hbar}\,\boldsymbol{\sigma}_x\, e^{-i\,H\,(i-1)\,\Delta\, t/\hbar} \\ &= \boldsymbol{\sigma}_x \cos\{(i-1)\,\omega\,\Delta\, t\} - \boldsymbol{\sigma}_y \sin\{(i-1)\,\omega\,\Delta\, t\} \end{aligned} \tag{1.39}$$

(these observables are dichotomic as their eigenvalues are ± 1). We obtain, $\langle \mathbf{Q}_1\,\mathbf{Q}_2\rangle = \langle \mathbf{Q}_2\,\mathbf{Q}_3\rangle = \cos(\omega\,\Delta\, t)$ and $\langle \mathbf{Q}_1\,\mathbf{Q}_3\rangle = \cos(2\,\omega\,\Delta\, t)$. Thus,

$$K_3 = 2\,\cos(\omega\,\Delta\, t) - \cos(2\,\omega\,\Delta\, t). \tag{1.40}$$

Maximum value of K_3 with this choice is 1.5, which violates the LGI. Fig 1.4 shows the violation of LG K_3 string.

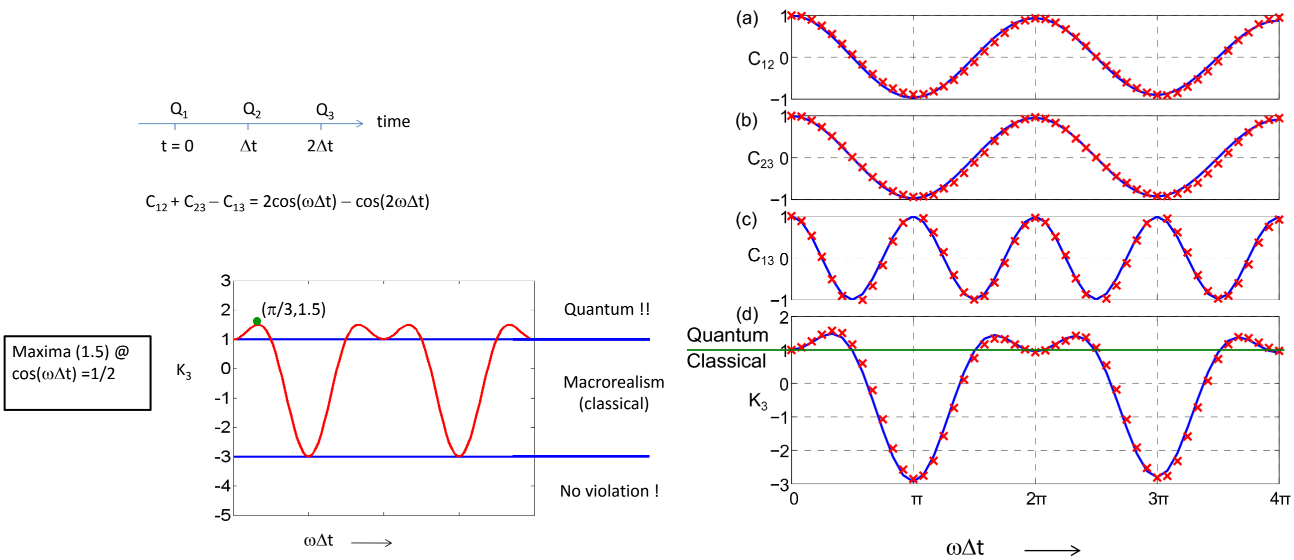

Figure 1.4: The left figure shows the theoretical result, i.e, Quantum violation of LG K_3 string. The right figure shows the experimental violation of the LG K_3 string. For more details on the experimental aspects see [82]

Off late, experimentalists have been giving increasing attention towards performing tests checking the validation of quantum systems adhering to the tenets of macrorealism. These experiments, however have concentrated at length scales which are characteristic of what is called as the microscopic regime [83, 84, 85, 82, 86] (also, see [87] for a more recent review concerning Leggett-Garg inequalities). It is the author's view that experimental propositions verifying the validity of macrorealism need to be performed at the length scale which is grey enough to be called neither micro nor the macro regime. This helps mainly in the better characterization of the transition from micro to the macro or vice versa. To this end, the content of Chapter 3 proposes a different yet stringent theoretical scheme to witness such a transition, the experimental realization of which could be performed at the mentioned length scale.

The last non-classical feature which we are going to introduce is the concept of *steering* or *non-local steering*. Recently, there have been a surge of research activity wherein the concept of non-local steering has been shown to be interlinked with that of the notion of *Joint Measurability*. A small digression regarding these developments is given here in brief.

1.3.3 Quantum Steering and Joint Measurability

Quantum Steering

The paradox of the EPR paper brought in the attention of *Erwin Schrödinger*. In fact, it was he who called it as a "paradox" as he was neither able to find a flaw in the EPR argument nor was he accepting quantum theory to be an incomplete description of nature. Furthermore, it was he who coined the word "Entanglement" for the non-factorizability or non-separability of composite pure states.

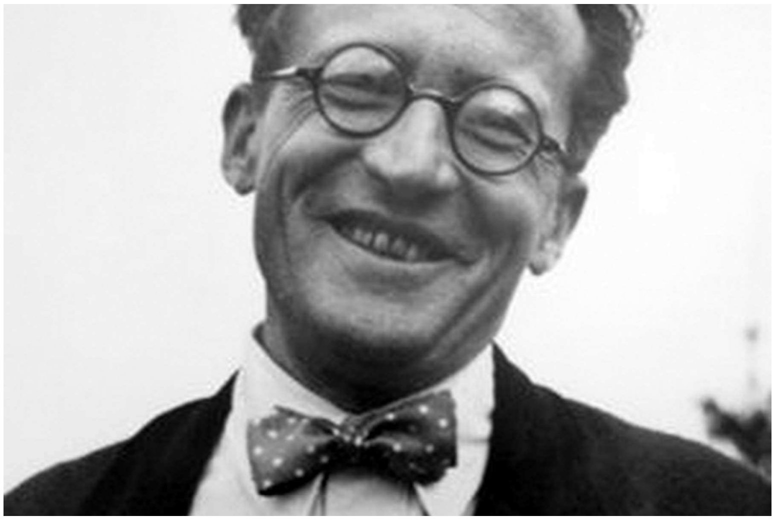

Figure 1.5: **Erwin Schrödinger** Pic credit: Timeline of the atom

Thus he remarked,

> "Quantum entanglement is the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought."

Moreover, he understood that this entanglement is broken (disentanglement) when a measurement of an observable is made on either of the parties sharing the composite state. As such, he puts the argument of EPR in the way that [88, 23]

> "Attention has recently [EPR] been called to the obvious but very disconcerting fact that even though we restrict the disentangling measurements to one system, the representative obtained for the *other* system is by no means independent of the particular choice of observations which we select for that purpose and which by the way are *entirely* arbitrary."

Consider non-separable pure states of a bi-partite system. Let the composite state be shared by the archetypal pair of Alice and Bob.

$$|\Psi\rangle = \sum_n c_n |\psi_n\rangle |u_n\rangle = \sum_n d_n |\phi_n\rangle |v_n\rangle$$

When Bob makes measurements at his end, he can steer Alice's state into either $|\psi_n\rangle$'s or $|\phi_n\rangle$'s depending upon his choice of measurement which is *random*. As such, Schrödinger introduced the term "steering" when he discerned that,

> "It is rather discomforting that the theory should allow a system to be steered ...... into one or the other type of state at the experimenters mercy in spite of having no access to it."

Thus, it is found that steering is yet another facet of the mystical world of Quantum Mechanics.
A formal modern approach to steering was initiated by M. D. Reid [89], who proposed the first experimentally testable criteria of nonlocal steering. Reid's criteria brought out that steering and the Einstein-Podolsky-Rosen paradox are equivalent notions of nonlocality. Further, H. M. Wiseman et al. [90] showed that steering constitutes a different class of nonlocality, which lies between entanglement and Bell nonlocality. Manifestation of steering in the form of different types of steering inequalities is presented by E. G. Cavalcanti et al. [88].

Joint Measurability

Bell and Leggett-Garg inequalities involve statistical outcomes of spatial and temporal correlations, the violation of which implies *neither* Local Realism *nor* macrorealism. Mainly, the violation of these inequalities points towards the *non-existence of a grand joint probability distribution* for the results of measurement made on quantum systems. [73, 91]. The characterization of this non-existence of a grander joint probability distribution forms the content of

Chapters 4 and 5.

Commutativity of projective measurements, representing two or more Hermitian observables, imply that they are jointly measurable (compatible) and via this way the existence of a grand joint probability distribution of measurement outcomes is ensured. However, compatibility of measurements with commutativity turns out to be limited in an extended framework where Positive Operator Valued Measures (POVM) have been analyzed to generalize the aspect of compatibility through the notion of *Joint Measurability*.

A joint measurement of commuting observables imply that by performing one measurement, we can produce the results for each of the two observables. But quantum mechanics places restrictions on how *sharply* two non-commuting observables can be measured jointly. Naturally one is lead to ask, "Are joint un-sharp measurements possible?" The orthodox notion of *sharp* projective valued (PV) measurements of hermitian observables gets broadened to include *unsharp* measurements of POV observables (observables "corresponding" to POVMs). This allows us to seek whether classical features emerge when one merely confines to measurements of *compatible unsharp observables*. Also, is it possible to classify physical theories based on the *fuzziness* required for joint measurability? The answers to some of these questions are provided in the Chapter 7.

Joint Measurability of POVMs

Mathematically, POVM is a set $\mathbb{E} = \{\mathbf{E}(x)\}$ comprising of positive self-adjoint operators $0 \leq \mathbf{E}(x) \leq 1$, called *effects*, satisfying $\sum_x \mathbf{E}(x) = \mathbb{I}$; x denotes the outcomes of measurement and $\mathbb{I}$ is the identity operator. The notion of a POVM

$\mathbf{E}$ to be a generalized observable provides a physical representation for any possible events (effects $\mathbf{E}(x)$) to occur as outcomes x in a measurement process.

When a quantum system is prepared in the state ρ, measurement of the observable $\mathbb{E}$ gives rise to generalized Lüder's transformation of the state i.e.,

$$\rho \longmapsto \sum_x \sqrt{\mathbf{E}(x)}\, \rho\, \sqrt{\mathbf{E}(x)} \tag{1.41}$$

and an outcome x occurs with probability $p(x) = \text{Tr}[\rho\, \mathbf{E}(x)]$. The expectation value of the observable is given by

$$\langle \mathbb{E} \rangle = \sum_x x\, \text{Tr}[\rho\, \mathbf{E}(x)] = \sum_x x\, p(x). \tag{1.42}$$

The usual scenario of PV measurements is recovered as a special case, when $\{\mathbf{E}(x)\}$ forms a set of complete, orthogonal projectors.

A finite collection of POVMs $\mathbf{E}_1, \mathbf{E}_2, \ldots, \mathbf{E}_n$ is said to be jointly measurable (or compatible), if there exists a *grand* POVM $\mathbb{G} = \{\mathbf{G}(\lambda);\ 0 \leq \mathbf{G}(\lambda) \leq \mathbb{I}, \sum_\lambda \mathbf{G}(\lambda) = \mathbb{I}\}$ from which the observables $\mathbf{E}_i$ can be obtained by post-processing as follows. Suppose a measurement of the global POVM $\mathbf{G}$ is carried out in a state ρ and the probability of obtaining the outcome λ is denoted by $p(\lambda) = \text{Tr}[\rho\, \mathbf{G}(\lambda)]$. If the effects $\mathbf{E}_i(x_i)$ constituting the POVM $\mathbb{E}_i$ can be obtained as *marginals* of the *grand* POVM $\mathbb{G} = \{\, \mathbf{G}(\lambda), \lambda \equiv \{x_1, x_2, \ldots\}$, (where λ corresponds to a collective index $\{x_1, x_2, \ldots\}$) i.e., if there exists a grand POVM $\mathbb{G}$ such that [12]

$$\begin{aligned}
\mathbf{E}_1(x_1) &= \sum_{x_2, x_3, \ldots} \mathbf{G}(x_1, x_2, \ldots, x_n) \\
\mathbf{E}_2(x_2) &= \sum_{x_1, x_3, \ldots} \mathbf{G}(x_1, x_2, \ldots, x_n)
\end{aligned}$$

$$\vdots$$

$$\mathbf{E}_n(x_n) \;=\; \sum_{x_1,x_3,\ldots} \mathbf{G}(x_1, x_2, \ldots, x_n), \tag{1.43}$$

the POVMs $\mathbf{E}_1, \mathbf{E}_2, \ldots, \mathbf{E}_n$ are said to be jointly measurable. Thus, a collection of compatible POVMs $\mathbf{E}_1, \mathbf{E}_2, \ldots, \mathbf{E}_n$ is obtained from a global POVM $\mathbf{G}$ via post processing of the form (1.43). We emphasize once again that compatibility of POVMs does not require their commutativity, but it demands the existence of a global POVM.

As an example, consider Pauli spin observables $\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_z$ of a qubit. Sharp measurements of the observables $\boldsymbol{\sigma}_x = \sum_{x=\pm1} x\, \mathbf{\Pi}_{\boldsymbol{\sigma}_x}(x)$ and $\boldsymbol{\sigma}_z = \sum_{z=\pm1} z\, \mathbf{\Pi}_{\boldsymbol{\sigma}_z}(z)$ is performed using the two outcome projection operators

$$\begin{aligned}
\mathbf{\Pi}_{\boldsymbol{\sigma}_x}(x) &= \frac{1}{2}\left(\mathbb{I} + x\,\boldsymbol{\sigma}_x\right), \\
\mathbf{\Pi}_{\boldsymbol{\sigma}_z}(z) &= \frac{1}{2}\left(\mathbb{I} + z\,\boldsymbol{\sigma}_z\right).
\end{aligned} \tag{1.44}$$

The observables $\boldsymbol{\sigma}_x$ and $\boldsymbol{\sigma}_z$ are non-commuting and hence can not be measured jointly using PV measurements. However, it is possible to consider joint fuzzy measurements of $\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_z$ in terms of their POVM counterparts, which are constructed by adding uniform white noise to the PV operators of (1.44). One then obtains binary POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x} = \{\mathbf{E}_{\boldsymbol{\sigma}_x}(x);\, x = \pm1\}$, $\mathbb{E}_{\boldsymbol{\sigma}_z} = \{\mathbf{E}_{\boldsymbol{\sigma}_z}(z);\, z = \pm1\}$, where

$$\begin{aligned}
\mathbf{E}_{\boldsymbol{\sigma}_x}(x) &= \eta\, \mathbf{\Pi}_{\boldsymbol{\sigma}_x}(x) + (1-\eta)\,\frac{\mathbb{I}}{2} \\
&= \frac{1}{2}\left(\mathbb{I} + \eta\, x\,\boldsymbol{\sigma}_x\right) \\
\mathbf{E}_{\boldsymbol{\sigma}_z}(z) &= \eta\, \mathbf{\Pi}_{\boldsymbol{\sigma}_z}(z) + (1-\eta)\,\frac{\mathbb{I}}{2} \\
&= \frac{1}{2}\left(\mathbb{I} + \eta\, z\,\boldsymbol{\sigma}_z\right)
\end{aligned} \tag{1.45}$$

where $0 \leq \eta \leq 1$ denotes the unsharpness parameter. It may be noted that when $\eta = 1$, the fuzzy POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x} = \{\mathbf{E}_{\boldsymbol{\sigma}_x}(x)\}, \mathbb{E}_{\boldsymbol{\sigma}_z} = \{\mathbf{E}_{\boldsymbol{\sigma}_z}(z)\}$ reduce to their corresponding *sharp* PV versions $\{\boldsymbol{\Pi}_{\boldsymbol{\sigma}_x}(x)\}, \{\boldsymbol{\Pi}_{\boldsymbol{\sigma}_z}(z)\}$.

The binary POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x}$, $\mathbb{E}_{\boldsymbol{\sigma}_z}$ are compatible if there exists a four element grand POVM $\mathbb{G} = \{\mathbf{G}(x, z);\ x, z = \pm 1\}$ satisfying

$$\begin{aligned}\sum_{z=\pm 1} \mathbf{G}(x,z) &= \mathbf{G}(x,1) + \mathbf{G}(x,-1) = \mathbf{E}_{\boldsymbol{\sigma}_x}(x) \\ \sum_{x=\pm 1} \mathbf{G}(x,z) &= \mathbf{G}(1,z) + \mathbf{G}(-1,z) = \mathbf{E}_{\boldsymbol{\sigma}_z}(z) \\ \sum_{x,z=\pm 1} \mathbf{G}(x,z) &= \mathbb{I}, \qquad \mathbf{G}(x,z) \geq 0. \end{aligned} \tag{1.46}$$

It has been shown [8, 12] that the POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x}$, $\mathbb{E}_{\boldsymbol{\sigma}_z}$ are compatible in the range $0 \leq \eta \leq 1/\sqrt{2}$ of the unsharpness parameter (see Appendix B), as it is possible to construct a global POVM $\mathbb{G}$ comprising of the effects

$$\mathbf{G}(x,z) = \frac{1}{4}\left(\mathbb{I} + \eta\, x\, \boldsymbol{\sigma}_x + \eta\, z\, \boldsymbol{\sigma}_z\right),\ 0 \leq \eta \leq 1/\sqrt{2} \tag{1.47}$$

satisfying the required conditions (1.46).

Measurement of a *single* generalized observable (POVM) $\mathbb{G}$ enables one to produce the results of measurement of both the POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x}$ and $\mathbb{E}_{\boldsymbol{\sigma}_z}$, when they are compatible. And, as a consequence, joint measurability of POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x}$, $\mathbb{E}_{\boldsymbol{\sigma}_y}$ ensures the existence of a joint probability distribution $p(x,z) = \mathrm{Tr}[\rho\, \mathbf{G}(x,z)]$ obeying $p(x) = \sum_z p(x,z) = \mathrm{Tr}[\rho \sum_z \mathbf{G}(x,z)] = \mathrm{Tr}[\rho\, \mathbf{E}_{\boldsymbol{\sigma}_x}(x)]$, $p(z) = \sum_x p(x,z) = \mathrm{Tr}[\rho \sum_x \mathbf{G}(x,z)] = \mathrm{Tr}[\rho\, \mathbf{E}_{\boldsymbol{\sigma}_z}(z)]$, over the measurement outcomes x, z of the unsharp POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x}$, $\mathbb{E}_{\boldsymbol{\sigma}_z}$ in any arbitrary quantum state ρ.

Triple-wise joint measurements of all the three Pauli observables $\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_y$ and $\boldsymbol{\sigma}_z$ can be envisaged by considering the fuzzy binary outcome POVMs $\mathbb{E}_{\boldsymbol{\sigma}_x} = \left\{\mathbf{E}_{\boldsymbol{\sigma}_x}(x) = \frac{1}{2}\left(\mathbb{I} + \eta\, x\, \boldsymbol{\sigma}_x\right);\, x = \pm 1\right\}$, $\mathbb{E}_{\boldsymbol{\sigma}_y} = \left\{\mathbf{E}_{\boldsymbol{\sigma}_y}(y) = \frac{1}{2}\left(\mathbb{I} + \eta\, y\, \boldsymbol{\sigma}_y\right);\, y = \pm 1\right\}$, $\mathbb{E}_{\boldsymbol{\sigma}_z} = \left\{\mathbf{E}_{\boldsymbol{\sigma}_z}(z) = \frac{1}{2}\left(\mathbb{I} + \eta\, z\, \boldsymbol{\sigma}_z\right);\, z = \pm 1\right\}$ in the range $0 \leq \eta \leq 1/\sqrt{3}$ of the unsharpness parameter [12, 17]. Further, it has also been shown [17] that the noisy versions $\mathbb{E}_{\vec{\boldsymbol{\sigma}}\cdot\hat{n}_k} = \left\{\mathbf{E}_{\vec{\boldsymbol{\sigma}}\cdot\hat{n}_k}(x_k = \pm 1) = \frac{1}{2}\left(\mathbb{I} + \eta\, x_k\, \vec{\boldsymbol{\sigma}}\cdot\hat{n}_k\right)\right\}$ of the qubit spin, oriented along the unit vectors $\hat{n}_k$, $k = 1, 2, 3$, which are equally separated in a plane (i.e., separated by an angle 120°), are pairwise jointly measurable if the unsharpness parameter, $\eta \leq \sqrt{3} - 1$, but are triple-wise jointly measurable when $\eta \leq 2/3$ (see Appendix B).

The interconnection between the concepts of non-local steering, joint measurability and entropic uncertainty forms the content of Chapter 7.

Chapter 2

The uncertainty product of position and momentum in classical dynamics

It is generally believed that the classical regime emerges as a limiting case of quantum theory. Exploring such quantum-classical correspondences provides a deeper understanding of foundational aspects and has attracted a great deal of attention since the early days of quantum theory. It has been proposed that since a quantum mechanical wave function describes an intrinsic statistical behavior, its classical limit must correspond to a classical ensemble—not to an individual particle. This idea leads us to ask how the uncertainty product of canonical observables in the quantum realm compares with the corresponding dispersions in the classical realm. In this Chapter, we explore parallels between the uncertainty product of position and momentum in stationary states of quantum systems and the corresponding fluctuations of these observables in the associated classical ensemble. We confine ourselves to one-dimensional conservative systems and show, with the help of suitably defined dimensionless physical quantities, that first and second moments of the canonical observables match with each other in the classical and quantum descriptions—resulting in identical structures for the uncertainty relations in both realms.

2.1 Introduction

It is imperative to retrieve classical dynamics as a limiting case—in its domain of validity—from quantum theory. The generally prevailing notion is that classical mechanics emerges in the limit $\hbar \to 0$. The applicability of this limit is reviewed critically in Refs. [34] and [92].

Another quantum-classical correspondence discussed widely is through the Ehrenfest's theorem [93]. This states that the equations of motion for the expectation values of the position and momentum are the same as those obeyed by a classical particle under certain conditions. More specifically, for a system with Hamiltonian $\mathbf{H} = \mathbf{p}^2/2m + V(\mathbf{x})$, the equations of motion for the expectation values of the position and momentum operators are

$$\frac{d\langle \mathbf{x} \rangle}{dt} = \frac{\langle \mathbf{p} \rangle}{m}, \tag{2.1}$$

$$\frac{d\langle \mathbf{p} \rangle}{dt} = -\left\langle \frac{dV(\mathbf{x})}{dx} \right\rangle = \langle \mathbf{F}(\mathbf{x}) \rangle, \tag{2.2}$$

where $\mathbf{F}(\mathbf{x}) = -dV(\mathbf{x})/dx$ is the force operator. Under the approximation $\langle \mathbf{F}(\mathbf{x}) \rangle \approx \mathbf{F}(\langle \mathbf{x} \rangle)$ (which is exact for linear and quadratic potentials), the equation of motion for $\langle \mathbf{p} \rangle$ reduces to

$$\frac{d\langle \mathbf{p} \rangle}{dt} = \mathbf{F}(\langle \mathbf{x} \rangle). \tag{2.3}$$

In other words, the quantum averages $\langle \mathbf{x} \rangle$ and $\langle \mathbf{p} \rangle$ satisfy the classical equations of motion (2.1) and (2.3). However, in order for these equations to lead to classical trajectories, the quantum wave function must be narrow compared to the typical length scale over which the force varies. Furthermore, for the stationary states of a Hamiltonian that is symmetric under $\mathbf{x} \leftrightarrow -\mathbf{x}$, both $\langle \mathbf{x} \rangle$ and $\langle \mathbf{p} \rangle$ are always zero and therefore Ehrenfest's theorem does not yield any useful information.

The discussions in many textbooks on quantum mechanics are essentially confined to the limit $\hbar \to 0$ and the Ehrenfest theorem in discussing the emergence of the classical regime. While both these quantum-classical correspondences operate in their own domains of applicability, it has been identified that they are not universally satisfactory [94, 95, 96, 97, 98, 99, 100]. In the absence of a commonly accepted notion of the classical limit, it is important to recognize the quantum features that are expected to leave their imprints in the classical regime.

It has been pointed out that the classical limit of a quantum state ought to correspond to an ensemble than a single particle [34, 96, 101]. Hence, it would be interesting to compute the averages, variances, and the higher-order moments of the quantum and classical probability distributions in the limiting case. Interestingly, considerable attention has been evinced recently in exploring the borderline between classical and quantum worlds via the uncertainty principle [1]. Conceptual advances in symplectic geometry and topology—followed by Gromov's discovery of *symplectic non-squeezing* phenomena [3]—shed light on the fact that there is an underlying uncertainty principle governing the classical Hamiltonian phase flows too [2].

In order to compare the statistical form of classical dynamics with the corresponding one in quantum dynamics, the phase space probability distribution of the classical ensemble (a counterpart of the corresponding quantum state) needs to be identified. The classical phase space probability distribution satisfies the Liouville equation and the phase space averages of the classical observables are shown to exhibit dynamical behaviour analogous to that of the corresponding quantum case—even when Ehrenfest's theorem breaks down [96]. More recently [102], it has been shown that starting from the Ehrenfest theorem, either the Liouville equation (if the momentum and coordinate commute), or the Schrödinger equation (if the momentum and coordinate obey the canonical commutation relation) would ensue.

It is pertinent to mention here another approach towards the classical limit, where one considers only stationary state solutions of the quantum Hamiltonian and graphically compare the probability density function $P^{(n)}_{\rm QM}(x) = |\psi_n(x)|^2$

with the corresponding classical probability distribution $P_{\mathrm{CL}}(x)$ of an ensemble; it is then recognized that the *envelope* of the quantum probability density approaches the classical one in the large-n limit [103].

In this Chapter, we show that the first and second moments of suitably defined *dimensionless* canonical variables evaluated for the stationary states of one-dimensional conservative quantum systems match with those associated with the corresponding classical ensemble. This, in turn, leads to *identical* structure for uncertainty relations of the dimensionless position and momentum variables in both classical and quantum domains—bringing out the underlying unity of the two formalisms—irrespective of their structurally different mathematical and conceptual nature.

2.2 Classical probability distributions corresponding to quantum mechanical stationary states

We begin by reviewing the classical probability distributions [103] for an ensemble of particles bound in a one-dimensional potential $V(x)$. The probability density function for the position x of a *single* particle, whose initial position and velocity are specified, is given by

$$P_{\mathrm{CL}}^{\mathrm{single}}(x,t) = \delta[x - x(t)], \tag{2.4}$$

where $x(t)$ denotes the deterministic trajectory of the particle at any instant of time t. However, the quantum mechanical probability density $P_{QM}^{(n)}(x) = |\psi_n(x)|^2$ associated with the stationary-state solution $\psi_n(x)$ is not expected to approach—in the classical limit— the single-particle probability density of Eq. (2.4). Rather, the locally averaged quantum probability density *does* approximate a probability distribution $P_{\mathrm{CL}}(x)$ of a classical ensemble of particles (of fixed energy E) in the large n limit [103].

Classical particles of fixed energy E in a statistical ensemble (microcanonical ensemble) are confined to move on a surface of constant energy E in the phase space and the associated phase space probability distribution $P_{\rm CL}(x,p)$ obeys the stationary state Liouville equation

$$\frac{dP_{\rm CL}(x,p)}{dt} = \{P_{\rm CL}(x,p), H\} = 0, \tag{2.5}$$

where $\{P_{\rm CL}(x,p), H\}$ is the Poisson bracket of $P_{\rm CL}(x,p)$ with the Hamiltonian $H = (p^2/2m) + V(x)$. In other words, the phase space distribution $P_{\rm CL}(x,p)$ is a function of the Hamiltonian H itself. The principle of equal *a priori* probability then corresponds to

$$P_{\rm CL}(x,p) \propto \delta\left[\frac{p^2}{2m} + V(x) - E\right]. \tag{2.6}$$

The position probability function is then obtained by integrating over the momentum variable p:

$$\begin{aligned} P_{\rm CL}(x) &= \int dp\, P_{\rm CL}(x,p) \\ &= \text{Constant} \cdot \int dp\, \delta\left[\frac{p^2}{2m} + V(x) - E\right]. \end{aligned} \tag{2.7}$$

Using the properties $\delta(ax) = \delta(x)/|a|$ and $\delta(x^2 - a^2) = [\delta(x+a) + \delta(x-a)]/2|a|$ of the Dirac delta function, the classical probability distribution reduces to

$$\begin{aligned} P_{\rm CL}(x) &= \text{Constant} \cdot \int dp\, 2m\, \delta\left(p^2 + 2m[V(x) - E]\right) \\ &= \text{Constant} \cdot \sqrt{\frac{2m}{[E - V(x)]}} \int dp\, \left[\delta\left(p + \sqrt{2m[E - V(x)]}\right)\right. \\ &\qquad \left. + \delta\left(p - \sqrt{2m[E - V(x)]}\right)\right] \\ &= \frac{\mathcal{N}}{\sqrt{E - V(x)}}, \end{aligned} \tag{2.8}$$

where $\mathcal{N}$ denotes the normalization factor, such that $\int_{x_1}^{x_2} dx\, P_{\rm CL}(x) = 1$ (the integration is taken between the classical turning points (x_1, x_2) as the probability distribution $P_{\rm CL}(x)$ vanishes outside the domain $x_1 \leq x \leq x_2$).

It may be readily seen that, by substituting $E = m\omega^2 A^2/2$ and $V(x) = m\omega^2 x^2/2$ in the familiar example of the harmonic oscillator, the classical position probability distribution (2.8) reduces to the well-known expression $P_{\rm CL}(x) = 1/\pi\sqrt{A^2 - x^2}$.

The phase space averages of any arbitrary function $F(x,p)$ of position and momentum variables get reduced to those evaluated with the position probability distribution function $P_{\rm CL}(x)$ as follows:

$$\begin{aligned}
\langle F(x,p)\rangle_{\rm CL} &= \int dx \int dp\, P_{\rm CL}(x,p)\, F(x,p) \\
&= \text{Constant} \cdot \int dx \int dp\, \delta\left(\frac{p^2}{2m} + V(x) - E\right) F(x,p) \\
&= \text{Constant} \cdot \int dx \sqrt{\frac{2m}{E - V(x)}} \int dp\, \left[\delta\left(p + \sqrt{2m[E - V(x)]}\right)\right. \\
&\qquad\qquad \left. + \delta\left(p - \sqrt{2m[E - V(x)]}\right)\right] F(x,p) \\
&= \text{Constant} \cdot \int dx \sqrt{\frac{2m}{E - V(x)}} \left[F(x, -\sqrt{2m[E - V(x)]})\right. \\
&\qquad\qquad \left. + F(x, \sqrt{2m[E - V(x)]})\right] \\
&= \frac{1}{2} \int dx\, P_{\rm CL}(x) \left[F\left(x, -\sqrt{2m[E - V(x)]}\right) + F\left(x, \sqrt{2m[E - V(x)]}\right)\right].
\end{aligned} \tag{2.9}$$

We define dimensionless (scaled) position and momentum variables,

$$X = \frac{x}{A}, \qquad P = \frac{p}{\sqrt{2mE}}, \tag{2.10}$$

such that $|X|$, $|P| \leq 1$ in a bounded system.

In the next section, we compute the first and second moments $\langle X\rangle_{\rm CL}$, $\langle X^2\rangle_{\rm CL}$, $\langle P\rangle_{\rm CL}$, and $\langle P^2\rangle_{\rm CL}$ of the classical probability distribution in three specific examples of one-dimensional bound systems. We then compare these classical averages with the quantum expectation values $\langle \mathbf{X}\rangle_{\rm QM}$, $\langle \mathbf{X}^2\rangle_{\rm QM}$, $\langle \mathbf{P}\rangle_{\rm QM}$, and $\langle \mathbf{P}^2\rangle_{\rm QM}$, evaluated for the stationary states $\psi_n(x)$, and show that they agree remarkably with each other in the classical limit.

2.3 Comparison of first and second moments of the classical distribution with the stationary state quantum moments

We focus now on three specific examples of one-dimensional bound systems: the harmonic oscillator, the infinite well, and the bouncing ball. We evaluate the first and second moments of the dimensionless position and momentum variables (Eq. (2.10)) and show that the quantum moments—evaluated for stationary eigenstates of the Hamiltonian—match their classical counterparts.

2.3.1 One-dimensional harmonic oscillator

As shown in the previous section, the classical probability density for finding a system of harmonic oscillators—all with the same amplitude A—between position x and $x+dx$ is given by

$$P_{\rm CL}(x) = \begin{cases} \dfrac{1}{\pi}\dfrac{1}{\sqrt{A^2-x^2}} & \text{for } |x| \le A, \\ 0 & \text{for } |x| > A. \end{cases} \tag{2.11}$$

We use scaled canonical variables $X = x/A$ and $P = p/\sqrt{2mE} = p/(m\omega A)$, and evaluate the averages of X, X^2, P, and P^2, making use of Eqs. (2.9) and (2.11):

$$\langle X\rangle_{\rm CL} = \frac{1}{A}\int dx\, P_{\rm CL}(x)\, x = \frac{1}{A\pi}\int_{-A}^{A} dx\, \frac{x}{\sqrt{A^2-x^2}} = 0; \tag{2.12}$$

$$\langle X^2\rangle_{\rm CL} = \frac{1}{A^2}\int dx\, P_{\rm CL}(x)\, x^2 = \frac{1}{A^2\pi}\int_{-A}^{A} dx\, \frac{x^2}{\sqrt{A^2-x^2}} = \frac{1}{2}; \tag{2.13}$$

$$\langle P\rangle_{\rm CL} = \frac{1}{2m\omega A}\int_{-A}^{A} dx\, P_{\rm CL}(x)\left(-\sqrt{2m\,[E-\tfrac{1}{2}m\omega^2\,x^2\,]}+\sqrt{2m\,[E-\tfrac{1}{2}m\omega^2\,x^2\,]}\right) = 0; \tag{2.14}$$

$$\begin{aligned}\langle P^2\rangle_{\rm CL} &= \frac{1}{m^2\omega^2A^2}\int_{-A}^{A} dx\, P_{\rm CL}(x)\, 2m\,[E-\tfrac{1}{2}m\omega^2x^2\,]\\ &= \frac{1}{A^2\pi}\int_{-A}^{A} dx\,\sqrt{A^2-x^2} = \frac{1}{2}.\end{aligned} \tag{2.15}$$

The variances of X and P are given by

$$\begin{aligned}(\Delta X)^2_{\rm CL} &= \langle X^2\rangle_{\rm CL} - \langle X\rangle^2_{\rm CL} = \frac{1}{2},\\ (\Delta P)^2_{\rm CL} &= \langle P^2\rangle_{\rm CL} - \langle P\rangle^2_{\rm CL} = \frac{1}{2},\end{aligned} \tag{2.16}$$

and hence the product of variances is

$$(\Delta X)^2_{\rm CL}\,(\Delta P)^2_{\rm CL} \equiv \frac{1}{4} \tag{2.17}$$

in a classical ensemble (characterized by the probability distribution (2.11)) of harmonic oscillators.

The stationary-state solutions of the quantum Hamiltonian $\mathbf{H} = [\mathbf{p}^2 + m^2\,\omega^2\,\mathbf{x}^2]/2m$ are given by

$$\psi_n(x) = \left(\frac{\sqrt{m\omega/\pi\hbar}}{2^n\,n!}\right)^{1/2} H_n(\sqrt{m\omega/\hbar}\,x)\,e^{-m\omega x^2/\hbar}, \tag{2.18}$$

where H_n are the Hermite polynomials of degree n. These states correspond to the energy eigenvalues $E_n = (n + 1/2)\,\hbar\omega$. The *classical turning points* associated with energy E_n are readily identified to be $A_n = \sqrt{2\,E_n/m\omega^2} = \sqrt{(2n+1)\,\hbar/m\omega}$.

We use scaled position and momentum operators, $\mathbf{X} = \mathbf{x}/A_n = \mathbf{x}\,\sqrt{m\omega/(2n+1)\,\hbar}$, $\mathbf{P} = \mathbf{p}/\sqrt{2\,m\,E_n} = \mathbf{p}/\sqrt{(2n+1)\,\hbar\,m\,\omega}$ (corresponding to their classical counterparts above), and evaluate the expectation values of $\mathbf{X}$, $\mathbf{X}^2$, $\mathbf{P}$, and $\mathbf{P}^2$ for the stationary states $\psi_n(x)$:

$$\langle \mathbf{X} \rangle_{QM} = \sqrt{\frac{m\omega}{(2n+1)\hbar}} \int_{-\infty}^{\infty} dx\, |\psi_n(x)|^2\, x = 0; \tag{2.19}$$

$$\langle \mathbf{X^2} \rangle_{QM} = \frac{m\omega}{(2n+1)\hbar} \int_{-\infty}^{\infty} dx\, |\psi_n(x)|^2\, x^2 = \frac{1}{2}; \tag{2.20}$$

$$\langle \mathbf{P} \rangle_{QM} = -i\sqrt{\frac{\hbar}{(2n+1)m\omega}} \int_{-\infty}^{\infty} dx\, \psi_n^*(x) \frac{d\psi_n(x)}{dx} = 0; \tag{2.21}$$

$$\langle \mathbf{P^2} \rangle_{QM} = \frac{-\hbar}{(2n+1)m\omega} \int_{-\infty}^{\infty} dx\, \psi_n^*(x) \frac{d^2\psi_n(x)}{dx^2} = \frac{1}{2}. \tag{2.22}$$

Clearly, these quantum expectation values match the classical ones given in Eqs. (2.12) through (2.15) and we obtain the uncertainty product, for *all* stationary-state solutions of the quantum oscillator,

$$(\Delta \mathbf{X})^2_{\mathrm{QM}}\, (\Delta \mathbf{P})^2_{\mathrm{QM}} \equiv \frac{1}{4}. \tag{2.23}$$

It is pertinent to point out here that the commutation relation

$$\begin{aligned} [\mathbf{X}, \mathbf{P}] &= \left[\sqrt{\frac{m\omega}{(2n+1)\hbar}}\mathbf{x}, \frac{\mathbf{p}}{\sqrt{\hbar m\omega(2n+1)}}\right] \\ &= \frac{1}{(2n+1)\hbar}\,[\mathbf{x}, \mathbf{p}] = \frac{i}{2n+1} \end{aligned} \tag{2.24}$$

leads to the uncertainty relation

$$(\Delta \mathbf{X})^2_{QM} (\Delta \mathbf{P})^2_{QM} \geq \frac{1}{4(2n+1)^2}. \tag{2.25}$$

In the large-n limit the right-hand side goes to zero, which would be expected in the classical regime. However Eq. (2.23) for the uncertainty product holds for *all* the stationary-state solutions; and strikingly, this result matches that of a classical ensemble of oscillators with fixed energy E (see Eq. (2.17)).

2.3.2 One dimensional infinite potential box

We consider a symmetric infinite potential well defined by

$$V(x) = \begin{cases} 0 & \text{for } -L/2 \leq x \leq L/2; \\ \infty & \text{for } |x| > L/2. \end{cases} \tag{2.26}$$

The particles move with a constant velocity within the box and get reflected back and forth. The position probability distribution for an ensemble of classical particles confined to move within the box is a constant (as can be readily seen by substituting Eq. (2.26) in Eq. (2.8)) and is given by [103]

$$P_{\mathrm{CL}}(x) = \begin{cases} 1/L & \text{for } |x| \leq L/2; \\ 0 & \text{for } |x| > L/2. \end{cases} \tag{2.27}$$

This distribution obeys $\int_{-L/2}^{L/2} P_{\mathrm{CL}}(x)\, dx = 1$.

In this example, the dimensionless position and momentum variables are

$$X = \frac{x}{L/2}, \qquad P = \frac{p}{\sqrt{2mE}} = \frac{p}{|p|}, \tag{2.28}$$

and the classical averages $\langle X\rangle_{\mathrm{CL}}$, $\langle X^2\rangle_{\mathrm{CL}}$, $\langle P\rangle_{\mathrm{CL}}$, and $\langle P^2\rangle_{\mathrm{CL}}$ are readily evaluated using the probability distribution (2.27):

$$\langle X\rangle_{\rm CL} = \int dx\, P_{\rm CL}(x)\frac{x}{L/2} = \frac{2}{L^2}\int_{-L/2}^{L/2} x\, dx = 0; \tag{2.29}$$

$$\langle X^2\rangle_{\rm CL} = \int dx\, P_{\rm CL}(x)\,\frac{x^2}{L^2/4} = \frac{4}{L^3}\int_{-L/2}^{L/2} dx\, x^2 = \frac{1}{3}; \tag{2.30}$$

$$\langle P\rangle_{\rm CL} = 0; \tag{2.31}$$

$$\langle P^2\rangle_{\rm CL} = 1. \tag{2.32}$$

So, the variances of X and P are $(\Delta X)^2_{\rm CL} = 1/3$ and $(\Delta P)^2_{\rm CL} = 1$ for the classical ensemble of particles of fixed energy E, confined within the infinite well. The product of the variances is

$$(\Delta X)^2_{\rm CL}\,(\Delta P)^2_{\rm CL} \equiv \frac{1}{3}. \tag{2.33}$$

The quantum mechanical stationary-state solutions (even and odd parity) for a particle confined in the one-dimensional infinite potential well are

$$\begin{aligned} \psi_n^{(+)}(x) &= \sqrt{\frac{2}{L}}\cos(n\pi x/L), \quad n = 1, 3, 5, \ldots, \\ \psi_n^{(-)}(x) &= \sqrt{\frac{2}{L}}\sin(n\pi x/L), \quad n = 2, 4, 6, \ldots, \end{aligned} \tag{2.34}$$

and the corresponding energy eigenvalues are

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{2.35}$$

The scaled dimensionless position and momentum operators are

$$\mathbf{X} = \frac{\mathbf{x}}{L/2}, \qquad \mathbf{P} = \frac{\mathbf{p}}{\sqrt{2\,m\,E_n}} = \frac{\mathbf{p}}{n\pi\hbar/L}. \tag{2.36}$$

The expectation values of $\mathbf{X}$, $\mathbf{X}^2, \mathbf{P}$, and $\mathbf{P}^2$ are evaluated in the stationary states (both even and odd) to obtain

$$\langle \mathbf{X} \rangle_{QM} = \frac{1}{L/2} \int_{-L/2}^{L/2} dx \, |\psi_n^{(+/-)}(x)|^2 \, x = 0; \tag{2.37}$$

$$\langle \mathbf{X^2} \rangle_{QM} = \frac{1}{L^2/4} \int_{-L/2}^{L/2} dx \, |\psi_n^{(+/-)}(x)|^2 \, x^2 = \frac{1}{3} - \frac{2}{n^2\pi^2}; \tag{2.38}$$

$$\langle \mathbf{P} \rangle_{QM} = -i\frac{L}{n\pi} \int_{-L/2}^{L/2} dx \, \psi_n^{(+/-)}(x) \frac{d\psi_n^{(+/-)}(x)}{dx} = 0; \tag{2.39}$$

$$\langle \mathbf{P^2} \rangle_{QM} = -\frac{L^2}{n^2\pi^2} \int_{-L/2}^{L/2} dx \, \psi_n^{(+/-)}(x) \frac{d^2\psi_n^{(+/-)}(x)}{dx^2} = 1. \tag{2.40}$$

It may be seen that $\langle \mathbf{X}^2 \rangle_{\mathrm{QM}}$ approaches the classical result, $\langle X^2 \rangle_{\mathrm{CL}} = 1/3$, in the large-$n$ limit. In this limit the uncertainty product becomes

$$\lim_{n\to\infty} (\Delta \, \mathbf{X})_{\mathrm{QM}} \, (\Delta \, \mathbf{P})_{\mathrm{QM}} = \frac{1}{3}. \tag{2.41}$$

Meanwhile, from the commutator relation,

$$[\mathbf{X}, \mathbf{P}] = \left[\frac{2}{L} \, \mathbf{x}, \frac{L}{n\pi\hbar} \, \mathbf{p} \right] = \frac{2\, i}{n\pi}, \tag{2.42}$$

it is clear that the uncertainty product obeys

$$(\Delta \, \mathbf{X})^2_{QM} \, (\Delta \, \mathbf{P})^2_{QM} \geq \frac{1}{n^2\pi^2}, \tag{2.43}$$

and in the large-n limit one recovers the expected result $(\Delta \, \mathbf{X})^2_{QM} \, (\Delta \, \mathbf{P})^2_{QM} \geq 0$. However, the stationary-state uncertainty product, Eq. (2.41), does not vanish in the limit $n \to \infty$. Instead it approaches the value 1/3, which coincides *exactly* with that associated with the classical ensemble (see Eq. (2.33)).

2.3.3 Bouncing ball

We now consider the example of a particle bouncing vertically up and down in a uniform gravitational field, which is described by the confining potential

$$V(z) = \begin{cases} \infty & \text{for } z < 0, \\ mgz & \text{for } \; z \geq 0. \end{cases} \tag{2.44}$$

A classical particle of total energy E, subject to this potential, bounces back and forth between $z = 0$ and a maximum height $z = A$, where $A = E/mg$.

An ensemble of bouncing balls of energy E is characterized by the classical position probability distribution [103]

$$P_{\mathrm{CL}}(z) = \begin{cases} \dfrac{1}{2\,A}\dfrac{1}{\sqrt{1-(z/A)}} & \text{for } \; 0 \leq z \leq A, \\ 0 & \text{otherwise.} \end{cases} \tag{2.45}$$

This expression follows from substituting Eq. (2.44) in Eq. (2.8).

Employing dimensionless position and momentum variables

$$Z = \frac{z}{A}, \qquad P = \frac{p}{\sqrt{2mE}} = \frac{p}{\sqrt{2m^2gA}} \tag{2.46}$$

(so that $0 \leq Z \leq 1$ and $-1 \leq P \leq 1$ for the bouncing particles), we obtain the classical moments:

$$\langle Z \rangle_{\mathrm{CL}} = \frac{1}{A}\int dz\, P_{\mathrm{CL}}(z)\, z = \frac{1}{2\,A^2}\int_0^A dz\, \frac{z}{\sqrt{1-(z/A)}} = \frac{2}{3}; \tag{2.47}$$

$$\langle Z^2 \rangle_{\mathrm{CL}} = \frac{1}{A^2}\int dz\, P_{\mathrm{CL}}(z)\, z^2 = \frac{1}{2A^3}\int_0^A dz\, \frac{z^2}{\sqrt{1-(z/A)}} = \frac{8}{15}; \tag{2.48}$$

$$\langle P \rangle_{\mathrm{CL}} = \frac{1}{2\sqrt{2m^2gA}}\int_0^A dz P_{\mathrm{CL}}(z)\,(-\sqrt{2m(E-mgz)} + \sqrt{2m(E-mgz)}\,) = 0; \tag{2.49}$$

$$\langle P^2\rangle_{\rm CL} = \frac{1}{2m^2gA}\int_0^A dz\, P_{\rm CL}(z)\, 2m(E-mgz)$$
$$= \frac{1}{2A}\int_0^A dz\,\sqrt{1-(z/A)} = \frac{1}{3}. \tag{2.50}$$

Thus, the variances of Z and P are $(\Delta Z)^2_{\rm CL} = 4/45$ and $(\Delta P)^2_{\rm CL} = 1/3$, leading to

$$(\Delta Z)^2_{\rm CL}\,(\Delta P)^2_{\rm CL} \equiv 4/135. \tag{2.51}$$

Stationary-state solutions of a quantum bouncing particle [104] are obtained by solving the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(z)}{dz^2} + mgz\,\psi_n(z) = E_n\,\psi_n(z), \tag{2.52}$$

with the boundary condition

$$\psi_n(0) = 0. \tag{2.53}$$

In terms of the characteristic *gravitational length* [104]

$$l_g = \left(\frac{\hbar^2}{2m^2g}\right)^{1/3}, \tag{2.54}$$

it is convenient to define dimensionless quantities

$$E'_n = \frac{E_n}{mgl_g}, \qquad z' = \frac{z}{l_g} - E'_n, \tag{2.55}$$

so that the Schrödinger equation (2.52) takes the standard form

$$\frac{d^2\psi_n(z')}{dz'^2} = z'\,\psi_n(z'), \tag{2.56}$$

which is the Airy differential equation. The solutions of Eq. (2.56) are two linearly independent sets of Airy functions, $\mathrm{Ai}(z')$ and $\mathrm{Bi}(z')$. However, the function $\mathrm{Bi}(z')$ diverges as its argument increases, and so it is not a physically admissible solution. The stationary state solutions of a quantum bouncer are thus given by

$$\psi_n(z') = N_n \,\mathrm{Ai}(z'), \quad z' \geq -E'_n, \quad n = 1,\ 2,\ 3,\ \ldots, \tag{2.57}$$

where N_n is a normalization constant. From the boundary condition (2.53), one obtains $\mathrm{Ai}(-E'_n) = 0$, indicating that the (scaled) energy eigenvalue E'_n is minus the nth zero of the Airy function. (The zeros of the Airy function are all negative.) The first few energy eigenvalues E'_n of the quantum bouncing ball are given in Table 2.1.

n	E'_n
1	2.3381
2	4.0879
3	5.5205
4	6.7867
5	7.9441

Table 2.1: The first few scaled energy eigenvalues E'_n of the quantum bouncing ball.

Identifying the classical turning point A_n associated with the energy eigenvalues E_n of the quantum bouncer to be

$$A_n = \frac{E_n}{mg} = l_g E'_n, \tag{2.58}$$

we define appropriately scaled position and momentum operators (which are quantum counterparts of Z and P defined in Eq. (2.46)) as

$$\mathbf{Z} = \frac{\mathbf{z}}{A_n} = \frac{\mathbf{z}}{l_g E'_n}, \qquad \mathbf{P} = \frac{\mathbf{p}}{\sqrt{2mE_n}} = \frac{l_g \mathbf{p}}{\hbar\sqrt{E'_n}}. \tag{2.59}$$

Further, substituting Eqs. (2.54) and (2.55) in Eq. (2.59), we may express the configuration representation of the operators $\mathbf{Z}$ and $\mathbf{P}$ in terms of z' and E'_n as

$$\mathbf{Z} \to \frac{1}{E'_n}(z' + E'_n), \qquad \mathbf{P} \to \frac{-i}{\sqrt{E'_n}} \frac{d}{dz'}. \tag{2.60}$$

The expectation values $\langle \mathbf{Z} \rangle_{QM}, \langle \mathbf{Z}^2 \rangle_{QM}$ may be evaluated analytically [105] in the eigenstates Eq. (2.57) of the quantum bouncing ball:

$$\begin{aligned} \langle \mathbf{Z} \rangle_{QM} &= \frac{1}{E'_n} \int_{-E'_n}^{\infty} dz' \, (z' + E'_n) \, |\psi_n(z')|^2 \\ &= \frac{N_n^2}{E'_n} \int_{-E'_n}^{\infty} dz' \, (z' + E'_n) \, \mathrm{Ai}^2(z') = \frac{2}{3}; \end{aligned} \tag{2.61}$$

$$\begin{aligned} \langle \mathbf{Z}^2 \rangle_{QM} &= \frac{1}{E_n'^2} \int_{-E'_n}^{\infty} dz' \, (z' + E'_n)^2 \, |\psi_n(z')|^2 \\ &= \frac{N_n^2}{E_n'^2} \int_{-E'_n}^{\infty} dz' \, (z' + E'_n)^2 \, \mathrm{Ai}^2(z') = \frac{8}{15}, \end{aligned} \tag{2.62}$$

which agree *exactly* with the corresponding moments in a classical ensemble of bouncing balls (see Eq. (2.47) and Eq. (2.48)).

The expectation value $\langle \mathbf{P} \rangle_{QM}$ is given by,

$$\begin{aligned} \langle \mathbf{P} \rangle_{QM} &= \frac{-i}{\sqrt{E'_n}} \int_{-E'_n}^{\infty} dz' \, \psi_n^*(z') \, \frac{d\psi_n(z')}{dz'} \\ &= \frac{-i \, N_n^2}{\sqrt{E'_n}} \int_{-E'_n}^{\infty} dz' \, \mathrm{Ai}(z') \, \frac{d\mathrm{Ai}(z')}{dz'} = 0 \end{aligned} \tag{2.63}$$

which can be readily identified with the help of integration by parts.

Further, we evaluate the expectation value $\langle \mathbf{P}^2 \rangle_{QM}$ as follows:

$$\begin{aligned} \langle \mathbf{P}^2 \rangle_{QM} &= -\frac{1}{E'_n} \int_{-E'_n}^{\infty} dz' \, \psi_n^*(z') \, \frac{d^2\psi_n(z')}{dz'^2} \\ &= -\frac{1}{E'_n} \int_{-E'_n}^{\infty} dz' \, \psi_n^*(z') \, \psi_n(z') \end{aligned}$$

$$\begin{aligned} &= -\frac{N_n^2}{E_n'}\int_{-E_n'}^{\infty} dz'\, z'\,\mathrm{Ai}^2(z') \\ &= 1 - \langle \mathbf{Z}\rangle_{QM} = \frac{1}{3}, \end{aligned} \tag{2.64}$$

where we have used Eq. (2.56) in the second line and Eq. (2.61) in the fourth line of Eq. (2.64).

The expectation values $\langle \mathbf{P}\rangle_{QM}, \langle \mathbf{P}^2\rangle_{QM}$ match identically with the corresponding moments Eq. (2.49) and Eq. (2.50) of scaled momentum variables in an ensemble of classical bouncing balls. This is indeed a novel identification, bringing forth the deep-rooted unifying features of the classical and quantum realms.

From Eqs. (2.61) through (2.64), we obtain the variances of $\mathbf{Z}$ and $\mathbf{P}$ for the stationary states to be $(\Delta\mathbf{Z})^2_{\mathrm{QM}} = 4/45$ and $(\Delta\mathbf{P})^2_{\mathrm{QM}} = 1/3$. Hence, the uncertainty product is

$$(\Delta\mathbf{Z})^2_{\mathrm{QM}}\,(\Delta\mathbf{P})^2_{\mathrm{QM}} \equiv \frac{4}{135}, \tag{2.65}$$

which exactly matches that of the classical ensemble of bouncing balls (see Eq. (2.51)).

It may be noted that the commutation relation

$$[\mathbf{Z},\mathbf{P}] = \left[\frac{\mathbf{z}}{l_g E_n'}, \frac{l_g\,\mathbf{p}}{\hbar\sqrt{E_n'}}\right] = \frac{i}{(E_n')^{3/2}} \tag{2.66}$$

would lead to the uncertainty relation $(\Delta\mathbf{Z})^2_{\mathrm{QM}}\,(\Delta\mathbf{P})^2_{\mathrm{QM}} \geq 1/4(E_n')^3$. In the large-$n$ limit $1/E_n' \to 0$ (as the energy eigenvalues obey the scaling relation [103] $E_n' \propto n^{2/3}$ for large n), thus resulting in the classical limit on the variance product $(\Delta\mathbf{Z})^2_{\mathrm{QM}}\,(\Delta\mathbf{P})^2_{\mathrm{QM}} \geq 0$. Equation (2.65), on the other hand, is exact for the energy eigenstates.

2.4 Conclusions

Emergence of classical behaviour from the corresponding quantum world has remained an enigmatic topic ever since the inception of quantum theory. It is shown here that in three specific examples of one-dimensional bound systems—harmonic oscillator, infinite square well and bouncing ball—the uncertainty products of position and momentum evaluated for stationary quantum states agree with those of the corresponding constant-energy classical ensembles. This identification points towards a deep underlying connectivity between the two formalisms, despite their mathematical and conceptual differences.

The uncertainty principle is one of the intrinsic trademarks of quantum theory and is not a feature of the classical deterministic motion of single particle. However, recent investigations [1]—motivated by Gromov's non-squeezing theorem [3]—have shown that, indeed, there are intrinsic uncertainties governed by the symplectic geometry of Hamiltonian phase space flows associated with classical ensembles. Our work establishes a remarkable agreement between the uncertainty product for quantum stationary states and the classical microcanonical ensemble of constant energy, for the three specific examples considered here. This agreement could be a reflection of subtle aspects of symplectic toplogy. It would be interesting to investigate the nature of quantum-classical uncertainties from a unifying point of view based on phase space topology [1].

According to the Eherenfest theorem, the dynamical equations of motion for the average values of the position and momentum coincide with the classical equations for linear and quadratic potentials. The three specific examples analyzed here focused on stationary-state solutions associated with linear and quadratic potentials, and this raises the question of whether the agreement between classical and quantum uncertainty products happens to be an indirect reflection of Ehrenfest theorem itself [106]. Yet another reason why the classical and quantum uncertainty relationships coincide might be because the quasi-classical (WKB) approximation is exact for the potentials considered [107]. It is therefore important to extend our results to the case of non-quadratic potentials, which will be taken up in future.

Chapter 3

Macrorealism from entropic Leggett-Garg inequalities

We formulate entropic Leggett-Garg inequalities, which place constraints on the statistical outcomes of temporal correlations of observables. The information theoretic inequalities are satisfied if macrorealism *holds. We show that the quantum statistics underlying correlations between time-separated spin component of a quantum rotor mimics that of spin correlations in two spatially separated spin-s particles sharing a state of zero total spin. This brings forth the violation of the entropic Leggett-Garg inequality by a rotating quantum spin-s system in a similar manner as does the entropic Bell inequality ([49]) by a pair of spin-s particles forming a composite spin singlet state.*

3.1 Introduction

Conflicting foundational features like non-locality [57] and contextuality [108] mark how quantum universe differs from classical one. Non-locality rules out that spatially separated systems have their own objective properties prior to measurements and that they do not get influenced by any local operations by the other parties. Violation of Clauser-Horne-Shimony-Holt (CHSH) - Bell correlation inequality [65] by entangled states reveals that local realism is untenable in the quantum scenario. On the other hand, quantum contextuality states that the measurement outcome of an observable depends on the set of compatible observables that are measured alongside it. In this sense, non-locality turns out to be a reflection of contextuality in spatially separated systems.

Yet another foundational concept of classical world that is at variance with the quantum description is *macrorealism* [4]. As the notion of *macrorealism* is already discussed in Chapter 1, let us directly go ahead with the construction of the Leggett-Garg (LG) inequality using Shannon entropy.

Probabilities associated with measurement outcomes in the quantum framework are fundamentally different from those arising in the classical statistical scenario - and this is pivotal in initiating multitude of debates on various contrasting implications in the two worlds [73, 74, 109]. A deeper understanding of these foundational conflicts requires investigations from as many independent ways as possible. The CHSH-Bell (LG) inequalities were originally formulated for dichotomic observables and they constrain certain linear combinations of correlation functions of measurements done on spatially (temporally) separated states. However, there have been extensions of correlation Bell inequalities to arbitrary measurement outcomes [110]. Information entropy too offers as a natural candidate to capture the puzzling features of quantum probabilities. It also offers operational tests demarcating the two domains in an elegant and an illustrative fashion [49, 111, 112]. The information entropic formulation is applicable to observables with any number of outcomes of measurements. Moreover, while the correlation inequalities define a convex polytope [109], the entropic inequalities form a convex cone [113], bringing out their geometrically distinct features. Entropic tests thus generalize and strengthen the platform to understand the basic differences between the quantum and classical world views.

It was noticed quite early by Braunstein and Caves (BC) that interpreting correlations between two spatially separated EPR entangled pair of particles based on Shannon information entropy results in contradiction with local realism [49]. They developed information theoretic Bell inequality applicable to any pair of spatially separated systems and showed that the inequality is violated by two spatially separated spin-s particles sharing a state of zero total angular momentum. More recently, Kurzyński et al. [112] constructed an entropic inequality to investigate the failure of non-contextuality in a *single* three level quantum system and they identified optimal measurements revealing violation of the inequality. Chaves and Fritz [114] framed a more general entropic framework [111] to analyze local realism and contextuality in quantum as well as post-quantum scenarios. Entropic inequalities provide, in general, a necessary but not sufficient criterion for local realism and non-contextuality [114, 112]. It is shown that for the n-cycle scenario with dichotomic outcomes, entropic inequalities also satisfy the sufficiency criterion. That is, the violations of entropic inequalities completely characterize non-local and contextual probabilities for the n-cycle scenario [115, 116]. Application of entropic inequality to test contextuality in four level quantum system has been proposed in Ref. [117].

It is highly relevant to address the question "*Does the macrorealistic tenet encrypted in the form of classical entropic inequality get defeated in the quantum realm*?" This issue gains increasing importance as questions on the role of quantum theory in biological molecular processes are being addressed in rigorous manner and LG type tests offer an operational approach in recognizing quantum effects in evolutionary biological processes [5]. Entropic formulation of macrorealism generalizes the scope and applicability of such bench-mark investigations.

Here, we formulate *entropic LG inequalities* to investigate the notion of macrorealism of a single system. We show that the entropic inequality is violated by a spin-s quantum rotor (prepared in a completely random state) in a manner similar to the information theoretic BC inequality for a counter propagating entangled pair of spin-s particles in a spin-singlet state. *To our knowledge, this is the first time that entropic considerations are applied to investigate macrorealism.*

3.2 Entropic Inequalities to test Macrorealism

Consider a macrorealistic system in which $Q(t_i)$ is a dynamical observable at time t_i. Let the outcomes of measurements of the observable $Q(t_i)$ be denoted by q_i and the corresponding probabilities $P(q_i)$. In a macrorealistic theory, the outcomes q_i of the observables $Q(t_i)$at all instants of time pre-exist irrespective of their measurement; this feature is mathematically validated in terms of a joint probability distribution $P(q_1, q_2, \ldots)$ characterizing the statistics of the outcomes; the joint probabilities yield the marginals $P(q_i)$ of individual observations at time t_i. Further, measurement invasiveness implies that the act of observation of $Q(t_i)$ at an earlier time t_i has no influence on its subsequent value at a later time $t_j > t_i$.
This demands that the joint probabilities be expressed as a convex combination of product of probabilities $P(q_i|\lambda)$, averaged over a hidden variable probability distribution $\rho(\lambda)$ [73, 79]:

$$P(q_1, q_2, \ldots, q_n) = \sum_{\lambda} \rho(\lambda)\, P(q_1|\lambda)P(q_2|\lambda)\ldots P(q_n|\lambda), \tag{3.1}$$

$$0 \leq \rho(\lambda) \leq 1,\ \sum_{\lambda} \rho(\lambda) = 1; 0 \leq P(q_i|\lambda) \leq 1,\ \sum_{q_i} P(q_i|\lambda) = 1.$$

Joint Shannon information entropy associated with the measurement statistics of the observable at two different times t_k, t_{k+l} is defined as, $H(Q_k, Q_{k+l}) = -\sum_{q_k, q_{k+l}} P(q_k, q_{k+l}) \log_2 P(q_k, q_{k+l})$. The conditional Shannon entropy carried by the observable Q_{k+l} at time t_{k+l}, given that it had assumed the values $Q_k = q_k$ at an earlier time is given by, $H(Q_{k+l}|Q_k = q_k) = -\sum_{q_{k+l}} P(q_{k+l}|q_k)$ $\log_2 P(q_{k+l}|q_k)$, where $P(q_{k+l}|q_k) = P(q_k, q_{k+l})/P(q_k)$ denotes the conditional probability. The conditional Shannon entropy is given by

$$\begin{aligned} H(Q_{k+l}|Q_k) &= \sum_{q_k} P(q_k)\, H(Q_{k+l}|Q_k = q_k) \\ &= H(Q_k, Q_{k+l}) - H(Q_k). \end{aligned} \tag{3.2}$$

The classical Shannon entropies obey the inequality [49]:

$$H(Q_{k+l}|Q_k) \leq H(Q_{k+l}) \leq H(Q_k, Q_{k+l}), \tag{3.3}$$

Extending (3.3) to three variables, and using the relation $H(Q_k, Q_{k+l}) = H(Q_{k+l}|Q_k) + H(Q_k)$, we obtain,

$$\begin{aligned} H(Q_k, Q_{k+m}) &\leq H(Q_k, Q_{k+l}, Q_{k+m}) = H(Q_{k+m}|Q_{k+l}, Q_k) + H(Q_{k+l}|Q_k) + H(Q_k) \\ &\Longrightarrow H(Q_{k+m}|Q_k) \leq H(Q_{k+m}|Q_{k+l}) + H(Q_{k+l}|Q_k). \end{aligned} \tag{3.4}$$

Here, the first line follows from the chain rule for entropies and the derivation is analogous to that given by BC [49].

The entropic inequality (3.4) is a reflection of the fact that knowing the value of the observable at three different times $t_k < t_{k+l} < t_{k+m}$ – via its information content – can never be smaller than the information about it at two time instants. Moreover, existence of a grand joint probability distribution $P(q_1, q_2, q_3)$

of the variables Q_1, Q_2, Q_3, consistent with a given set of marginal probability distributions $P(q_1, q_2)$, $P(q_2, q_3)$, $P(q_1, q_3)$ of pairs of observables, imposes non-trivial conditions on the associated Shannon information entropies. Violation of the inequality points towards the lack of a legitimate grand joint probability distribution for all the measured observables, such that the family of probability distributions associated with measurement outcomes of pairs of observables belong to it as marginals [111].

$\Big($**Remark**: Consider *quantum* sequential measurement of the observables $\mathbf{Q}_1$, $\mathbf{Q}_2$ and $\mathbf{Q}_3$ resulting in the measurement outcomes q_1, q_2, q_3 in a quantum system prepared in the state ρ. With measurements of only $\mathbf{Q}_1, \mathbf{Q}_2$, the probabilities $P(q_1, q_2) = P(q_1)\, P(q_2|q_1)$ with $P(q_2|q_1) = Tr[\mathbf{\Pi}_{q_2}\, \rho_{q_1}]$, where $\rho_{q_1} = [\mathbf{\Pi}_{q_1} \rho\, \mathbf{\Pi}_{q_1}]/P(q_1)$; $P(q_1) = \mathrm{Tr}[\rho\, \mathbf{\Pi}_{q_1}]$. A consequent measurement of $\mathbf{Q}_3$ yields the probabilities $P(q_1, q_2, q_3) = P(q_1, q_2)\, P(q_3|q_1, q_2); P(q_3|q_1, q_2) = \mathrm{Tr}[\mathbf{\Pi}_{q_3}\, \rho_{q_1\, q_2}]$ and $\rho_{q_1\, q_2} = \mathbf{\Pi}_{q_2}\, \rho_{q_1}\, \mathbf{\Pi}_{q_2}/P(q_1, q_2)$. After simplification, the three variable joint probabilities reduce to the form, $P(q_1, q_2, q_3) = P(q_1, q_2)\, P(q_2, q_3)/P(q_2)$. It is easy to see that the three variable probabilities $P(q_1, q_2, q_3)$ associated with the sequential measurement of the observables $\mathbf{Q}_1$, $\mathbf{Q}_2$, and $\mathbf{Q}_3$ are not consistent with the pairwise probabilities $P(q_1, q_3)$. Absence of a legitimate grand joint probability distribution, consistent with all pairwise probabilities reflects itself in the violation of entropic inequality [111].$\Big)$

The same reasoning, which lead to a three term entropic inequality (3.4), could be extended to construct an entropic inequality for n consecutive measurements $Q_1, Q_2, \ldots, Q_n$ at time instants $t_1 < t_2 < \ldots < t_n$:

$$H(Q_n|Q_1) \leq H(Q_n|Q_{n-1}) + H(Q_{n-1}|Q_{n-2}) + \ldots + H(Q_2|Q_1). \tag{3.5}$$

The macrorealistic information underlying the statistical outcomes of the observable at n different times must be consistent with the information associated with pairwise non-invasive measurements as given in (3.5).

Note that for even values of n, there is a one-to-one correspondence between the entropic inequality (3.5) of a single system and the information theoretic BC inequality [49] for two spatially separated parties (Alice and Bob). More specifically, let us consider $n = 4$ in (3.5) and associate temporal observable Q_i with Alice's (Bob's) observables A', A (B', B) as $Q_1 \leftrightarrow B$, $Q_2 \leftrightarrow A'$, $Q_3 \leftrightarrow B'$, $Q_4 \leftrightarrow A$ to obtain the BC inequality [49] for a set of four correlations: $H(A|B) \leq H(A|B') + H(B'|A') + H(A'|B)$, which is satisfied by any *local realistic* model of spatially separated pairs. It may be identified that Eq. (3.1) is essentially analogous to the local hidden variable model (Bell scenario for spatially separated systems) as well as to the non-contextual model, while the interpretation here is towards macrorealism. Moreover, we emphasize that the logical reasoning in formulating the entropic LG inequalities (3.5) is synonymous to that of BC [49], which indeed offers a unified approach to address non-locality, contextuality and non-macrorealism.

3.3 Violation of Entropic Leggett-Garg Inequality by a quantum rotor

We now proceed to show that entropic LG inequality is violated by a quantum spin-s system. Consider a quantum rotor prepared initially in a maximally mixed state

$$\rho = \frac{1}{2s+1} \sum_{m=-s}^{s} |s, m\rangle\langle s, m| = \frac{\mathbb{I}}{2s+1} \tag{3.6}$$

where $|s, m\rangle$ are the simultaneous eigenstates of the squared spin operator $\mathbf{S}^2 = \mathbf{S}_x^2 + \mathbf{S}_y^2 + \mathbf{S}_z^2$ and the z-component of spin $\mathbf{S}_z$ (with respective eigenvalues $s(s+1)\,\hbar^2$ and $m\hbar$); $\mathbb{I}$ denotes the $(2s+1)\times(2s+1)$ identity matrix. We consider the Hamiltonian

$$\mathbf{H} = \omega\,\mathbf{S}_y, \tag{3.7}$$

resulting in the unitary evolution $\mathbf{U}(t) = e^{-i\omega t\,\mathbf{S}_y/\hbar}$ of the system (which corresponds to a rotation about the y-axis by an angle $\omega\,t$). We choose the z-component of spin $\mathbf{Q}(t) = \mathbf{S}_z(t) = \mathbf{U}^\dagger(t)\,\mathbf{S}_z\,\mathbf{U}(t)$ as the dynamical observable for our investigation of macrorealism. Let us suppose that the observable $\mathbf{Q}_k = \mathbf{S}_z(t_k)$ takes the value m_k at time t_k. Correspondingly, at a later instant of time t_{k+l} if the spin component $\mathbf{S}_z(t_{k+l})$ assumes the value m_{k+l}, the quantum mechanical joint probability is given by [79]

$$P(m_k, m_{k+l}) = P_{m_k}(t_k)\,P(m_{k+l}, t_{k+l}|m_k, t_k). \tag{3.8}$$

Here, $P_{m_k}(t_k) = \mathrm{Tr}[\rho\,\mathbf{\Pi}_{m_k}(t_k)]$ is the probability of obtaining the outcome m_k at time t_k, $P(m_{k+l}, t_{k+l}|m_k, t_k) = \mathrm{Tr}[\mathbf{\Pi}_{m_k}(t_k)\rho\mathbf{\Pi}_{m_k}(t_k)\,\mathbf{\Pi}_{m_{k+l}}(t_{k+l})]/P_{m_k}(t_k)$ denotes the conditional probability of obtaining the outcome m_{k+l} for the spin component $\mathbf{S}_z$ at time t_{k+l}, given that it had taken the value m_k at an earlier time t_k; $\mathbf{\Pi}_m(t) = \mathbf{U}^\dagger(t)\,|s, m\rangle\langle s, m|\,\mathbf{U}(t)$ is the projection operator measuring the outcome m for the spin component at time t. For the maximally mixed initial state (3.6), we obtain the quantum mechanical joint probabilities as,

$$\begin{aligned} P(m_k, m_{k+l}) &= \frac{1}{2s+1}\,\mathrm{Tr}[\mathbf{\Pi}_{m_k}(t_k)\,\mathbf{\Pi}_{m_{k+l}}(t_{k+l})] \\ &= \frac{1}{2s+1}\,|\langle\, s, m_{k+l}|e^{-i\omega(t_{k+l}-t_k)\,\mathbf{S}_y/\hbar}\,|s, m_k\rangle|^2 \\ &= \frac{1}{2s+1}\,|\,d^s_{m_{k+l},m_k}(\theta_{kl})|^2 \end{aligned} \tag{3.9}$$

where $d^s_{m',m}(\theta_{kl}) = \langle s, m'|e^{-i\theta_{kl}\,\mathbf{S}_y/\hbar}|s, m\rangle$ are the matrix elements of the $2s+1$ dimensional irreducible representation of rotation [118] about y-axis by an angle $\theta_{kl} = \omega(t_{k+l} - t_k)$. The marginal probability of the outcome m_k for the observable $\mathbf{Q}_k$ is readily obtained by making use of the unitarity property of d matrices: $P(m_k) = \sum_{m_{k+l}} P(m_k, m_{k+l}) = \frac{1}{2s+1}\sum_{m_{k+l}} |\, d^s_{m_{k+l},m_k}(\theta_{kl})|^2 = \frac{1}{2s+1}$.

Clearly, the temporal correlation probability (3.9) of quantum rotor is similar to the quantum mechanical pair probability [49]

$$
\begin{aligned}
P(m_a, m_b) &= [{}_{\mathbf{a}}\langle s, m_a| \otimes_{\mathbf{b}} \langle s, m_b|]\ |\Psi_{AB}\rangle \\
&= \frac{1}{2s+1}\,|d^s_{m_a,-m_b}(\theta_{ab})|^2
\end{aligned}
\tag{3.10}
$$

that Alice's measurement of spin component $\vec{\mathbf{S}}\cdot\mathbf{a}$ yields the value m_a and Bob's measurement of $\vec{\mathbf{S}}\cdot\mathbf{b}$ results in the outcome m_b in a spin singlet state $|\Psi_{AB}\rangle = \frac{1}{\sqrt{2s+1}}\sum_{m=-s}^{s}(-1)^{s-m}\ |s, m\rangle \otimes |s, -m\rangle$ of a spatially separated pair of spin-s particles. (Here θ_{ab} is the angle between the unit vectors $\mathbf{a}$ and $\mathbf{b}$). In other words, *quantum statistics of temporal correlations in a single spin-s rotor mimics that of spatial correlations in an entangled counter propagating pair of spin-s particles.*

Let us consider measurements at equidistant time intervals $\Delta t = t_{k+1} - t_k,\ k = 1, 2, \ldots n$ and denote $\theta = (n-1)\omega\,\Delta t$. The quantum mechanical information entropy depends only on the time separation, specified by the angle θ and is given by,

$$
\begin{aligned}
H(\mathbf{Q}_k|\mathbf{Q}_{k+1}) &\equiv H[\theta/(n-1)] \\
&= -\frac{1}{2s+1}\sum_{m_k, m_{k+1}} |d^s_{m_{k+1},m_k}[\theta/(n-1)]|^2 \\
&\times\ \log_2 |d^s_{m_{k+1},m_k}[\theta/(n-1)]|^2.
\end{aligned}
\tag{3.11}
$$

The n-term entropic inequality (3.5) for observations at equidistant time steps assumes the form,

$$\begin{aligned}(n-1)\,H[\theta/(n-1)] - H(\theta) \;=\; & -\frac{1}{2s+1}\sum_{m_k,m_{k+1}} \Big([(n-1)\,|d^s_{m_{k+1},m_k}[\theta/(n-1)]|^2 \\ & \times\; \log_2 |d^s_{m_{k+1},m_k}[\theta/(n-1)]|^2] \\ & -\; [|d^s_{m_{k+1},m_k}(\theta)|^2 \log_2 |d^s_{m_{k+1},m_k}(\theta)|^2]\Big) \\ & \geq\; 0. \end{aligned} \tag{3.12}$$

We introduce information deficit, measured in units of $\log_2(2s+1)$ bits, as

$$\mathcal{D}_n(\theta) = \frac{(n-1)\,H[\theta/(n-1)] - H(\theta)}{\log_2(2s+1)} \tag{3.13}$$

so that the violation of the LG entropic inequality (3.12) is implied by negative values of $\mathcal{D}_n(\theta)$. The units $\log_2(2s+1)$ for the quantity $\mathcal{D}_n(\theta)$ imply that the base of the logarithm for evaluating the entropies of a spin s system is chosen appropriately to be $(2s+1)$. For a spin-1/2 rotor, it is in bits.

In Fig. 3.1, we have plotted information deficit $\mathcal{D}_n(\theta)$ for $n = 3$ (Fig. 3.1a) and $n = 6$ (Fig. 3.1b) as a function of $\theta = (n-1)\,\omega\,\Delta t$ for spin values $s = 1/2, 1, 3/2$ and 2. The results illustrate that the information deficit assumes negative values, though the range of violation (i.e., the value of the angle θ for which the violation occurs) and also the strength (maximum negative value of $D_n(\theta)$) of the entropic violation reduces [119] with the increase of spin s. This implies the emergence of macrorealism for the dynamical evolution of a quantum rotor in the limit of large spin s. It may be noted that Kofler and Brukner [80] had shown violation of the correlation LG inequality – corresponding to the measurement outcomes of a dichotomic parity observable in the example of a quantum rotor – persists even for large values of spin if the eigenvalues of spin can be experimentally resolved by sharp quantum measurements. However, under the restriction of coarse-grained measurements classical realm emerges in the large spin limit. An experiment corroborating these theoretical findings have been performed on NMR systems [120].

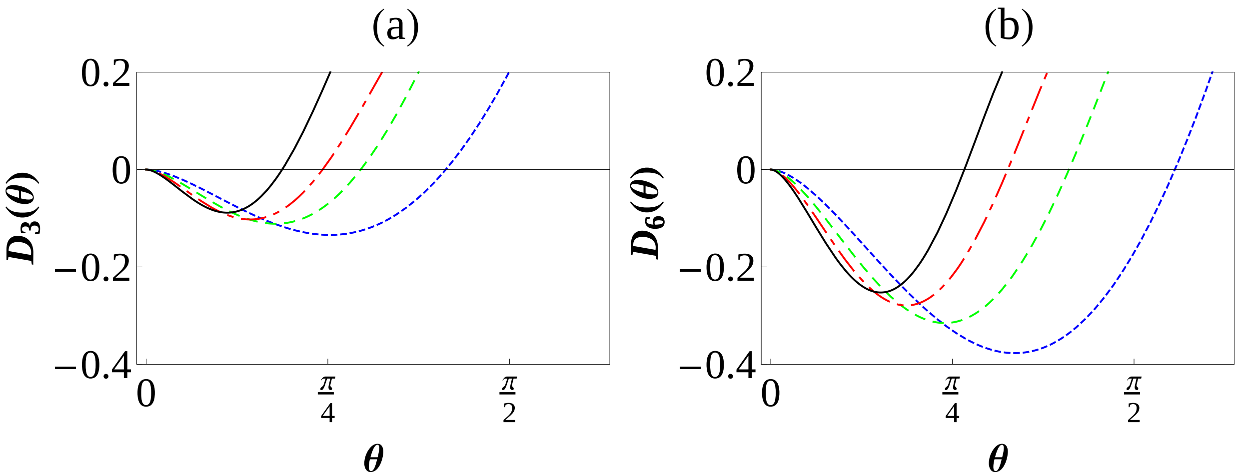

Figure 3.1: LG Information deficit $\mathcal{D}_n(\theta)$ of (3.13)) – in units of $\log_2(2s+1)$ bits – corresponding to the measurement of the spin component $\mathbf{S}_z(t)$ of a quantum rotor, at equidistant time steps $\Delta t = \frac{\theta}{(n-1)\,\omega}$, number of observations being (a) $n=3$ and (b) $n=6$ during the total time interval specified by the angle $\theta = (n-1)\,\omega\,\Delta t$. Conflict with macrorealism is recorded by the negative value of $\mathcal{D}_n(\theta)$. Maximum negative value and also the range i.e., the value of θ over which the information deficit is negative, grows with the increase in the number n of observations. However, for a given n, both the strength and the range of violation reduce with the increase of spin value (spin-1/2: dotted; spin-1: dashed; spin-3/2: dot-dashed; spin-2: solid curve). The strength of violation may be related to how much inconsistent Shannon information entropies could be – when the associated probabilities of outcomes of pairs of dynamical observables have their origin in noisy quantum measurements – compared to those arising within a classical macrorealistic premise. All quantities are dimensionless.

macrorealism requires that a consistently larger information content $H[\theta/(n-1)]$ has to be carried by the system, when number of observations n is increased and small steps of time interval are employed; however, quantum situation does not comply with this constraint. More specifically, in the classical premise, knowing the observable at almost all time instants provides more information content, whereas, quantum realm results in less information with large number of observations. To see this explicitly, consider the limit of $n \to \infty$ and infinitesimal time steps $\omega\,\Delta t \to 0$. Quantum statistics leads to vanishingly small information i.e., $H(\frac{\theta}{n-1}) \to 0$ – a signature of quantum Zeno effect. In this limit, the information deficit (see (3.13)) $D_n(\theta) \to \frac{-H(\theta)}{\log_2(2s+1)}$ is negative – thus violating the entropic LG inequality. The entropic test clearly brings forth the severity of macrorealistic demands towards *knowing* the observable in a non-invasive manner under such miniscule time scale observations.

3.4 Conclusion

We have formulated entropic LG inequality, which places bounds on the amount of information associated with non-invasive measurement of a macroscopic observable. The entropic formulation can be applied to any observables – not necessarily dichotomic ones – and it puts to test macrorealism i.e., a combined demand for the pre-existence of definite values of the measurement outcomes of a given dynamical observable at different instants of time – together with the assumption that act of observation at an earlier instant does not influence the subsequent evolution. The information entropic perspective provides a unified approach to test local realism, non-contextuality and macrorealism.

The classical notion of macrorealism demands that statistical outcomes of measurement of an observable at consecutive time intervals originate from a valid grand joint probability, presumably of the form (3.1). Non-existence of a legitimate joint probability, such that the family of probability distributions associated with the measurement outcomes of every pair of observables belong to it as marginals, reflects through the violation of the entropic inequality. The violation also brings forth the fact that more information is associated with the knowledge of the observable at more instants of time in the classical macro realistic realm – however, more number of observations correspond to less information in the quantum case.

In order to demonstrate the violation of the entropic inequality, we considered the dynamical evolution of a quantum spin system prepared initially in a maximally mixed state. We have demonstrated that the entropic violation in a quantum rotor system is similar to that of a spatially separated pair of spin-s particles sharing a state of total spin zero [49]. Furthermore, we have illustrated that the information content of a rotor grows with the increase of spin s such that it is consistent with the requirements of macrorealism.

Chapter 4

Moment Inversion and joint probabilities in quantum sequential measurements

A sequence of moments obtained from statistical trials encodes a classical probability distribution. However, it is well-known that an incompatible set of moments arise in the quantum scenario, when correlation outcomes associated with measurements on spatially separated entangled states are considered. This feature viz., the incompatibility of moments with a joint probability distribution is reflected in the violation of Bell inequalities. Here, we focus on sequential measurements on a single quantum system and investigate if moments and joint probabilities are compatible with each other. By considering sequential measurement of a dichotomic dynamical observable at three different time intervals, we explicitly demonstrate that the moments and the probabilities are inconsistent with each other.

4.1 Introduction

The issue of determining a probability distribution uniquely in terms of its moment sequence – known as *classical moment problem* – has been developed for more than 100 years [121, 122]. In the case of discrete distributions with the associated random variables taking finite values, moments faithfully capture the essence of the probabilities i.e., the probability distribution is moment determinate [123].

In the special case of classical random variables X_i assuming dichotomic values $x_i = \pm 1$, it is easy to see that the sequence of moments [124]

$$\mu_{n_1\,n_2\,\ldots n_k} = \langle X_1^{n_1} X_2^{n_2}\ldots X_k^{n_k}\rangle = \sum_{x_1,x_2,\ldots\, x_k=\pm 1} x_1^{n_1}\, x_2^{n_2}\ldots\, x_k^{n_k}\, P(x_1,x_2,\ldots,x_k)$$

where $n_1, n_2, \ldots, n_k = 0, 1$, can be readily inverted to obtain the joint probabilities $P(x_1, x_2, \ldots, x_k)$ uniquely. More explicitly, the joint probabilities $P(x_1, x_2, \ldots, x_k)$ are given in terms of the 2^k moments $\mu_{n_1\,n_2\,\ldots n_k}, \quad n_1, n_2, \ldots n_k = 0, 1$ as,

$$\begin{aligned} P(x_1,x_2,\ldots,x_k) &= \frac{1}{2^k}\sum_{n_1,\ldots n_k=0,1} x_1^{n_1}x_2^{n_2}\ldots x_k^{n_k}\,\mu_{n_1\ldots n_k} \\ &= \frac{1}{2^k}\sum_{n_1,\ldots,n_k=0,1} x_1^{n_1}x_2^{n_2}\ldots x_k^{n_k}\,\langle X_1^{n_1}X_2^{n_2}\ldots X_k^{n_k}\rangle. \quad (4.1)\end{aligned}$$

Does this feature prevail in the quantum scenario? The answer is in the negative as it is well known that the moments associated with the outcomes of measurements done on spatially separated parties are not compatible with the corresponding joint probability distribution. This feature reflects itself in the violation of Bell inequalities.

Here, we investigate whether moment-indeterminacy persists when we focus on sequential measurements on a single quantum system. We show that the discrete joint probabilities originating in the sequential measurement of a single qubit dichotomic observable $\mathbf{X}(t_i) = \mathbf{X}_i$ at different time intervals are not consistent with the ones reconstructed from the moments. More explicitly, considering sequential measurements of $\mathbf{X}_1$, $\mathbf{X}_2$, $\mathbf{X}_3$, we reconstruct the trivariate joint probabilities $P_\mu(x_1, x_2, x_3)$ based on the set of eight moments

$$\{1, \langle \mathbf{X}_1\rangle, \langle \mathbf{X}_2\rangle, \langle \mathbf{X}_3\rangle, \langle \mathbf{X}_1\,\mathbf{X}_2\rangle, \langle \mathbf{X}_2\,\mathbf{X}_3\rangle, \langle \mathbf{X}_1\,\mathbf{X}_3\rangle, \langle \mathbf{X}_1\,\mathbf{X}_2\,\mathbf{X}_3\rangle\}$$

and prove that they do not agree with the three-time joint probabilities (TTJP) $P_d(x_1, x_2, x_3)$ evaluated directly based on the correlation outcomes in the sequential measurement of all the three observables. Interestingly, the moments and TTJP can be independently extracted experimentally in NMR systems – demonstrating the difference between moment inverted three time probabilities with the ones directly drawn from experiment, in agreement with the theory. For obtaining TTJP directly one can use the procedure of Ref.[120] and for extracting the moments, extension of the Moussa protocol [125] to a set of non-commutating observables can be done. More details regarding the experimental scheme can be found in [126].

Disagreement between moment inverted joint probabilities with the ones based on measurement outcomes in turn reflects the inherent inconsistency that the family of all marginal probabilities do not arise from the grand joint probabilities. The non-existence of a legitimate grand joint probability distribution, consistent with the set of all pairwise marginals is attributed to be the common origin of a wide range of no-go theorems on non-contextuality, locality and macrorealism in the foundations of quantum theory [73, 58, 108, 127, 128, 4, 129, 91]. The absence of a valid grand joint probability distribution in the sequential measurement on a single quantum system is brought out here in terms of its mismatch with moment sequence.

4.2 Reconstruction of joint probability of classical dichotomic random variables from moments

Let X denote a dichotomic random variable with outcomes $x = \pm 1$. The moments associated with statistical outcomes involving the variable X are given by

$$\mu_n = \langle X^n \rangle = \sum_{x=\pm 1} x^n \, P(x), \;\; n = 0, 1, 2, 3, \ldots$$

where

$$0 \leq P(x = \pm 1) \leq 1; \sum_{x=\pm 1} P(x) = 1$$

are the corresponding probabilities. Given the moments μ_0 and μ_1 from a statistical trial, one can readily obtain the probability mass function:

$$\begin{aligned} P(1) &= \frac{1}{2}(\mu_0 + \mu_1) = \frac{1}{2}(1 + \mu_1) \\ P(-1) &= \frac{1}{2}(\mu_0 - \mu_1) = \frac{1}{2}(1 - \mu_1), \end{aligned}$$

i.e., moments determine the probabilities uniquely.

In the case of two dichotomic random variables X_1, X_2, the moments

$$\mu_{n_1, n_2} = \langle X_1^{n_1} \, X_2^{n_2} \rangle = \sum_{x_1=\pm 1, x_2=\pm 1} x_1^{n_1} \, x_2^{n_2} \, P(x_1, x_2), \;\; n_1, n_2 = 0, 1 \ldots$$

encode the bivariate probabilities $P(x_1, x_2)$. Explicitly,

$$\begin{aligned} \mu_{00} &= \sum_{x_1, x_2 = \pm 1} P(x_1, x_2) = P(1,1) + P(1,-1) + P(-1,1) + P(-1,-1) = 1, \\ \mu_{10} &= \sum_{x_1, x_2 = \pm 1} x_1 \, P(x_1, x_2) = \sum_{x_1 = \pm 1} x_1 \; P(x_1), \end{aligned}$$

$$
\begin{aligned}
&= P(1,1) + P(1,-1) - P(-1,1) - P(-1,-1) \\
\mu_{01} &= \sum_{x_1,x_2=\pm 1} x_2\, P(x_1,x_2) = \sum_{x_2} x_2\, P(x_2) \\
&= P(1,1) - P(1,-1) + P(-1,1) - P(-1,-1) \\
\mu_{11} &= \sum_{x_1,x_2=\pm 1} x_1\, x_2\, P(x_1,x_2) \\
&= P(1,1) - P(1,-1) - P(-1,1) + P(-1,-1).
\end{aligned} \tag{4.2}
$$

Note that the moments μ_{10}, μ_{01} involve the marginal probabilities $P(x_1) = \sum_{x_2=\pm 1} P(x_1,x_2)$, $P(x_2) = \sum_{x_1=\pm 1} P(x_1,x_2)$ respectively and they could be evaluated based on statistical trials drawn independently from the two random variables X_1 and X_2.

Given the moments $\mu_{00}, \mu_{10}, \mu_{01}, \mu_{11}$ the reconstruction of the probabilities $P(x_1,x_2)$ is straightforward:

$$
\begin{aligned}
P(x_1,x_2) &= \frac{1}{4} \sum_{n_1,n_2=0,1} x_1^{n_1} x_2^{n_2}\, \mu_{n_1\, n_2} \\
&= \frac{1}{4} \sum_{n_1,n_2=0,1} x_1^{n_1} x_2^{n_2}\, \langle X_1^{n_1}\, X_2^{n_2} \rangle.
\end{aligned} \tag{4.3}
$$

Further, a reconstruction of trivariate joint probabilities $P(x_1,x_2,x_3)$ requires the following set of eight moments: $\{\mu_{000} = 1, \mu_{100} = \langle X_1 \rangle,\ \mu_{010} = \langle X_2 \rangle, \mu_{010} = \langle X_3 \rangle, \mu_{110} = \langle X_1\, X_2 \rangle, \mu_{011} = \langle X_2\, X_3 \rangle, \mu_{101} = \langle X_1\, X_3 \rangle,\ \mu_{111} = \langle X_1\, X_2\, X_3 \rangle\}$. The probabilities are retrieved faithfully in terms of the eight moments as,

$$
\begin{aligned}
P(x_1,x_2,x_3) &= \frac{1}{8} \sum_{n_1,n_2,n_3=0,1} x_1^{n_1} x_2^{n_2} x_3^{n_3}\, \mu_{n_1\, n_2\, n_3} \\
&= \frac{1}{8} \sum_{n_1,n_2,n_3=0,1} x_1^{n_1} x_2^{n_2} x_3^{n_3}\, \langle X_1^{n_1}\, X_2^{n_2}\, X_3^{n_3} \rangle.
\end{aligned} \tag{4.4}
$$

It is implicit that the moments $\mu_{100}, \mu_{010}, \mu_{001}$ are determined through independent statistical trials involving the random variables X_1, X_2, X_3 separately; $\mu_{110}, \mu_{011}, \mu_{101}$ are obtained based on the correlation outcomes of (X_1, X_2), (X_2, X_3) and (X_1, X_3) respectively. More specifically, in the classical probability setting there is a tacit underlying assumption that the set of all marginal probabilities $P(x_1), P(x_2), P(x_3), P(x_1, x_2), P(x_2, x_3), P(x_1, x_3)$ are consistent with the trivariate joint probabilities $P(x_1, x_2, x_3)$. This underpinning does not get imprinted automatically in the quantum scenario. Suppose the observables $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$ are non-commuting and we consider their sequential measurement. The moments $\mu_{100} = \langle \mathbf{X}_1 \rangle, \mu_{010} = \langle \mathbf{X}_2 \rangle, \mu_{001} = \langle \mathbf{X}_3 \rangle$ may be evaluated from the measurement outcomes of dichotomic observables $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$ independently; the correlated statistical outcomes in the sequential measurements of $(\mathbf{X}_1, \mathbf{X}_2)$, $(\mathbf{X}_2, \mathbf{X}_3)$ and $(\mathbf{X}_1, \mathbf{X}_3)$ allow one to extract the set of moments $\mu_{110} = \langle \mathbf{X}_1 \mathbf{X}_2 \rangle, \mu_{011} = \langle \mathbf{X}_2 \mathbf{X}_3 \rangle, \mu_{101} = \langle\, \mathbf{X}_1 \mathbf{X}_3 \rangle$; further the moment $\mu_{111} = \langle \mathbf{X}_1\, \mathbf{X}_2\, \mathbf{X}_3 \rangle$ is evaluated based on the correlation outcomes when all the three observables are measured sequentially. The joint probabilities $P_\mu(x_1, x_2, x_3)$ retrieved from the moments as given in (4.4) differ from the ones evaluated directly in terms of the correlation outcomes in the sequential measurement of all the three observables. We illustrate this inconsistency appearing in the quantum setting in the next section.

4.3 Quantum three-time joint probabilities and moment inversion

Let us consider a spin-1/2 system, the dynamical evolution of which is governed by the Hamiltonian

$$\mathbf{H} = \frac{1}{2}\, \hbar\, \omega \boldsymbol{\sigma}_x. \tag{4.5}$$

We choose the z-component of spin as our dynamical observable:

$$\begin{aligned}\mathbf{X}_i &= \mathbf{X}(t_i) = \boldsymbol{\sigma}_z(t_i) \\ &= \mathbf{U}^\dagger(t_i)\,\boldsymbol{\sigma}_z\,\mathbf{U}(t_i) \\ &= \boldsymbol{\sigma}_z\,\cos\omega\,t_i + \boldsymbol{\sigma}_y\,\sin\omega\,t_i,\end{aligned} \tag{4.6}$$

where $\mathbf{U}(t_i) = e^{-i\,\boldsymbol{\sigma}_x\,\omega\,t_i/2} = \mathbf{U}_i$, and consider sequential measurements of the observable $\mathbf{X}_i$ at three different times $t_1 = 0, t_2 = \Delta t, t_3 = 2\,\Delta t$:

$$\begin{aligned}\mathbf{X}_1 &= \boldsymbol{\sigma}_z \\ \mathbf{X}_2 &= \boldsymbol{\sigma}_z(\Delta t) = \boldsymbol{\sigma}_z\,\cos(\omega\Delta t) + \boldsymbol{\sigma}_y\,\sin(\omega\Delta t) \\ \mathbf{X}_3 &= \boldsymbol{\sigma}_z(2\Delta t) = \boldsymbol{\sigma}_z\,\cos(2\omega\Delta t) + \boldsymbol{\sigma}_y\,\sin(2\omega\Delta t).\end{aligned} \tag{4.7}$$

Note that these three operators are not commuting in general.

The moments $\langle\mathbf{X}_1\rangle, \langle\mathbf{X}_2\rangle, \langle\mathbf{X}_3\rangle$ are readily evaluated to be

$$\begin{aligned}\mu_{100} &= \langle\mathbf{X}_1\rangle = \mathrm{Tr}[\rho_{\rm in}\,\boldsymbol{\sigma}_{\rm z}] = 0, \\ \mu_{010} &= \langle\mathbf{X}_2\rangle = \mathrm{Tr}[\rho_{\rm in}\,\boldsymbol{\sigma}_{\rm z}(\Delta \mathrm{t})] = 0, \\ \mu_{001} &= \langle\mathbf{X}_3\rangle = \mathrm{Tr}[\rho_{\rm in}\,\boldsymbol{\sigma}_{\rm z}(2\Delta \mathrm{t})] = 0\end{aligned} \tag{4.8}$$

when the system density matrix is prepared initially in a maximally mixed state $\rho_{in} = \frac{\mathbb{I}}{2}$. The probabilities of outcomes $x_i = \pm 1$ in the completely random initial state are given by $P(x_i = \pm 1) = \mathrm{Tr}[\rho_{\rm in}\,\mathbf{\Pi}_{\rm x_i}] = \frac{1}{2}$, where $\mathbf{\Pi}_{x_i} = |x_i\rangle\langle x_i|$ is the projection operator corresponding to measurement of the observable $\mathbf{X}_i$.

The two-time joint probabilities arising in the sequential measurements of the observables $\mathbf{X}_i, \mathbf{X}_j,\ j > i$ are evaluated as follows. The measurement of the observable $\mathbf{X}_i$ yielding the outcome $x_i = \pm 1$ projects the density operator to $\rho_{x_i} = \frac{\mathbf{\Pi}_{x_i}\,\rho_{\rm in}\,\mathbf{\Pi}_{x_i}}{\mathrm{Tr}[\rho_{\rm in}\,\mathbf{\Pi}_{x_i}]}$. Further, a sequential measurement of $\mathbf{X}_j$ leads to the two-time joint probabilities as,

$$
\begin{aligned}
P(x_i, x_j) &= P(x_i)\, P(x_j|x_i) \\
&= \mathrm{Tr}[\rho_{\rm in}\, \mathbf{\Pi}_{x_i}]\; \mathrm{Tr}[\rho_{x_i}\, \mathbf{\Pi}_{x_j}] \\
&= \mathrm{Tr}[\mathbf{\Pi}_{x_i}\, \rho_{\rm in}\, \mathbf{\Pi}_{x_i} \mathbf{\Pi}_{x_j}] \\
&= \langle x_i|\, \rho_{\rm in}\, |x_i\rangle\, |\langle x_i|x_j\rangle|^2 \qquad (4.9)
\end{aligned}
$$

We evaluate the two-time joint probabilities associated with the sequential measurements of $(\mathbf{X}_1, \mathbf{X}_2)$, $(\mathbf{X}_2, \mathbf{X}_3)$, and $(\mathbf{X}_1, \mathbf{X}_3)$ explicitly:

$$P(x_1, x_2) = \frac{1}{4}\,[1 + x_1\, x_2\, \cos(\omega \Delta t)] \qquad (4.10)$$

$$P(x_2, x_3) = \frac{1}{4}\,[1 + x_2\, x_3\, \cos(\omega \Delta t)] \qquad (4.11)$$

$$P(x_1, x_3) = \frac{1}{4}\,[1 + x_1\, x_3\, \cos(2\omega \Delta t)]. \qquad (4.12)$$

We then obtain two-time correlation moments as,

$$
\begin{aligned}
\mu_{110} = \langle\, \mathbf{X}_1 \mathbf{X}_2 \rangle &= \sum_{x_1, x_2 = \pm 1} x_1\, x_2\, P(x_1, x_2) \\
&= \cos(\omega \Delta t) \\
\mu_{011} = \langle\, \mathbf{X}_2 \mathbf{X}_3 \rangle &= \sum_{x_2, x_3 = \pm 1} x_2\, x_3\, P(x_2, x_3) \\
&= \cos(\omega \Delta t) \qquad (4.13) \\
\mu_{101} = \langle\, \mathbf{X}_1 \mathbf{X}_3 \rangle &= \sum_{x_1, x_3 = \pm 1} x_1\, x_3\, P(x_1, x_3) \\
&= \cos(2\, \omega \Delta t).
\end{aligned}
$$

Further, the three-time joint probabilities $P(x_1, x_2, x_3)$ arising in the sequential measurements of $\mathbf{X}_1, \mathbf{X}_2$, followed by $\mathbf{X}_3$ are given by

$$\begin{aligned} P(x_1, x_2, x_3) &= P(x_1)\, P(x_2|x_1)\, P(x_3|x_1, x_2) \\ &= \mathrm{Tr}[\rho_{\rm in}\, \mathbf{\Pi}_{x_1}]\, \mathrm{Tr}[\rho_{x_1}\, \mathbf{\Pi}_{x_2}]\, \mathrm{Tr}[\rho_{x_2}\, \mathbf{\Pi}_{x_3}] \end{aligned} \tag{4.14}$$

where $\rho_{x_2} = \frac{\mathbf{\Pi}_{x_2}\, \rho_{x_1}\, \mathbf{\Pi}_{x_2}}{\mathrm{Tr}[\rho_{x_1}\, \mathbf{\Pi}_{x_2}]}$. We obtain,

$$\begin{aligned} P(x_1, x_2, x_3) &= \mathrm{Tr}[\mathbf{\Pi}_{x_2}\, \mathbf{\Pi}_{x_1}\, \rho_{\rm in}\, \mathbf{\Pi}_{x_1}\, \mathbf{\Pi}_{x_2}\, \mathbf{\Pi}_{x_3}] \\ &= \langle x_1|\, \rho_{\rm in}\, |x_1\rangle\, |\langle x_1|x_2\rangle|^2\, |\langle x_2|x_3\rangle|^2 \\ &= \frac{P(x_1, x_2)\, P(x_2, x_3)}{\langle x_2|\, \rho_{\rm in}\, |x_2\rangle} \\ &= \frac{P(x_1, x_2)\, P(x_2, x_3)}{P(x_2)} \end{aligned} \tag{4.15}$$

where in the third line of (4.15) we have used (4.9).

The three-time correlation moment is evaluated to be,

$$\begin{aligned} \mu_{111} = \langle \mathbf{X}_1\, \mathbf{X}_2\, \mathbf{X}_3 \rangle &= \sum_{x_1, x_2, x_3 = \pm 1} x_1\, x_2\, x_3\, P(x_1, x_2, x_3) \\ &= 0. \end{aligned} \tag{4.16}$$

From the set of eight moments (4.8), (4.13), (4.16) together with $\mu_{000} = 1$, we construct the TTJP (see (4.4)) as,

$$\begin{aligned} P_\mu(1,1,1) &= P_\mu(-1,-1,-1) = \frac{1}{8}\, [1 + 2\cos(\omega \Delta t) + \cos(2\omega \Delta t)], \\ P_\mu(-1,1,1) &= P_\mu(-1,-1,1) = P_\mu(1,1,-1) = P_\mu(1,-1,-1) \\ &= \frac{1}{8}\, [1 - \cos(2\omega \Delta t)] \\ P_\mu(1,-1,1) &= P_\mu(-1,1,-1) = \frac{1}{8}\, [1 - 2\cos(\omega \Delta t) + \cos(2\omega \Delta t)]. \end{aligned} \tag{4.17}$$

On the other hand, the three dichotomic variable quantum probabilities $P(x_1, x_2, x_3)$

evaluated directly are given by,

$$
\begin{aligned}
P_d(1,1,1) &= P_d(-1,-1,-1) = \frac{1}{8}\,[1+\cos(\omega\,\Delta t)]^2, \\
P_d(-1,1,1) &= P_d(-1,-1,1) = P_d(1,1,-1) = P_d(1,-1,-1) \\
&= \frac{1}{8}\,[1-\cos^2(\omega\,\Delta t)] \\
P_d(1,-1,1) &= P_d(-1,1,-1) = \frac{1}{8}\,[1-\cos(\omega\,\Delta t)]^2. \qquad (4.18)
\end{aligned}
$$

Clearly, there is no agreement between the moment inverted TTJP (4.17) and the ones of (4.18) directly evaluated. In other words, the TTJP realized in a sequential measurement are not invertible in terms of the moments – which in turn reflects the incompatibility of the set of all marginal probabilities with the grand joint probabilities $P_d(x_1, x_2, x_3)$. In fact, it may be explicitly verified that $P(x_1, x_3) \neq \sum_{x_2=\pm 1} P_d(x_1, x_2, x_3)$. Moment-indeterminacy points towards the absence of a valid grand probability distribution consistent with all the marginals.

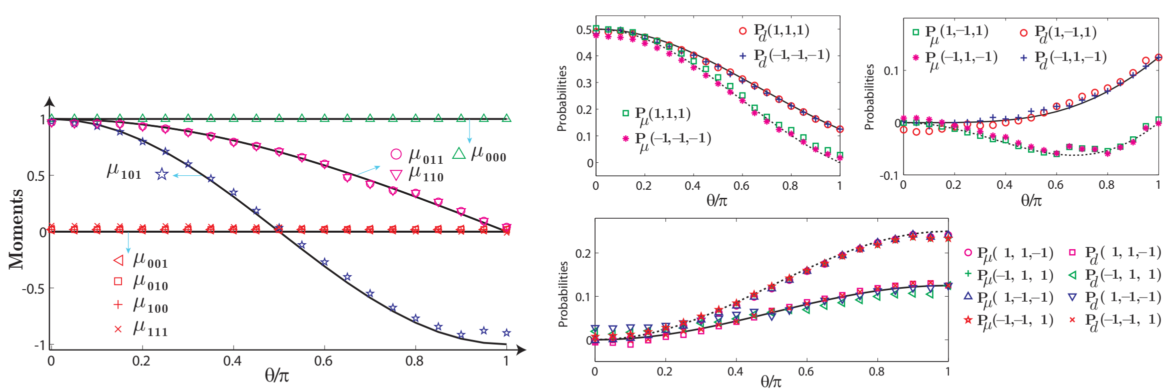

Figure 4.1: The left figure shows the moment extraction in the experiment, which are used to construct the probabilities. The right figure shows the incompatibility between the moment inverted probabilities P_μ and that of the experimental ones P_d. This is a signature of the non-classical nature of the probabilities arising in the quantum scenario. For more details on the experimental aspects see [126].

The TTJP and moments can be independently extracted experimentally using NMR methods on an ensemble of spin-1/2 nuclei. The experimental approach and results are reported in [126]. The experimental verification using a nuclear magnetic resonance (NMR) system corroborating these theoretical observations viz., the incompatibility of the three-time joint probabilities with those extracted from the moment sequence when sequential measurements on a single qubit system is shown in fig 4.1.

4.4 Conclusion

In classical probability setting, statistical moments associated with dichotomic random variables determine the probabilities uniquely. When the same issue is explored in the quantum context – with random variables replaced by Hermitian observables (which are in general non-commuting) and the statistical outcomes of observables in sequential measurements are considered – it is shown that the joint probabilities do not agree with the ones inverted from the moments. This is explicitly illustrated by considering sequential measurements of a dynamical variable at three different times in the specific example of a spin-1/2 system. An experimental investigation based on NMR methods, where moments and the joint probabilities are extracted independently, demonstrates the moment indeterminacy of probabilities, concordant with theoretical observations.

The failure to revert joint probability distribution from its moments points towards its inherent incompatibility with the family of all marginals. In turn, the moment indeterminacy reveals the absence of a legitimate joint probability distribution compatible with the set of all marginal distributions – a common underpinning of various no-go theorems in the foundational aspects of quantum theory.

Chapter 5

Characterizing non-classicality via the positivity of Moment Matrix

We investigate if a given set of moments, arising from correlation measurements of three dichotomic observables in the quantum scenario, is compatible with a legitimate grand joint probability distribution. A valid sequence of correlations (moments) requires that the corresponding moment matrix is positive. We find an interesting link between moment matrix and the structure of admissible joint probability distribution: positivity of the moment matrix necessarily enforces that the associated joint probabilities are of the hidden variable form (convex sum of the product form).*Examples of spatial and temporal correlations arising within the quantum framework demonstrate that the moment matrix constructed out of these correlations (moments) is negative. This in turn strengthens our realization of the link between moment matrix and the structure of the underlying joint probability distribution.*

5.1 Introduction

Probabilities of measurement outcomes within the quantum framework are fundamentally different from those arising in the classical statistical scenario. This has invoked a wide range of debates on the foundational conflicts about the quantum-classical worldviews of nature [109, 73, 74]. Pioneering investigations by Bell [57], Kochen-Specker [108], Leggett-Garg [4] tied the puzzling non-classical (quantum) features with various no-go theorems. The common theme underlying the proofs of these no-go theorems points towards the non-existence of a joint probability distribution for the outcomes of all possible measurements performed on a quantum system [73, 57, 108, 4, 129, 91].

On an entirely different perspective, *classical moment problem* [121, 122] addresses the issue of determining a probability distribution given a sequence of statistical moments. Essentially, classical moment problem brings forth that a given sequence of real numbers qualify to be the moment sequence of a legitimate probability distribution if and only if the associated moment matrix is positive. In other words, *existence of a valid joint probability distribution* consistent with a given sequence of *moments* gets linked with the moment matrix positivity.

Here, we investigate the positivity of a 8×8 moment matrix to verify the existence of a valid joint probability distribution for the outcomes of the measurement of three dichotomic observables in the quantum scenario. This results in an interesting identification: *positivity of the moment matrix implies that the associated joint probabilities assume the convex sum of the product form.* In other words, *hidden variable structure for the joint probabilities emerges naturally – bringing forth a necessary and sufficient condition for non-classicality of correlations via moment matrix positivity criterion.*

Examples of

(a). Temporal correlations of a single qubit dichotomic observable measured at three different times, when the quantum system is evolving under a coherent unitary dynamics corresponding to the Leggett-Garg macrorealism.

(b). Correlation measurements of dichotomic observables performed on spatially separated systems corresponding to the Bell local realism.

(c). Correlation measurements of three dichotomic observables on a qubit forming a contextual scenario

are considered.

5.2 Positivity of a Moment Matrix

Consider a set $\{a_1, a_2, a_3, b_1, b_2, b_3, c\}$ where all the seven elements lie between ± 1. Our task is to verify if they correspond to a sequence of moments $\{\langle X_1\rangle, \langle X_2\rangle, \langle X_3\rangle, \langle X_1\, X_2\rangle, \langle X_2\, X_3\rangle, \langle X_1\, X_3\rangle, \langle X_1 X_2 X_3\rangle\}$ of a probability distribution $P(x_1, x_2, x_3)$. Here, $x_1, x_2, x_3 = \pm 1$ are three *classical* dichotomic random variables. The validation is done by arranging the given sequence in the form of a 8×8 moment matrix and verifying its positivity. (Moment matrix is positive iff there exists a probability distribution of which the sequence of numbers $\{a_1, a_2, a_3, b_1, b_2, b_3, c\}$ *do* correspond to the moments $\{\langle X_1\rangle, \langle X_2\rangle, \langle X_3\rangle, \langle X_1\, X_2\rangle, \langle X_2\, X_3\rangle, \langle X_1\, X_3\rangle, \langle X_1 X_2 X_3\rangle\}$) .

Moment matrix of a *valid* sequence of moments is constructed as follows: Consider a column vector,

$$\xi = \begin{pmatrix} 1 \\ X_1 \\ X_2 \\ X_3 \\ X_1 X_2 \\ X_2 X_3 \\ X_1 X_3 \\ X_1 X_2 X_3 \end{pmatrix}. \tag{5.1}$$

The associated real positive moment matrix is defined as $M = \langle \xi\, \xi^T \rangle$, which, by construction, is a real, positive matrix.

$$M=\langle \xi\,\xi^T\rangle=\begin{pmatrix} 1 & \langle X_1\rangle & \langle X_2\rangle & \langle X_3\rangle & \langle X_1X_2\rangle & \langle X_2X_3\rangle & \langle X_1X_3\rangle & \langle X_1X_2X_3\rangle \\ \langle X_1\rangle & 1 & \langle X_1X_2\rangle & \langle X_1X_3\rangle & \langle X_2\rangle & \langle X_1X_2X_3\rangle & \langle X_3\rangle & \langle X_2X_3\rangle \\ \langle X_2\rangle & \langle X_1X_2\rangle & 1 & \langle X_2X_3\rangle & \langle X_1\rangle & \langle X_3\rangle & \langle X_1X_2X_3\rangle & \langle X_1X_3\rangle \\ \langle X_3\rangle & \langle X_1X_3\rangle & \langle X_2X_3\rangle & 1 & \langle X_1X_2X_3\rangle & \langle X_2\rangle & \langle X_1\rangle & \langle X_1X_2\rangle \\ \langle X_1X_2\rangle & \langle X_2\rangle & \langle X_1\rangle & \langle X_1X_2X_3\rangle & 1 & \langle X_1X_3\rangle & \langle X_2X_3\rangle & \langle X_3\rangle \\ \langle X_2X_3\rangle & \langle X_1X_2X_3\rangle & \langle X_3\rangle & \langle X_2\rangle & \langle X_1X_3\rangle & 1 & \langle X_1X_2\rangle & \langle X_1\rangle \\ \langle X_1X_3\rangle & \langle X_3\rangle & \langle X_1X_2X_3\rangle & \langle X_1\rangle & \langle X_2X_3\rangle & \langle X_1X_2\rangle & 1 & \langle X_2\rangle \\ \langle X_1X_2X_3\rangle & \langle X_2X_3\rangle & \langle X_1X_3\rangle & \langle X_1X_2\rangle & \langle X_3\rangle & \langle X_1\rangle & \langle X_2\rangle & 1 \end{pmatrix}. \tag{5.2}$$

(Here, we have used the condition that square of the dichotomic variable X_i^2 assumes the value 1 i.e., $X_i^2\equiv 1$.)

Let us consider a special case where single variable averages $\langle X_1\rangle$, $\langle X_2\rangle$ and $\langle X_3\rangle$ as well as the three variable correlation $\langle X_1X_2X_3\rangle$ are zero. Let us denote the two variable correlations $\langle X_1X_2\rangle = a$, $\langle X_2X_3\rangle = b$ and $\langle X_1X_3\rangle = c$. The moment matrix reduces to the form,

$$M=\begin{pmatrix} 1 & 0 & 0 & 0 & a & b & c & 0 \\ 0 & 1 & a & c & 0 & 0 & 0 & b \\ 0 & a & 1 & b & 0 & 0 & 0 & c \\ 0 & c & b & 1 & 0 & 0 & 0 & a \\ a & 0 & 0 & 0 & 1 & c & b & 0 \\ b & 0 & 0 & 0 & c & 1 & a & 0 \\ c & 0 & 0 & 0 & b & a & 1 & 0 \\ 0 & b & c & a & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.3}$$

The eigenvalues of the moment matrix are given by,

$$\begin{array}{ll} 1+a-b-c & \text{(twice)} \\ 1-a+b-c & \text{(twice)} \\ 1-a-b+c & \text{(twice)} \\ 1+a+b+c & \text{(twice)} \end{array}$$

Positivity of the moment matrix imply the following conditions:

$$1 + a - b - c \geq 0 \tag{5.4}$$

$$1 - a + b - c \geq 0 \tag{5.5}$$

$$1 - a - b + c \geq 0 \tag{5.6}$$

$$1 + a + b + c \geq 0. \tag{5.7}$$

5.3 Mapping of moment matrix positivity with the positivity of a partially transposed two qubit density matrix

Let us consider a two qubit density matrix:

$$\rho_{AB} = \frac{1}{4}[\mathbb{I} \otimes \mathbb{I} + \vec{\boldsymbol{\sigma}} \cdot \vec{r} \times \mathbb{I} + \mathbb{I} \otimes \vec{\boldsymbol{\sigma}} \cdot \vec{s} + \sum_{i,j=x,y,z} \boldsymbol{\sigma}_i \otimes \boldsymbol{\sigma}_j \, t_{ij}] \tag{5.8}$$

where $r_i = \mathrm{Tr}[\rho_{AB}\boldsymbol{\sigma}_i \otimes \mathbb{I}]$, $s_i = \mathrm{Tr}[\rho_{AB}\, \mathbb{I} \otimes \boldsymbol{\sigma}_i]$ and $t_{ij} = \mathrm{Tr}[\rho_{AB}\boldsymbol{\sigma}_i \otimes \boldsymbol{\sigma}_j]$ denote 15 parameters characterizing the two qubit density matrix. When $r_i = s_i = 0$ and $t_{ij} = t_i\delta_{i,j}$, we find that the eigenvalues of the density matrix are given by,

$$1 - t_1 + t_2 + t_3 \tag{5.9}$$

$$1 + t_1 - t_2 + t_3 \tag{5.10}$$

$$1 + t_1 + t_2 - t_3 \tag{5.11}$$

$$1 - t_1 - t_2 - t_3. \tag{5.12}$$

Note that the parameters lie in the range $-1 \leq t_i \leq 1$. However, under the partial transpose of the density matrix, we have $t_i \to -t_i$.

As such, the eigenvalues of the partially transposed density matrix are given by,

$$1 + t_1 - t_2 - t_3 \tag{5.13}$$

$$1 - t_1 + t_2 - t_3 \tag{5.14}$$

$$1 - t_1 - t_2 + t_3 \tag{5.15}$$

$$1 + t_1 + t_2 + t_3. \tag{5.16}$$

Note that the eigenvalues of the moment matrix and that of the partially transposed density matrix match identically if we map $a \rightarrow t_1, b \rightarrow t_2$ and $c \rightarrow t_3$. In other words, positivity of the moment matrix is *equivalent* to the positivity of the partially transposed density matrix. Furthermore, positivity of the partially transposed density matrix implies that the two qubit density matrix is *separable* i.e.,

$$\rho_{AB} = \sum_\lambda p_\lambda \, \rho_{A\lambda} \otimes \rho_{B\lambda}$$

Hence, positivity of the moment matrix thus implies that the two variable correlations can be expressed as

$$\begin{aligned} a &= \sum_\lambda p_\lambda \, \mathrm{Tr}[\rho^T_{A\lambda} \boldsymbol{\sigma}_x] \, \mathrm{Tr}[\rho_{B\lambda} \boldsymbol{\sigma}_x] \\ &= \sum_\lambda p_\lambda \, \mathrm{Tr}[\rho^T_{A\lambda} \{ \sum_{m_1 = \pm 1} m_1 \, \mathbf{\Pi}^{(x)}_{m_1} \}] \, \mathrm{Tr}[\rho_{B\lambda} \{ \sum_{m_2 = \pm 1} m_2 \, \mathbf{\Pi}^{(x)}_{m_2} \}] \\ &= \sum_{m_1, m_2 = \pm 1} P^{(x)}(m_1, m_2) \, m_1 \, m_2 \end{aligned}$$

where $\mathbf{\Pi}^{(x)}_{m_1} = \frac{1}{2} [\mathbb{I} + m_1 \, \boldsymbol{\sigma}_x]$, $\mathbf{\Pi}^{(x)}_{m_2} = \frac{1}{2} [\mathbb{I} + m_2 \, \boldsymbol{\sigma}_x]$ and

$$P^{(x)}(m_1, m_2) = \sum_\lambda p_\lambda \, P^{(x)}_\lambda(m_1) Q^{(x)}_\lambda(m_2) \tag{5.17}$$

with $P^{(x)}_\lambda(m_1) = \mathrm{Tr}[\rho^T_{A\lambda}\boldsymbol{\sigma}_x]$, $Q^{(x)}_\lambda(m_2) = \mathrm{Tr}[\rho_{B\lambda}\boldsymbol{\sigma}_x]$. Similarly, one can express

$$b = \sum_{m_2, m_3 = \pm 1} P^{(y)}(m_2, m_3)\, m_2\, m_3$$

and

$$c = \sum_{m_1, m_3 = \pm 1} P^{(z)}(m_1, m_3)\, m_1\, m_3$$

where,

$$\begin{aligned} P^{(y)}(m_2, m_3) &= \sum_\lambda p_\lambda\, P^{(y)}_\lambda(m_2) Q^{(y)}_\lambda(m_3) \\ P^{(z)}(m_1, m_3) &= \sum_\lambda p_\lambda\, P^{(z)}_\lambda(m_1) Q^{(z)}_\lambda(m_3). \end{aligned}$$

Thus, the *separable* (convex sum of the product) form for the probabilities turns out to be both the necessary as well as sufficient condition for the positivity of the moment matrix. Furthermore, this condition is in tune with the requirement of the hidden variable theories underlying local realism, non-contextuality and macrorealism requiring the joint (classical) probabilities to be in the separable (convex sum of the product) form.

5.4 Moment matrix associated with temporal correlations

Consider a qubit, the dynamical evolution of which is governed by the Hamiltonian $\mathbf{H} = \frac{1}{2}\hbar\omega\boldsymbol{\sigma}_x$. We consider measurement of three observables $\mathbf{X}_i = \boldsymbol{\sigma}_z(t_i)$, $t_1 = 0, t_2 = \Delta t, t_3 = 2\,\Delta t$ (the dynamical observable $\boldsymbol{\sigma}_z$ at different times is given explicitly by, $\boldsymbol{\sigma}_z(t_i) = e^{i\mathbf{H}t_i}\boldsymbol{\sigma}_z e^{-i\mathbf{H}t_i} = \boldsymbol{\sigma}_z\,\cos(\omega t_i) + \boldsymbol{\sigma}_y\,\sin(\omega t_i)$). When the qubit is initially prepared in a maximally mixed state $\rho_{\rm in} = \mathbb{I}/2$, sequential measurements of $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$ lead to

$$\begin{aligned}
\langle \mathbf{X}_1 \rangle &= \langle \boldsymbol{\sigma}_z \rangle = 0 \\
\langle \mathbf{X}_2 \rangle &= \langle \boldsymbol{\sigma}_z(\Delta t) \rangle = 0 \\
\langle \mathbf{X}_3 \rangle &= \langle \boldsymbol{\sigma}_z(2\Delta t) \rangle = 0 \\
\langle \mathbf{X}_1\, \mathbf{X}_2 \rangle &= \langle \{\boldsymbol{\sigma}_z, \boldsymbol{\sigma}_z(\Delta t)\} \rangle = \cos(\omega \Delta t) \\
\langle \mathbf{X}_2\, \mathbf{X}_3 \rangle &= \langle \{\boldsymbol{\sigma}_z(\Delta t), \boldsymbol{\sigma}_z(2\Delta t)\} \rangle = \cos(\omega \Delta t) \\
\langle \mathbf{X}_1\, \mathbf{X}_3 \rangle &= \langle \{\boldsymbol{\sigma}_z, \boldsymbol{\sigma}_z(2\Delta t)\} \rangle = \cos(2\omega \Delta t) \\
\langle \mathbf{X}_1\, \mathbf{X}_2\, X_3 \rangle &= 0.
\end{aligned}$$

In other words, the parameters $a = \cos(\omega\Delta t),\ b = \cos(\omega\Delta t)$ and $c = \cos(2\omega\Delta t)$. Positivity of the eigenvalues of the moment matrix (and that of the corresponding partially transposed density matrix) results in the conditions:

$$\begin{aligned}
1 - \cos(2\omega\Delta t) &\geq 0 \\
1 - 2\cos(\omega\Delta t) + \cos(\omega\Delta t) &\geq 0 \\
1 + 2\cos(\omega\Delta t) + \cos(\omega\Delta t) &\geq 0.
\end{aligned}$$

The moment matrix is thus identified to be negative for any choice of Δt.

5.5 Moment matrix associated with spatial correlations

Consider a spatially separated two qubit system in a Bell state $|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left[|0_A, 1_B\rangle - |1_A, 0_B\rangle\right]$. We consider measurements of three observables $\mathbf{X}_1 = \vec{\boldsymbol{\sigma}} \cdot \mathbf{a} \otimes \mathbf{I}$, $\mathbf{X}_2 = \mathbf{I} \otimes \vec{\boldsymbol{\sigma}} \cdot \mathbf{b}$ and $\mathbf{X}_3 = \vec{\boldsymbol{\sigma}} \cdot \mathbf{a}' \otimes \mathbf{I}$. We obtain,

$$\begin{aligned}
\langle \mathbf{X}_1 \rangle &= 0 \\
\langle \mathbf{X}_2 \rangle &= 0
\end{aligned}$$

$$\begin{aligned}
\langle \mathbf{X}_3 \rangle &= 0 \\
\langle \mathbf{X}_1 \, \mathbf{X}_2 \rangle &= -\mathbf{a} \cdot \mathbf{b} = -\cos\theta_{ab} \\
\langle \mathbf{X}_2 \, \mathbf{X}_3 \rangle &= -\mathbf{a}' \cdot \mathbf{b} = -\cos\theta_{a'b} \\
\langle \mathbf{X}_1 \, \mathbf{X}_3 \rangle &= \mathbf{a} \cdot \mathbf{a}' = \cos\theta_{aa'} \\
\langle \mathbf{X}_1 \, \mathbf{X}_2 \, \mathbf{X}_3 \rangle &= 0.
\end{aligned}$$

Choosing coplanar geometry for $\mathbf{a}, \mathbf{b}, \mathbf{a}'$ such that $\theta_{ab} = \pi - \phi$, $\theta_{a'b} = \pi - \phi$ and $\theta_{aa'} = 2\pi - 2\phi$, we obtain,

$$a = \cos\phi, b = \cos\phi, c = \cos 2\phi, \tag{5.18}$$

which results in an analogous conclusion as in the case of temporal correlations (i.e., moment matrix is negative for any arbitrary values of ϕ).
Note that $[\mathbf{X}_1, \mathbf{X}_2] = 0 = [\mathbf{X}_2, \mathbf{X}_3]$ whereas $[\mathbf{X}_1, \mathbf{X}_3] \neq 0$. As $\mathbf{X}_2$ commutes with both $\mathbf{X}_1$ and $\mathbf{X}_3$, it provides the *context* in the measurement of the other two observables, which do not commute. As such, the above example reveals the contextuality amongst the three observables $\mathbf{X}_1$, $\mathbf{X}_2$ and $\mathbf{X}_3$.

5.6 Conclusion

Discerning the strikingly different nature of statistical features of the classical and quantum worlds has been a long studied problem. Various no-go theorems from the foundational works of Bell [57], Kochen-Specker [108], Leggett-Garg [4] and others signify the non-classical features of quantum theory. Furthermore, the advancement in technology has motivated results which have an operational expression in addition to the theoretical results characterizing the contrasting nature of the two worldviews. To this end, one such proposition is through the verification of the positivity of the moment matrix. In classical probability theory, the moment problem [121, 122] validates a sequence of real numbers to be the "statistical moments" of a (discrete) probability distribution through the positivity of the moment matrix. This addresses the issue of the existence of a probability distribution given a "sequence of statistical moments". That is, the *existence of a valid joint probability distribution* consistent with a given sequence of moments gets linked with moment matrix positivity. Here, we investigated the positivity of a 8×8 moment matrix to verify the existence of a valid joint probability distribution of three di-chotomic observables in the quantum scenario. An important identification that the *positivity of the moment matrix implies the separable (convex sum of the product) form for the associated joint probabilities* is noted. This establishes as a *necessary* as well a *sufficient* criterion for checking the separability of the joint probability distribution concerned. This is in tune with the requirement of the *hidden variable theories* underlying local realism, non-contextuality and macrorealism.

Chapter 6

Entropic Uncertainty assisted by temporal memory

The uncertainty principle brings out intrinsic quantum bounds on the precision of measuring non-commuting observables. Statistical outcomes in the measurement of incompatible observables reveal a trade-off on the sum of corresponding entropies. Maassen-Uffink entropic uncertainty relation [6] constrains the sum of entropies associated with incompatible measurements. The entropic uncertainty principle in the presence of quantum memory [7] brought about a fascinating twist by showing that quantum side information, enabled due to entanglement, helps in beating the uncertainty of non-commuting observables. Here we explore the interplay between temporal correlations and uncertainty. We show that with the assistance of a prior quantum temporal information achieved by sequential observations on the same quantum system at different times, the uncertainty bound on entropies gets reduced.

6.1 Introduction

The uncertainty principle marks an astounding departure from classical determinism by setting fundamental limits on the precision achievable in *knowing* non-commuting observables of a particle. Robertson [38] quantified this limit in knowing the values of non-commuting observables $\mathbf{X}$, $\mathbf{Z}$ as

$$(\Delta\mathbf{X})_\rho\,(\Delta\mathbf{Z})_\rho \geq \frac{1}{2}\,|\langle[\mathbf{X},\mathbf{Z}]\rangle_\rho|. \tag{6.1}$$

It has been identified subsequently that Shannon entropies of the probabilities of measurement outcomes of the observables $\mathbf{X}$, $\mathbf{Z}$ given by, $H_\rho(\mathbf{X}) = -\sum_x P(x)\log_2 P(x)$, $H_\rho(\mathbf{Z}) = -\sum_z P(z)\log_2 P(z)$ offer a more general framework to quantify the *intrinsic ignorance* associated with incompatible measurements. Here, x (z) are the measurement outcomes of the observable $\mathbf{X}$ ($\mathbf{Z}$) and $P(x) = \langle x|\rho|x\rangle$ ($P(z) = \langle z|\rho|z\rangle$) denote the probability of outcomes x (z); $\{|x\rangle\}$ ($\{|z\rangle\}$) is the set of eigenvectors of $\mathbf{X}$ ($\mathbf{Z}$). For any arbitrary quantum state ρ (both pure and mixed), the Entropic Uncertainty Relation (EUR) given by Maassen and Uffink [6] is:

$$H_\rho(\mathbf{X}) + H_\rho(\mathbf{Z}) \geq -2\log_2 C(\mathbf{X},\mathbf{Z}), \tag{6.2}$$

where $C(\mathbf{X},\mathbf{Z}) = \max_{x,y}|\langle x|z\rangle|$. The lower bound limiting the sum of entropies (6.2) is independent of the state ρ. The term $C(\mathbf{X},\mathbf{Z})$ can assume a maximum value $\frac{1}{\sqrt{d}}$ resulting in the maximum entropic bound of $\log_2 d$, where d denotes the dimension of the system.

A recent uplifting happened with the extension of the EUR assisted by the presence of a quantum memory [7], which refined the lower bound of (6.2). Here, an observer Bob, whose task is to minimize the uncertainty of Alice's measurement of the observables $\mathbf{X}$, $\mathbf{Z}$, is allowed to share an entangled quantum state ρ_{AB} with the qubit in Alice's possession. The uncertainty principle, when Bob possesses a quantum memory, is given by [7]

$$S(\mathbf{X}|B) + S(\mathbf{Z}|B) \geq -2\log_2 C(\mathbf{X},\mathbf{Z}) + S(A|B), \tag{6.3}$$

where

$$S(\mathbf{X}|B) = S(\rho_{AB}^{(\mathbf{X})}) - S(\rho_B), S(\mathbf{Z}|B) = S(\rho_{AB}^{(\mathbf{Z})}) - S(\rho_B)$$

are the conditional von Neumann entropies of the post measured states

$$\rho_{AB}^{(\mathbf{X})} = \sum_x (\mathbf{\Pi}_x \otimes I_B)\rho_{AB}(\mathbf{\Pi}_x \otimes I_B), \quad \rho_{AB}^{(\mathbf{Z})} = \sum_z (\mathbf{\Pi}_z \otimes I_B)\rho_{AB}(\mathbf{\Pi}_z \otimes I_B)$$

obtained after the measurements of $\mathbf{X}$, $\mathbf{Z}$ performed by Alice on the system A; $\mathbf{\Pi}_x = |x\rangle\langle x|$, $\mathbf{\Pi}_z = |z\rangle\langle z|$; and $S(A|B) = S(\rho_{AB}) - S(\rho_B)$ is the conditional von Neumann entropy. When Alice's system is in a maximally entangled state with Bob's quantum memory, the second term on the right hand side of (6.3) takes negative value: $S(A|B) = -\log_2 d$ and as $-2\log_2 C(\mathbf{X},\mathbf{Z}) \leq \log_2 d$, one can achieve a trivial lower bound of zero. Thus, with the help of a quantum memory maximally entangled with Alice's state, Bob can beat the uncertainty bound and can predict the outcomes of incompatible observables $\mathbf{X}$, $\mathbf{Z}$ precisely.

Statistics of quantum correlations between the outcomes of spatially separated systems get mimicked in an interesting fashion by that of temporally separated observables measured sequentially in a single quantum system [4, 130, 131, 129, 87]. Non-classicality of *temporal correlations* between outcomes of sequentially measured observables is reflected by the violation of Leggett-Garg inequality [4] (also termed as temporal Bell inequality [132]), experimental verification of which has gained momentum recently [133, 82, 86, 134, 85, 120]. Sequential measurements on the *same* quantum system result in the transmission of *temporal* information. Temporal correlations resulting from consecutive observations on a single quantum system (in contrast to measurements on spatially separated systems) draw a surge of interest in foundational investigations on quantum vs classical world view [135, 136]. Further, information gained from correlations between the outcomes of subsequent measurements on the same quantum system is shown to be advantageous in quantum communication tasks involving state discrimination [137] and in quantum cryptography [138, 139].

Here, we raise the question, 'analogous to spatial correlations, do temporal correlations arising in sequential measurement of observables, play a distinct role in reducing the uncertainty of incompatible observables?' This boils down to explore if the sum of conditional Shannon entropies $H_\rho(\mathbf{X}|\mathbf{X}_0) + H_\rho(\mathbf{Z}|\mathbf{Z}_0)$ is always smaller than the Maassen-Uffink bound of $-2\log_2 C(\mathbf{X}, \mathbf{Z})$. In other words, would measurements of incompatible observables $\mathbf{X}$, $\mathbf{Z}$, conditioned by outcomes of prior time measurements of $\mathbf{X}_0$, $\mathbf{Z}_0$ respectively lead to better precision?

We show that the uncertainty does get reduced in the presence of a quantum temporal memory due to correlations between the outcomes of $\mathbf{X}_0$ *(*$\mathbf{Z}_0$*) and* $\mathbf{X}$ *(*$\mathbf{Z}$*) – whereas it is impossible to beat the uncertainty bound if the temporal correlations are classical.*

6.2 An example of a Conditioned EUR

Let us consider a qubit prepared in a completely random mixture given by $\rho = \mathbb{I}/2$ ($\mathbb{I}$ denotes 2×2 identity matrix). Measurements of the observables $\mathbf{X} = \boldsymbol{\sigma}_x$ and $\mathbf{Z} = \boldsymbol{\sigma}_z$ in this state leads to Shannon entropies of measurement $H_\rho(\mathbf{X}) = H_\rho(\mathbf{Z}) = 1$; $C(\mathbf{X}, \mathbf{Z}) = \frac{1}{\sqrt{2}}$ and the uncertainty bound (6.2) is $-2\log_2 C(\mathbf{X}, \mathbf{Z}) = 1$; the Maassen-Uffink relation is satisfied.

Let us envisage the following scenario: A dichotomic observable $\mathbf{X}_0 = \cos\theta\, \boldsymbol{\sigma}_z + \sin\theta\, \boldsymbol{\sigma}_x$ is measured in the quantum state followed by which $\mathbf{X} = \boldsymbol{\sigma}_x$ is sequentially measured; the probabilities of realizing the outcomes $x_0 = \pm 1$

for $\mathbf{X}_0$ and $x = \pm 1$ for $\mathbf{X}$ in the sequential measurement is given by

$$P(x_0, x) = \text{Tr}[\mathbf{\Pi}_{x_0} \rho \mathbf{\Pi}_{x_0} \mathbf{\Pi}_x] = \frac{1}{4}[1 + x_0 x \, \cos\theta]$$

where the projectors associated with dichotomic observables $\mathbf{X}_0$ and $\mathbf{X}$ are given by

$$\mathbf{\Pi}_{x_0} = \frac{1}{2}[\mathbb{I} + x_0 \mathbf{X}_0], \mathbf{\Pi}_x = \frac{1}{2}[\mathbb{I} + x\mathbf{X}]$$

Further, measurement of $\mathbf{Z} = \boldsymbol{\sigma}_z$ preceded by that of another dichotomic observable $\mathbf{Z}_0 = \cos\phi \; \boldsymbol{\sigma}_z + \sin\phi \; \boldsymbol{\sigma}_x$ results in the probabilities

$$P(z_0, z) = \text{Tr}[\mathbf{\Pi}_{z_0} \rho \mathbf{\Pi}_{z_0} \mathbf{\Pi}_z] = \frac{1}{4}[1 + z_0 z \, \cos\phi]$$

The conditional Shannon entropy associated with the sequential measurement of $\mathbf{X}_0$ and $\mathbf{X}$ is given by

$$H_\rho(\mathbf{X}|\mathbf{X}_0) = -\sum_{x_0, x = \pm 1} P(x_0, x) \log_2[P(x|x_0)] = H[\cos^2(\theta/2)]$$

(where the conditional probability $P(x|x_0) = P(x_0, x)/P(x_0)$; $H(p) = -p\log_2 p - (1-p)\log_2(1-p)$; $0 \leq p \leq 1$ denotes the binary entropy, which is bounded by $0 \leq H(p) \leq 1$). Similarly, one gets the conditional Shannon entropy

$$H_\rho(\mathbf{Z}|\mathbf{Z}_0) = H[\cos^2(\phi/2)]$$

associated with the sequential measurement of $\mathbf{Z}_0$, $\mathbf{Z}$. Clearly, the sum of conditional Shannon entropies

$$H_\rho(\mathbf{X}|\mathbf{X}_0) + H_\rho(\mathbf{Z}|\mathbf{Z}_0) = H[\cos^2(\theta/2)] + H[\cos^2(\phi/2)]$$

beats the uncertainty bound $-2\log_2 C(\mathbf{X}, \mathbf{Z}) = 1$.

More specifically, the uncertainty relation (6.2) no longer holds for entropies of $\mathbf{X}$ and $\mathbf{Z}$ conditioned by the information in the *temporal memory* obtained by prior measurements $\mathbf{X}_0$, $\mathbf{Z}_0$. While conditioning in general reduces the information entropy i.e.,

$$H_\rho(\mathbf{X}|\mathbf{X}_0) \leq H_\rho(\mathbf{X}),\ H_\rho(\mathbf{Z}|\mathbf{Z}_0) \leq H_\rho(\mathbf{Z})$$

we prove here that the temporal correlations between the sequential measurement outcomes of $\mathbf{X}$, $\mathbf{X}_0$ and $\mathbf{Z}$, $\mathbf{Z}_0$ must necessarily be *non-classical* in order to beat the uncertainty bound of (6.2), which operates in the absence of any temporal side information.

6.3 Conditioned EUR

We proceed to prove the EUR assisted by temporal correlations. Consider a single quantum system prepared in the state ρ. In the absense of any other assisting information, the uncertainty in the observables $\mathbf{X}$ and $\mathbf{Z}$ is bounded by (6.2). A temporal memory is created by first noting down the outcome x_0 (z_0) of an observable $\mathbf{X}_0$ ($\mathbf{Z}_0$) at an earlier time before recording the measurement outcomes x (z) of $\mathbf{X}$ ($\mathbf{Z}$). Then, the ignorance about the measurement outcome of $\mathbf{X}$ conditioned on the information about $\mathbf{X}_0$ stored in temporal memory is quantified in terms of the conditional Shannon entropy $H_\rho(\mathbf{X}|\mathbf{X}_0)$:

$$\begin{aligned} H_\rho(\mathbf{X}|\mathbf{X}_0) &= H_\rho(\mathbf{X}_0, \mathbf{X}) - H_\rho(\mathbf{X}_0) \\ &= H_\rho(\mathbf{X}) - H_\rho(\mathbf{X}_0 : \mathbf{X}) \end{aligned} \tag{6.4}$$

which is expressed in terms of the mutual information entropies $H_\rho(\mathbf{X}_0 : \mathbf{X}) = H_\rho(\mathbf{X}) + H_\rho(\mathbf{X}_0) - H_\rho(\mathbf{X}, \mathbf{X}_0)$ and the unconditioned entropies $H_\rho(\mathbf{X})$. Similarly, entropy of $\mathbf{Z}$, conditioned by the outcomes of $\mathbf{Z}_0$ is given by,

$$H_\rho(\mathbf{Z}|\mathbf{Z}_0) = H_\rho(\mathbf{Z}) - H_\rho(\mathbf{Z} : \mathbf{Z}_0). \tag{6.5}$$

The entropic uncertainty relation in the presence of temporal memory is then obtained by identifying the lower bound on the sum of conditional entropies $H_\rho(\mathbf{X}|\mathbf{X}_0) + H_\rho(\mathbf{Z}|\mathbf{Z}_0)$. Combining (6.4), (6.5), using the minimum value

$$[H_\rho(\mathbf{X}) + H_\rho(\mathbf{Z})]_{\rm min} = -2\log_2 C(\mathbf{X},\mathbf{Z})$$

(as given by (6.2)) and the maximum values

$$[H_\rho(\mathbf{X}_0 : \mathbf{X})]_{\rm max}\,,\ [H_\rho(\mathbf{Z}_0 : \mathbf{Z})]_{\rm max}$$

of the mutual information entropies, we obtain,

$$\begin{aligned} H_\rho(\mathbf{X}|\mathbf{X}_0) + H_\rho(\mathbf{Z}|\mathbf{Z}_0) &\geq \max\left[0, -2\log_2 C(\mathbf{X},\mathbf{Z}) - \{H_\rho(\mathbf{X}_0 : \mathbf{X})\}_{\rm max} - \{H_\rho(\mathbf{Z}_0 : \mathbf{Z})\}_{\rm max}\right] \\ &\geq \max\left[0, -2\log_2 C(\mathbf{X},\mathbf{Z}) - H_\rho^{(\rm min)}(\mathbf{X}) - H_\rho^{(\rm min)}(\mathbf{Z})\right] \end{aligned} \quad (6.6)$$

The second line of the inequality (6.6) follows by noting that the mutual information entropy of two variables $\mathbf{X}$, $\mathbf{X}'$ can at the most be equal to the minimum of marginal entropies of $\mathbf{X}$ or $\mathbf{X}'$ [140] i.e.,

$$H(\mathbf{X} : \mathbf{X}') \leq \min[H(\mathbf{X}), H(\mathbf{X}')]$$

denoting

$$\min[H_\rho(\mathbf{X}), H_\rho(\mathbf{X}_0)] = H_\rho^{(\rm min)}(\mathbf{X}), \ \ \min[H_\rho(\mathbf{Z}), H_\rho(\mathbf{Z}_0)] = H_\rho^{(\rm min)}(\mathbf{Z})$$

we thus express

$$[H_\rho(\mathbf{X}_0 : \mathbf{X})]_{\rm max} = H_\rho^{(\rm min)}(\mathbf{X}) \ \ \text{and} \ \ [H_\rho(\mathbf{Z}_0 : \mathbf{Z})]_{\rm max} = H_\rho^{(\rm min)}(\mathbf{Z})$$

Further, since $-2\log_2 C(\mathbf{X},\mathbf{Z})$ cannot exceed $\log_2 d$ and the largest values of the marginal entropies $H_\rho^{(\rm min)}(\mathbf{X}), H_\rho^{(\rm min)}(\mathbf{Z})$ being $\log_2 d$ [140], the right hand side of the conditioned entropic uncertainty (6.6) is expressed as the maximum of the trivial value zero and $-2\log_2 C(\mathbf{X},\mathbf{Z}) - H_\rho^{(\min)}(\mathbf{X}) - H_\rho^{(\min)}(\mathbf{Z})$.

6.4 Conditioning with classical temporal correlations

Temporal correlation between the sequential outcomes x_0 and x of the observables $\mathbf{X}_0$, $\mathbf{X}$ is *classical* [141] iff the joint probabilities $P(x_0, x)$ can be expressed as a convex combination of the product of probabilities,

$$P(x_0, x) = \sum_\lambda p_\lambda\, P_\lambda(x_0)\, Q_\lambda(x), \tag{6.7}$$

$$\sum_{x_0} P_\lambda(x_0) = 1, \ \sum_x Q_\lambda(x) = 1 \tag{6.8}$$

$$\sum_\lambda p_\lambda = 1, \ \ 0 \le p_\lambda \le 1.$$

Quantum temporal memory requires that the correlation outcomes of the observables at different time instants are *not* governed by the joint probabilities of the form (6.7).

We now prove the following theorem.

Theorem: *If temporal correlations of the outcomes of* $\mathbf{X}_0$*,* $\mathbf{X}$ *and those of* $\mathbf{Z}_0$*,* $\mathbf{Z}$ *obtained from sequential measurement runs on the quantum state are* classical *(the correlation probabilities are of the form (6.7)), the sum of conditional Shannon entropies obey an* ***entropic temporal steering inequality*** [142]

$$H_\rho(\mathbf{X}|\mathbf{X}_0) + H_\rho(\mathbf{Z}|\mathbf{Z}_0) \ge -2\log_2 C(\mathbf{X},\mathbf{Z}). \tag{6.9}$$

Proof: Let us consider the conditional information for the measurement outcomes of the observable $\mathbf{X}$, given that a prior measurement $\mathbf{X}_0$ has taken the value x_0:

$$H_\rho(\mathbf{X}|\mathbf{X}_0 = x_0) = -\sum_x P(x|x_0)\,\log_2 P(x|x_0) \tag{6.10}$$

The conditional probability $P(x|x_0) = P(x_0, x)/P(x_0)$ corresponding to *classical* temporal correlations (see (6.7)) is given by,

$$\begin{aligned} P(x|x_0) &= \frac{\sum_\lambda p_\lambda\, P_\lambda(x_0)\, Q_\lambda(x)}{\sum_{\lambda'} p_{\lambda'}\, P_{\lambda'}(x_0)} \\ &= \sum_\lambda p_{\lambda,x_0}\, Q_\lambda(x) \end{aligned} \tag{6.11}$$

where we have denoted $p_{\lambda,x_0} = \frac{p_\lambda\, P_\lambda(x_0)}{\sum_{\lambda'} p_{\lambda'}\, P_{\lambda'}(x_0)}$. Note that $\sum_\lambda p_{\lambda,x_0} = 1$, and $0 \leq p_{\lambda,x_0} \leq 1$.

Consider the relative entropy $D(\mathcal{P}_{x_0}||\mathcal{Q}_{x_0})$ of the probabilitiy distributions $\mathcal{P}_{x_0}(\lambda, x) = p_{\lambda,x_0}\, Q_\lambda(x)$ and $\mathcal{Q}_{x_0}(\lambda, x) = p_{\lambda,x_0}\, P(x|x_0)$. Positivity of the relative entropy leads to the following identification [143]:

$$\begin{aligned} D(\mathcal{P}_{x_0}||\mathcal{Q}_{x_0}) &= \sum_\lambda \sum_x p_{\lambda,x_0}\, Q_\lambda(x)\, \log_2\left[\frac{Q_\lambda(x)}{P(x|x_0)}\right] \geq 0 \\ &\Rightarrow\ H_\rho(\mathbf{X}|x_0) \geq \sum_\lambda p_{\lambda,x_0}\ H^{(\lambda)}_\rho(\mathbf{X}) \end{aligned} \tag{6.12}$$

where $H^{(\lambda)}_\rho(\mathbf{X}) = -\sum_x Q_\lambda(x)\, \log_2 Q_\lambda(x)$. Thus, the average conditional information $H_\rho(\mathbf{X}|\mathbf{X}_0) = -\sum_{x_0} P(x_0)\ H_\rho(\mathbf{X}|x_0)$, $P(x_0) = \sum_x P(x, x_0) = \sum_\lambda p_\lambda\, P_\lambda(x_0)$ should obey the constraint

$$\begin{aligned} H_\rho(\mathbf{X}|\mathbf{X}_0) &\geq \sum_{x_0} P(x_0) \sum_\lambda p_{\lambda,x_0}\ H^{(\lambda)}_\rho(\mathbf{X}) \\ &\geq \sum_\lambda p_\lambda\ H^{(\lambda)}_\rho(\mathbf{X}), \end{aligned} \tag{6.13}$$

Similarly, we obtain

$$H_\rho(\mathbf{Z}|\mathbf{Z}_0) \geq \sum_\lambda p_\lambda H_\rho^{(\lambda)}(\mathbf{Z}). \tag{6.14}$$

Thus, the sum of conditional entropies are constrained by

$$\begin{aligned} H_\rho(\mathbf{X}|\mathbf{X}_0) + H_\rho(\mathbf{Z}|\mathbf{Z}_0) &\geq \sum_\lambda p_\lambda [H_\rho^{(\lambda)}(\mathbf{X}) + H_\rho^{(\lambda)}(\mathbf{Z})] \\ &= -2\log_2 C(\mathbf{X},\mathbf{Z}). \end{aligned} \tag{6.15}$$

In the second line of (6.15) we have employed the Maassen-Uffink relation $H_\rho^{(\lambda)}(\mathbf{X}) + H_\rho^{(\lambda)}(\mathbf{Z}) \geq -2\log_2 C(\mathbf{X},\mathbf{Z})$.

This identification reveals the crucial significance of *quantum temporal memory* to achieve *sharpened* predictions of incompatible observables.

6.5 An example illustrating the reduction of uncertainty due to temporal memory

We illustrate how temporal correlations assist in reducing the entropic spread of non-commuting observables by considering an example of a spin-s quantum rotor prepared initially in a state

$$\rho = \frac{1}{2s+1} \sum_{m_z=-s}^{s} |s, m_z\rangle\langle s, m_z| = \frac{\mathbb{I}_{2s+1}}{2s+1}.$$

Here $|s, m_z\rangle$ are the simultaneous eigenstates of the squared spin operator $\mathbf{S}^2 = \mathbf{S}_x^2 + \mathbf{S}_y^2 + \mathbf{S}_z^2$ and the z-component of spin $\mathbf{S}_z$ (with respective eigenvalues $s(s+1)$ and m_z); $\mathbb{I}_{2s+1}$ is the $(2s+1)\times(2s+1)$ identity matrix.

Measurement of non-commuting observables $\mathbf{X} = \mathbf{S}_x$ and $\mathbf{Z} = \mathbf{S}_z$ results in the probabilities of outcomes $-s \leq m_x, m_z \leq s$ as,

$$P(m_x) = \mathrm{Tr}[\rho\, \mathbf{\Pi}_{m_x}] = \frac{1}{2s+1}; P(m_z) = \mathrm{Tr}[\rho\, \mathbf{\Pi}_{m_z}] = \frac{1}{2s+1}$$

where $\mathbf{\Pi}_m$ denotes the projection operator of the corresponding observable. The *spread* in the completely random measurement outcomes is revealed in terms of the corresponding Shannon entropies of measurement $H_\rho(\mathbf{X}) = \log_2(2s+1)$ and $H_\rho(\mathbf{Z}) = \log_2(2s+1)$, which obey the trade-off relation (6.2) – the largest value of the uncertainty bound on the right hand side being $\log_2(2s+1)$.

In order to identify how the EUR for $\mathbf{S}_x$ and $\mathbf{S}_z$, assisted by prior conditioning, can reveal enhanced precision of the observables, we consider dynamical evolution of the system governed by the Hamiltonian $\mathbf{H} = \omega\, \mathbf{S}_y$. Under the Hamiltonian dynamics, the evolution of z component of spin is given by

$$\mathbf{S}_z(t) = e^{i\mathbf{S}_y \omega t}\, \mathbf{S}_z\, e^{-i\mathbf{S}_y \omega t} = \mathbf{S}_z\, \cos(\omega\, t) + \mathbf{S}_x\, \sin(\omega\, t)$$

We consider sequential measurement of $\mathbf{S}_z(t)$ at different times as follows:

In the first run, the observable $\mathbf{S}_z(t)$ is measured at time $t = t_{x0}$ and consequently at $t_x = \pi/2\omega$. This corresponds to sequential measurement of observables

$$\mathbf{X}_0 = \mathbf{S}_z \cos(\omega\, t_{x0}) + \mathbf{S}_x \sin(\omega t_{x0}) \quad \text{and} \quad \mathbf{X} = \mathbf{S}_x$$

with a dimensionless time separation $\theta = \omega t_{x0} - \pi/2$.
The sequential measurements enable the observer to record the temporal correlation probabilities $P(m_{x_0}, m_x; \theta)$ of the outcomes $-s \leq m_{x_0}, m_x \leq s$ of the observables $\mathbf{X}_0 = \mathbf{S}_z(t_{x0})$ and $\mathbf{X} = \mathbf{S}_x$.
Then, in one more round of observations, $\mathbf{S}_z$ is measured sequentially at two

different time instants t_{z0} and $t_z = \pi/\omega$.That is, a measurement of

$$\mathbf{Z}_0 = \mathbf{S}_z\cos(\omega\, t_{z0}) + \mathbf{S}_x\sin(\omega t_{z0}) \;\; \text{and} \;\; \mathbf{Z} = \mathbf{S}_z$$

separated by a dimensionless time parameter $\phi = \omega\, t_{z0} - \pi$ is performed and the correlation probabilities $P(m_{z_0}, m_z; \phi)$ of the $(2s+1)^2$ outcomes $-s \le m_{z_0}, m_z \le s$ are noted down.

The probabilities of sequential measurement outcomes of $\mathbf{S}_z(t)$ at two different times t_{x0} and $t_x = \pi/2\omega$ are given by [129],

$$\begin{aligned}
P(m_{x_0}, m_x; \theta) &= P(m_{x_0}; t_{x0})\, P(m_x; t_x | m_{x_0}; t_{x0}) \\
&= \mathrm{Tr}[\rho\, \mathbf{\Pi}_{m_{x_0}}(t_{x0})]\, \frac{\mathrm{Tr}[\mathbf{\Pi}_{m_{x_0}}(t_{x0})\rho\, \mathbf{\Pi}_{m_{x_0}}(t_{x0})\, \mathbf{\Pi}_{m_x}(t_x)]}{P(m_{x_0}; t_{x0})} \\
&= \frac{1}{2s+1}\, \mathrm{Tr}[\mathbf{\Pi}_{m_{x_0}}(t_{x0})\, \mathbf{\Pi}_{m_x}(t_x)] \\
&= \frac{1}{2s+1}\, |\langle\, s, m_{x_0}| e^{-i\omega(t_{x0}-t_x)\,\mathbf{S}_y}\, |s, m_x\rangle|^2 \\
&= \frac{1}{2s+1}\, |\, d^s_{m_x, m_{x_0}}(\theta)|^2 \qquad (6.16)
\end{aligned}$$

where $\mathbf{\Pi}_m(t) = e^{i\omega t\,\mathbf{S}_y}\, |s, m\rangle\langle s, m|\, e^{-i\omega t\,\mathbf{S}_y}$ is the projection operator measuring the outcome m of the spin component $\mathbf{S}_z(t)$; and $d^s_{m_x, m_{x0}}(\theta) = \langle s, m_x| e^{-i\theta\,\mathbf{S}_y}|s, m_{x_0}\rangle$ are the matrix elements of the $2s+1$ dimensional irreducible representation of rotation [118] about y-axis by an angle $\theta = \omega(t_{x0} - t_x)$.

The marginal probability associated with measuring $\mathbf{S}_z(t_{x_0})$ is readily obtained as

$$P(m_{x_0}; t_{x_0}) = \mathrm{Tr}[\rho\, \mathbf{\Pi}_{m_{x_0}}(t_{x0})] = \frac{1}{2s+1}$$

Similarly, the correlation probabilities in the second run of sequential measurements are obtained as, $P(m_{z_0}, m_z; \phi) = \frac{1}{2s+1} \,|\, d^s_{m_z, m_{z_0}}(\phi)|^2$ and the marginal probabilities $P(m_{z_0}; t_{z_0}) = 1/(2s+1)$.

The conditional entropies of measurement (which depend only on the time separations $\theta,\ \phi$) $H_\rho(\mathbf{X}|\mathbf{X}_0) = \mathcal{H}(\theta)$ and $H_\rho(\mathbf{Z}|\mathbf{Z}_0) = \mathcal{H}(\phi)$ are given by,

$$\begin{aligned}\mathcal{H}(\theta) &= -\frac{1}{2s+1} \sum_{m_{x_0}, m_x} |d^s_{m_{x_0}, m_x}(\theta)|^2 \, \log_2 |d^s_{m_{x_0}, m_x}(\theta)|^2 \\ \mathcal{H}(\phi) &= -\frac{1}{2s+1} \sum_{m_{z_0}, m_z} |d^s_{m_{z_0}, m_z}(\phi)|^2 \, \log_2 |d^s_{m_{z_0}, m_z}(\phi)|^2.\end{aligned} \tag{6.17}$$

We define a quantity $\mathcal{M}_s(\theta, \phi)$ as the difference between the sum of conditional entropies and the Maassen-Uffink uncertainty bound $-2\log_2 C(\mathbf{X}, \mathbf{Z})$

$$\begin{aligned}\mathcal{M}_s(\theta, \phi) &= H_\rho(\mathbf{X}|\mathbf{X}_0) + H_\rho(\mathbf{Z}|\mathbf{Z}_0) + 2\,\log_2 C(\mathbf{X}, \mathbf{Z}) \\ &= \mathcal{H}(\theta) + \mathcal{H}(\phi) + 2\,\log_2 C(\mathbf{X}, \mathbf{Z})\end{aligned} \tag{6.18}$$

in order to demonstrate improved precision in the measurement of the spin components $\mathbf{X} = \mathbf{S}_x$ and $\mathbf{Z} = \mathbf{S}_z$.

While a *classical* temporal side information results in $\mathcal{M}_s(\theta, \phi)$ being necessarily positive, presence of a *quantum temporal memory*, created by appropriate sequential measurements, can reveal itself in non-positive values of $\mathcal{M}_s(\theta, \phi)$.

In Fig. 6.1, we have plotted the quantity $\mathcal{M}_s(\theta, \phi)$ as a function of θ and ϕ for spin values $s = 1/2, 1, 3/2$ and 2. The results clearly demonstrate reduction in the uncertainties of the non-commuting spin components $\mathbf{S}_x,\ \mathbf{S}_z$ (in the region where $\mathcal{M}_s$ is negative) – in the presence of a *quantum temporal memory.* We note that the range of time-separation θ and ϕ, over which $\mathcal{M}_s$ assumes negative values, reduces with the increase of spin s – thus indicating a quantum to classical transition of the temporal memory in the limit of large spin s.

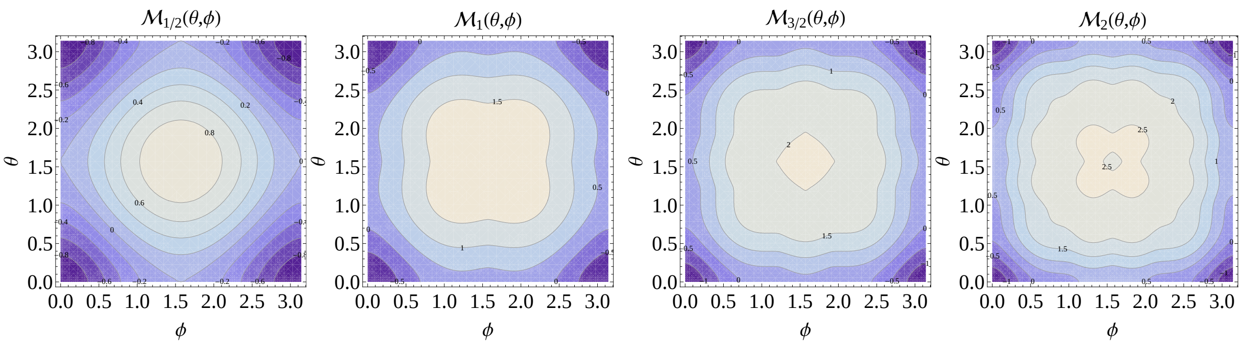

Figure 6.1: A contour plot of the quantity $\mathcal{M}_s(\theta, \phi)$ (defined by (6.18)) constructed based on two runs of sequential measurements of the spin component $\mathbf{S}_z(t)$ of a quantum rotor, with dimensionless time separations θ and ϕ for spin values $s = 1/2$, $s = 1$, $s = 3/2$, $s = 2$. Negative values of $\mathcal{M}_s$ imply that the uncertainties about the outcomes of the spin components $\mathbf{S}_x$, $\mathbf{S}_z$ (conditioned on the information of outcomes of $\mathbf{S}_z(t_{x0})$, $\mathbf{S}_z(t_{z0})$ of prior measurements) get reduced in the presence of quantum temporal memory. It may be seen that the range of values of the dimensionless time-separation parameters θ and ϕ, over which $\mathcal{M}_s$ is negative, reduces with the increase of spin s indicating a quantum to classical transition of temporal correlations. All quantities are dimensionless.

6.6 Conclusions

Uncertainty principle reflects the inevitability inbuilt within the quantum framework in realizing deterministic outcomes for non-commuting observables of a particle. Entropic uncertainty relation [6] captures the trade-off in the *spread* of the outcomes of incompatible observables. However, a deterministic prediction is ensured when the particle is entangled maximally with another party. Berta et al., [7] brought out the subtle interplay between uncertainty and entanglement by extending the entropic uncertainty principle in the presence of quantum side information. In this work, we have explored the interesting association between temporal correlations and uncertainty. Our entropic uncertainty relation reveals that the presence of quantum temporal side information too plays a significant role in beating the uncertainty bound. More specifically, our results offer a unified view that a prior *quantum* knowledge, achieved with the help of suitable spatially/temporally separated observations, empower a deterministic prediction of non-commuting observables.

Chapter 7

Joint measurability, steering and entropic uncertainty

There has been a surge of research activity recently on the role of joint measurability of unsharp observables on non-local features viz., violation of Bell inequality and EPR steering. Here, we investigate the entropic uncertainty relation for a pair of non-commuting observables (of Alice's system), when an entangled quantum memory of Bob is restricted to record outcomes of jointly measurable POVMs. We show that with this imposed constraint of joint measurability at Bob's end, the entropic uncertainties associated with Alice's measurement outcomes – conditioned by the results registered at Bob's end – obey an entropic steering inequality. Thus, Bob's non-steerability is intrinsically linked with his inability in predicting the outcomes of Alice's pair of non-commuting observables with better precision, even when they share an entangled state.

7.1 Introduction

In the classical domain, physical observables commute with each other and they can all be jointly measured. In contrast, measurements of observables, which do not commute are usually declared to be *incompatible* in the quantum scenario. However, the notion of *compatibility* of measurements is captured entirely by *commutativity* of the observables if one restricts only to *sharp* projective valued (PV) measurements. In an extended framework, which include measurements of *unsharp* generalized observables, comprised of positive operator valued measures (POVM), the concept of *joint measurability* gets delinked from that of commutativity [8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Though non-commuting observables do not admit simultaneous *sharp* values through their corresponding PV measurements, it is possible to assign *unsharp* values jointly to compatible positive operator valued (POV) observables. Active research efforts are dedicated [8, 10, 11, 12, 14, 144, 145, 18, 19] to explore clear, operationally significant criteria for the *joint measurability* of two or more POVMs and also to identify that incompatible measurements, which cannot be implemented jointly, are necessary to bring out *non-classical* features. In this context, it has already been recognized [8, 10, 11, 12, 14, 144, 18, 19] that if one merely confines to local compatible POVMs on parts of an entangled quantum system, it is not possible to witness non-local quantum features like steering (see Chapter 1) and violation of Bell inequality. More specifically, incompatible measurements are instrumental in bringing to surface the violations of various no-go theorems in the quantum world.

Here, we investigate the entropic uncertainty relation associated with Alice's measurements of a pair of non-commuting discrete observables with d outcomes, in the presence of Bob's quantum memory [7] – by restricting to compatible (jointly measurable) POVMs at Bob's end. We first establish that the sum of entropies of Alice's measurement results, when conditioned by the outcomes of compatible *unsharp* POVMs recorded in Bob's quantum memory, is constrained to *obey* an *entropic steering inequality* derived in [146, 147]. This essentially brings out the intrinsic equivalence between the violation of an entropic steering inequality and the possibility of reducing the entropic uncertainty bound of a pair of non-commuting observables with the help of an entangled quantum memory. And as violation of a steering inequality requires

[18, 19] that (i) the parties share a steerable entangled state and also that (ii) the measurements by one of the parties (Bob) [148] is incompatible, it becomes evident that information stored in Bob's entangled quantum memory is of no use in reducing the uncertainty of Alice's pair of non-commuting observables, when Bob can measure only compatible POVMs.

To this end, following the notion of joint measurability of POVMs already introduced in the introductory chapter and the Entropic uncertainty relation for Alice's pair of discrete observables in the presence of Bob's quantum memory discussed in Chapter 6, we show that when Bob is restricted to employ only jointly measurable POVMs, it is not possible to achieve enhanced precision for predicting Alice's measurement outcomes, even if entangled state is shared between them.

7.2 Joint Measurability

We begin by recollecting the brief outline of joint measurability of observables in terms of POVMs. Mathematically, POVM is a set $\mathbb{E} = \{\mathbf{E}(x)\}$ comprising of positive self-adjoint operators $0 \leq \mathbf{E}(x) \leq 1$, called *effects*, satisfying $\sum_x \mathbf{E}(x) = \mathbb{I}$; x denotes the outcomes of measurement and $\mathbb{I}$ is the identity operator. When a quantum system is prepared in the state ρ, measurement of $\mathbf{E}$ gives an outcome x with probability $p(x) = \mathrm{Tr}[\rho\, \mathbf{E}(x)]$. If $\{\mathbf{E}(x)\}$ is a set of complete, orthogonal projectors, then the measurement reduces to the special case of PV measurement.

A finite collection of POVMs $\mathbf{E}_1, \mathbf{E}_2, \ldots, \mathbf{E}_n$ is said to be jointly measurable (or compatible), if there exists a *grand* POVM $\mathbb{G} = \{\mathbf{G}(\lambda);\ 0 \leq \mathbf{G}(\lambda) \leq 1, \sum_\lambda \mathbf{G}(\lambda) = \mathbb{I}\}$ from which the observables $\mathbf{E}_i$ can be obtained by post-processing as follows. Suppose a measurement of the global POVM $\mathbf{G}$ is carried out in a state ρ and the probability of obtaining the outcome λ is denoted by $p(\lambda) = \mathrm{Tr}[\rho\,\mathbf{G}(\lambda)]$. If the effects $\mathbf{E}_i(x_i)$ constituting the POVM $\mathbb{E}_i$ can be obtained as *marginals* of the *grand* POVM $\mathbb{G} = \{\,\mathbf{G}(\lambda), \lambda \equiv \{x_1, x_2, \ldots\}$, (where λ corresponds to a collective index $\{x_1, x_2, \ldots\}$) i.e., if there exists a grand POVM $\mathbb{G}$ such that [12, 19, 149]

$$\begin{aligned}
\mathbf{E}_1(x_1) &= \sum_{x_2, x_3, \ldots} \mathbf{G}(x_1, x_2, \ldots, x_n) \\
\mathbf{E}_2(x_2) &= \sum_{x_1, x_3, \ldots} \mathbf{G}(x_1, x_2, \ldots, x_n) \\
&\vdots \\
\mathbf{E}_n(x_n) &= \sum_{x_1, x_3, \ldots} \mathbf{G}(x_1, x_2, \ldots, x_n),
\end{aligned} \tag{7.1}$$

the POVMs $\mathbf{E}_1, \mathbf{E}_2, \ldots, \mathbf{E}_n$ are said to be jointly measurable [8]. Thus, a collection of compatible POVMs $\mathbf{E}_1, \mathbf{E}_2, \ldots, \mathbf{E}_n$ is obtained from a global POVM $\mathbf{G}$ via post processing of the form (7.1). We emphasize once again that compatibility of POVMs does not require their commutativity, but it demands the existence of a global POVM.

More specifically, measurements of compatible POVMs $\mathbf{E}_i$ can be interpreted in terms of a single *grand* POVM $\mathbf{G}$ (i.e., given the positive numbers $p(x_i|i, \lambda)$, one can construct the probabilities of measuring compatible POVMs $\mathbf{E}_i$ solely based on the results of measurement of $\mathbf{G}$, i.e,

$$p(x_i|i) = \mathrm{Tr}[\rho\,\mathbf{E}_i(x_i)] = \mathrm{Tr}[\rho \sum_{\lambda} p(x_i|i, \lambda)\, G(\lambda)] = \sum_{\lambda} p(\lambda)\, p(x_i|i, \lambda).$$

Here, x_i is the outcome of measuring the POV observable $\mathbf{E}_i(x_i)$.)

Reconciling to joint measurability within quantum theory results in subsequent manifestation of classical features [19]. In particular, as measurement of a single *grand* POVM can be used to construct results of measurements of all compatible POVMs, joint measurability entails a joint probability distribution for all compatible observables (though for *unsharp* values of the observables) in *every* quantum state. Existence of joint probabilities in turn implies that the set of all Bell inequalities are satisfied [73], when only compatible measurements are employed. Wolf et al. [14] have shown that incompatible measurements of a pair of POVMs with dichotomic outcomes are necessary and sufficient for the violation of Clauser-Horne-Shimony-Holt (CHSH) Bell inequality. Further, Quintino et al. [18] and Uola et al. [19] have established a more general result that a set of POVMs (with arbitrarily many outcomes) are not jointly measurable if and only if they are useful for non-local quantum steering. It is of interest to explore the limitations imposed by joint measurability on quantum information tasks. In the following, we study the implications of joint measurability on entropic uncertainty relation in the presence of quantum memory.

7.3 Entropic uncertainty relation in the presence of quantum memory

The Shannon entropies $H(\mathbf{X}) = -\sum_x p(x)\log_2 p(x)$, $H(\mathbf{Z}) = -\sum_z p(z)\log_2 p(z)$, associated with the probabilities $p(x) = \mathrm{Tr}\,[\rho\,\mathbf{E}_{\mathbf{X}}(\mathrm{x})]$, $p(z) = \mathrm{Tr}\,[\rho\,\mathbf{E}_{\mathbf{Z}}(\mathrm{z})]$ of measurement outcomes x, z of a pair of POV observables $\mathbf{X} \equiv \{E_{\mathbf{X}}(x) |\, 0 \leq \mathbf{E}_{\mathbf{X}} \leq 1;\ \sum_x \mathbf{E}_{\mathbf{X}} = \mathbb{I}\}$, $\mathbf{Z} \equiv \{\mathbf{E}_{\mathbf{Z}}(z) |\, 0 \leq E_{\mathbf{Z}} \leq 1;\ \sum_z \mathbf{E}_{\mathbf{Z}} = \mathbb{I}\}$, quantify the uncertainties of predicting the measurement outcomes in a quantum state ρ. Trade-off between the entropies of observables $\mathbf{X}$ and $\mathbf{Z}$ in a finite level quantum system is quantified by the Entropic Uncertainty Relation

[6, 150]:

$$H(\mathbf{X}) + H(\mathbf{Z}) \geq -2\log_2 C(\mathbf{X}, \mathbf{Z}), \tag{7.2}$$

where $C(\mathbf{X}, \mathbf{Z}) = \max_{\mathrm{x,z}} ||\sqrt{\mathbf{E_X}(\mathrm{x})}\,\sqrt{\mathbf{E_Z}(\mathrm{z})}||$. (Here, $||\mathbf{A}|| = \mathrm{Tr}[\sqrt{\mathbf{A}^\dagger\,\mathbf{A}}]$).

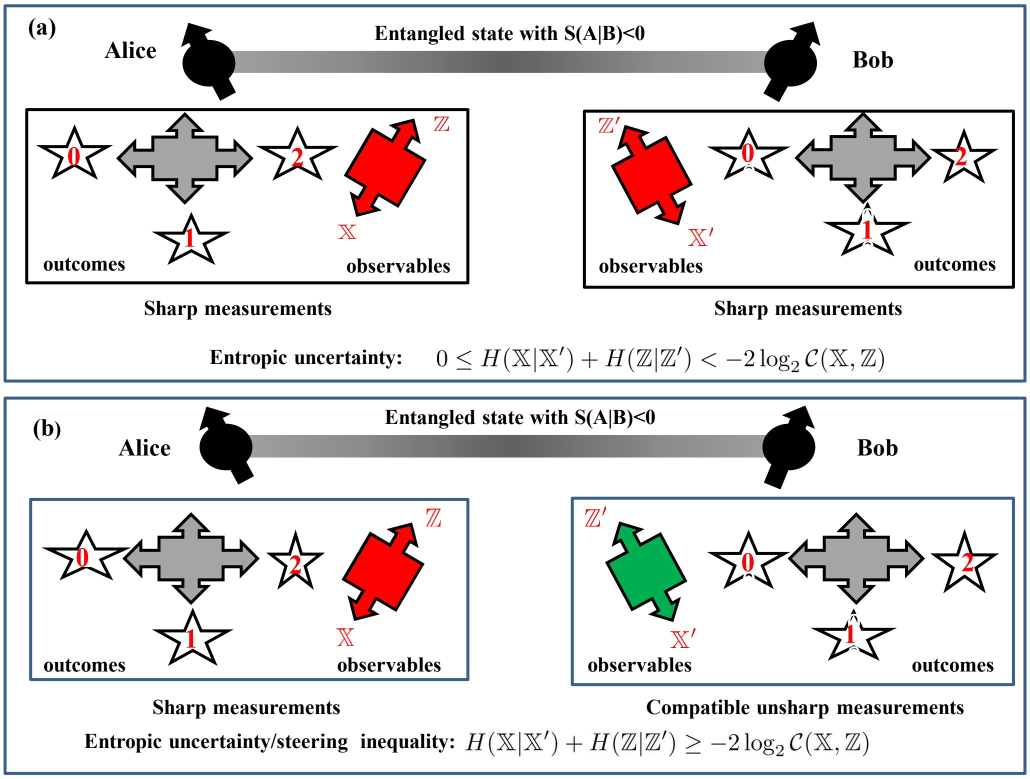

Figure 7.1: Alice and Bob decide on a pair of non-commuting observables $\mathbf{X}$, $\mathbf{Z}$. Bob prepares an entangled state ρ_{AB} and sends the subsystem A to Alice. Alice measures $\mathbf{X}$ or $\mathbf{Z}$ randomly and conveys her choice to Bob. At his end, Bob measures $\mathbf{X}'$ or $\mathbf{Z}'$ and predicts Alice's outcomes. (a) Alice and Bob both perform sharp measurements. In this case, Bob can predict Alice's outcomes with an enhanced precision, as the entropic uncertainty bound (see (7.4)) can be smaller than $-2\log_2 C(\mathbf{X}, \mathbf{Z})$, when the conditional von Neumann entropy $S(A|B)$ of the entangled state ρ_{AB} is negative. (b) Alice performs sharp measurements of the chosen observables $\mathbf{X}$ or $\mathbf{Z}$, while Bob correspondingly records outcomes of compatible unsharp measurements of $\mathbf{X}'$ or $\mathbf{Z}'$. In the joint measurability range of $\mathbf{X}'$, $\mathbf{Z}'$, Bob's quantum memory fails to predict Alices outcomes more precisely because the sum of entropies $H(\mathbf{X}|\mathbf{X}')$, $H(\mathbf{Z}|\mathbf{Z}')$ is constrained to obey an entropic steering inequality: $H(\mathbf{X}|\mathbf{X}') + H(\mathbf{Z}|\mathbf{Z}') \geq -2\log_2 C(\mathbf{X}, \mathbf{Z})$.

Consider the following uncertainty game [7]: two players Alice and Bob agree to measure a pair of observables $\mathbf{X}$ and $\mathbf{Z}$. Bob prepares a quantum state of his choice and sends it to Alice. Alice measures $\mathbf{X}$ or $\mathbf{Z}$ randomly and communicates her choice of measurements to Bob. To win the game, Bob's initial preparation of the quantum state should be such that he is able to predict Alice's measurement outcomes of the chosen pair of observables $\mathbf{X}$ or $\mathbf{Z}$ with as much precision as possible, when Alice announces which of the pair of observables is measured. In other words, Bob's task is to minimize the uncertainties in the measurements of a pair of observables $\mathbf{X}$, $\mathbf{Z}$ that were agreed upon initially, with the help of an optimal quantum state. The uncertainties of $\mathbf{X}$, $\mathbf{Z}$ are bounded as in (7.2), when Bob has only classical information about the state. On the other hand, with the help of a quantum memory (where Bob prepares an entangled state and sends one part of the state to Alice) Bob can beat the uncertainty bound of (7.2).

The entropic uncertainty relation, when Bob possesses a quantum memory, was put forth by Berta et al., [7]:

$$S(\mathbf{X}|B) + S(\mathbf{Z}|B) \geq -2\log_2 C(\mathbf{X},\mathbf{Z}) + S(A|B), \tag{7.3}$$

where $S(\mathbf{X}|B) = S\left(\rho_{AB}^{(\mathbf{X})}\right) - S(\rho_B)$, $S(\mathbf{Z}|B) = S\left(\rho_{AB}^{(\mathbf{Z})}\right) - S(\rho_B)$ are the conditional von Neumann entropies of the post measured states $\rho_{AB}^{(\mathbf{X})} = \sum_x |x\rangle\langle x| \otimes \rho_B^{(x)}$ with $\rho_B^{(x)} = \mathrm{Tr}_A[\rho_{AB}(\mathbf{E}_\mathbf{X}(x) \otimes \mathbb{I}_B)]$ and $\rho_{AB}^{(\mathbf{Z})} = \sum_z |z\rangle\langle z| \otimes \rho_B^{(z)}$ with $\rho_B^{(z)} = \mathrm{Tr}_A[\rho_{AB}(\mathbf{E}_\mathbf{Z}(z) \otimes \mathbb{I}_B)]$, obtained after Alice's measurements of $\mathbf{X}$, $\mathbf{Z}$ on her system. (Here, the measurement outcomes of the effects $\mathbf{E}_\mathbf{X}(x)$ ($\mathbf{E}_\mathbf{Z}(z)$) are encoded in an orthonormal basis $\{|x\rangle\}$ ($\{|z\rangle\}$) and the probability of measurement outcome x (z) is given by $p(x) = \mathrm{Tr}[\rho_\mathrm{B}^{(\mathrm{x})}]$ ($p(z) = \mathrm{Tr}[\rho_\mathrm{B}^{(\mathrm{z})}]$); $S(A|B) = S(\rho_{AB}) - S(\rho_B)$ is the conditional von Neumann entropy of the state ρ_{AB}).

When Alice's system is in a maximally entangled state with Bob's quantum memory, the second term on the right hand side of (7.3) takes the value $S(A|B) = -\log_2 d$ and as $-2\log_2 C(\mathbf{X},\mathbf{Z}) \leq \log_2 d$ (which can be realized when Alice employs pairs of unbiased projective measurements [151]), a trivial lower bound of zero is obtained in the entropic uncertainty relation. In other words, by sharing an entangled state with Alice, Bob can beat the uncertainty bound given by (7.2) and can predict the outcomes of a pair of observables $\mathbf{X}$, $\mathbf{Z}$ with improved precision by performing suitable measurements on his part of the state.

Let us denote $\mathbf{X}'$ or $\mathbf{Z}'$ as the POVMs which Bob choses to measure, when Alice announces her choice of measurements of the observables $\mathbf{X}$ or $\mathbf{Z}$. The uncertainty relation (7.3) can be recast in terms of the conditional entropies [152] $H(\mathbf{X}|\mathbf{X}')$, $H(\mathbf{Z}|\mathbf{Z}')$ of Alice's measurement outcomes of the observables $\mathbf{X}$, $\mathbf{Z}$, conditioned by Bob's measurements of $\mathbf{X}'$, $\mathbf{Z}'$. As measurements always increase entropy i.e., $H(\mathbf{X}|\mathbf{X}') \geq S(\mathbf{X}|B)$, $H(\mathbf{Z}|\mathbf{Z}') \geq S(\mathbf{Z}|B)$, the entropic uncertainty relation in the presence of quantum memory can be expressed in the form [7]

$$H(\mathbf{X}|\mathbf{X}') + H(\mathbf{Z}|\mathbf{Z}') \geq -2\log_2 C(\mathbf{X}, \mathbf{Z}) + S(A|B). \tag{7.4}$$

On the other hand, the conditional entropies $H(\mathbf{X}|\mathbf{X}')$, $H(\mathbf{Z}|\mathbf{Z}')$ are constrained to obey the *entropic steering inequality* [146, 147],

$$H(\mathbf{X}|\mathbf{X}') + H(\mathbf{Z}|\mathbf{Z}') \geq -2\log_2 C(\mathbf{X}, \mathbf{Z}) \tag{7.5}$$

if Bob is unable to remotely steer Alice's state by his local measurements. And, as has been proved recently [18, 19], measurements at Bob's end can result in the violation of any steering inequality if and only if they are incompatible (in addition that the state shared between Alice and Bob is entangled so as to be steerable). In other words, the entropic inequality (7.5) can never be violated if Bob's measurements $\mathbf{X}'$, $\mathbf{Z}'$ are compatible. Violation of the steering inequality (7.5) would in turn correspond to a reduced bound in the entropic uncertainty relation (7.4) in the presence of quantum memory (reduction in the bound is realized when Alice and Bob share an entangled state with $S(A|B) < 0$). If Bob is constrained to perform compatible measurements on his system, he cannot beat the uncertainty bound of (7.2) and win the *uncertainty game* by predicting the outcomes as precisely as possible, even when he shares a maximally entangled state with Alice (See Fig. 7.1).

7.3.1 An example

We illustrate the entropic uncertainty relation (7.3) for a pair of qubit observables $\mathbf{X} = |0\rangle\langle 1| + |1\rangle\langle 0|$ and $\mathbf{Z} = |0\rangle\langle 0| - |1\rangle\langle 1|$, when Alice and Bob share a maximally entangled two-qubit state $|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|0_A,\ 1_B\rangle - |1_A,\ 0_B\rangle\right)$. Alice performs one of the *sharp* PV measurements

$$\begin{aligned}\mathbf{\Pi}_{\mathbf{X}}(x) &= \frac{1}{2}\left(\mathbb{I} + x\,\mathbf{X}\right),\ x = \pm 1,\\ \mathbf{\Pi}_{\mathbf{Z}}(z) &= \frac{1}{2}\left(\mathbb{I} + z\,\mathbf{Z}\right),\ z = \pm 1,\end{aligned} \tag{7.6}$$

of the observables $\mathbf{X}$ or $\mathbf{Z}$ randomly on her qubit and announces her choice of measurement, while Bob tries to predict Alice's outcomes by performing *unsharp* compatible measurements of the POVMs $\{\mathbf{E}_{\mathbf{X}'}(x'),\ x' = \pm 1\}$ or $\{E_{\mathbf{Z}'}(z'),\ z' = \pm 1\}$ on his qubit. The effects $\mathbf{E}_{\mathbf{X}'}(x'), \mathbf{E}_{\mathbf{Z}'}(z')$ (corresponding to binary *unsharp* measurements of the observables $\mathbf{X}'$, $\mathbf{Z}'$) are given by,

$$\begin{aligned}\mathbf{E}_{\mathbf{X}'}(x') &= \frac{1}{2}\left(\mathbb{I} + \eta\, x'\,\mathbf{X}'\right),\\ \mathbf{E}_{\mathbf{Z}'}(z') &= \frac{1}{2}\left(\mathbb{I} + \eta\, z'\,\mathbf{Z}'\right),\end{aligned} \tag{7.7}$$

where x', z' are the measurement outcomes and $0 \leq \eta \leq 1$ denotes the *unsharpness* of the fuzzy measurements. Clearly, when $\eta = 1$, the POVM elements $\mathbf{E}_{\mathbf{X}'}(x')$, $E_{\mathbf{Z}'}(z')$ reduce to their corresponding *sharp* PV versions (see (7.6)) $\mathbf{\Pi}_{\mathbf{X}'}(x'), \mathbf{\Pi}_{\mathbf{Z}'}(z')$.

The joint probabilities $p(x, x')$ (or $p(z, z')$) of Alice's *sharp* outcome x (or z)

and Bob's *unsharp* outcome x' (or z'), when they both choose to measure the same observable $\mathbf{X}$ (or $\mathbf{Z}$) at their ends, is obtained to be,

$$\begin{aligned} p(x,x') &= \langle\psi_{AB}|\mathbf{\Pi_X}(x)\otimes \mathbf{E_X}(x')|\psi_{AB}\rangle \\ &= \frac{1}{4}\,(1-\eta\, x\, x')) \\ p(z,z') &= \langle\psi_{AB}|\Pi_{\mathbf{Z}}(z)\otimes E_{\mathbf{Z}}(z')|\psi_{AB}\rangle \\ &= \frac{1}{4}\,(1-\eta\, z\, z')) \end{aligned} \tag{7.8}$$

While the right-hand side of the entropic uncertainty relation (7.4) reduces to zero in this case, the left-hand side can be simplified (see [152]) to obtain,

$$\begin{aligned} H(\mathbf{X}|\mathbf{X}')+H(\mathbf{Z}|\mathbf{Z}') &= -\sum_{x,x'=\pm 1} p(x,x')\log_2 p(x|x') - \sum_{z,z'=\pm 1} p(z,z')\log_2 p(z|z') \\ &= 2\,H[(1+\eta)/2] \end{aligned} \tag{7.9}$$

where $H(p) = -p\,\log_2 p - (1-p)\,\log_2(1-p)$ is the binary entropy. As the binary entropy function $H[(1+\eta)/2]$ vanishes only when $\eta = 1$, the trivial lower bound of the uncertainty relation (7.4) can be reached if Bob too performs *sharp* PV measurements of the observables $\mathbf{X}$ and $\mathbf{Z}$ at his end. In other words, Bob can predict the outcomes of Alice's measurements of $\mathbf{X}$ and $\mathbf{Z}$ precisely when he employs *sharp* PV measurements of the same observables. But *sharp* measurements of $\mathbf{X}$ and $\mathbf{Z}$ are not compatible. The joint measurability of the unsharp POVMs $\{\mathbf{E_X}(x')\}$ and $\{\mathbf{E_Z}(z')\}$ sets the limitation [8, 12] $\eta \leq 1/\sqrt{2}$ on the *unsharpness* parameter (see Appendix B).

If Bob confines only to the joint measurability range $0 \leq \eta \leq 1/\sqrt{2}$, the entropic steering inequality (7.5)

$$H(\mathbf{X}|\mathbf{X}')+H(\mathbf{Z}|\mathbf{Z}') \geq 1 \tag{7.10}$$

is always satisfied [153]. In turn, it implies that Bob cannot beat the entropic uncertainty bound of (7.2) – even with the help of an entangled state he shares with Alice – if he is constrained to employ jointly measurable POVMs.

The result demonstrated here in the specific example of $d = 2$ (qubits) holds in principle for any d dimensional POVMs. An illustration in the d dimensional example, however, requires that the compatibility/incompatibility range of the unsharpness parameter η is known. However, optimal values of the unsharpness parameter (η) of a set of POVMs is known only for qubits (See Appendix B).

7.4 Conclusion

Measurement outcomes of a pair of non-commuting observables reveal a trade-off, which is quantified by uncertainty relations. Entropic uncertainty relation [6] constrains the sum of entropies associated with the probabilities of outcomes of a pair of observables. An extended entropic uncertainty relation [7] brought out that it is possible to beat the lower bound on uncertainties when the system is entangled with a quantum memory. In this Chapter, we have explored the entropic uncertainty relation when the entangled quantum memory is restricted to record the outcomes of jointly measurable POVMs only. With this constraint on the measurements, the entropies satisfy an entropic steering inequality [146]. Thus, we identify that an entangled quantum memory, which is limited to record results of compatible POVMs, cannot assist in beating the entropic uncertainty bound.

Chapter 8

Conclusions and future directions

Finally, I form the overall conclusions and possible future directions based on the work carried out as a part of this thesis. I have tried to explore foundational notions like locality, macro-realism, non-contextuality, uncertainty, in terms of the underlying structure of probabilities, based on the theoretical perspective of quantum information. Starting from the observation of the reflection of the uncertainties in the classical realm, in the classical limit, when the (intrinsically statistical) quantum mechanical wave function is paralleled to the corresponding classical ensemble but not to an individual particle, I have formulated the entropic version of the Leggett-Garg inequality. This is the first time that entropic considerations have been applied to study macro realism. Furthermore, I have worked on the framing of the necessary and sufficiency criterion for the non-classicality of the probability distributions arising in the various (quantum) temporal and spatial scenarios in terms of the moment matrix and moment inversion tests. The precision guaranteed in the measurement of two non-commuting observables when they are sequentially measured on a single quantum system due to the presence of temporal correlations is captured in the Chapter 6. Lastly, the interplay amongst the concepts of uncertainty, quantum steering and joint measurability is also explored wherein we have shown that the presence of the tradeoff term in the entropic uncertainty relation (calculated on an entangled state) is attributed to the projective measurements (measurement incompatibility) and would vanish if jointly measurable set of POVMs are employed.

Further, as part of the future work, we would like to explore Quasi Probability Distributions(QPD) of discrete non-commuting observables using the moments of their compatible POVMs. Quantum mechanical QPDs have been developed for non-commuting observables based on different operator correspondence rules. As they can assume negative values, one cannot treat them as true probabilities from the point of view of classical probability theory. Nevertheless, these functions offer a classical-like perspective of quantum scenario. We would like to investigate how bona fide joint probability distributions result when the POVMs turn out to be compatible.

Furthermore, we wish to investigate quantum thermodynamic work distribution function and the associated Crooks-Jarzynski fluctuation relation (and hence the second law of thermodynamics) when the initial and final energy measurements are compatible. This study sheds light on the emergence of classicality from a quantum scenario, when joint measurability is invoked. We also plan to investigate contextuality, nonlocality, uncertainty relations and information theoretic quantum thermodynamics aspects based on the joint probability distributions, within the purview of joint measurability.

Appendix A

Joint Probability Distribution for observables

A.1 Joint probability distribution for a pair of commuting observables

Consider two commuting observables $\mathbf{A}$ and $\mathbf{B}$, whose eigenvalues are denoted respectively by a, b. Quantum mechanics predicts the joint probability of obtaining the outcomes a, b (in an arbitrary quantum state ρ) as,

$$\begin{aligned} p(a,b) &= p(a)\, q(b|a) \\ \text{where} \;\; p(a) &= \mathrm{Tr}[\rho\, \mathbf{\Pi}_a], \quad q(b|a) = \mathrm{Tr}[\mathbf{\Pi}_a\, \rho\, \mathbf{\Pi}_a\, \mathbf{\Pi}_b]/p(a), \end{aligned} \tag{A.1}$$

and $\mathbf{\Pi}_a = |a\rangle\langle a|, \mathbf{\Pi}_b = |b\rangle\langle b|$ are complete, orthogonal eigen projectors of $\mathbf{A}$ and $\mathbf{B}$; further, for commuting observables $\mathbf{A}$ and $\mathbf{B}$, we have simultaneous eigenstates, and so, we have, $\mathbf{\Pi}_a\mathbf{\Pi}_b = \mathbf{\Pi}_a\, \delta_{a,b}$.

$\Big($A small digression about joint (sequential) projective measurement is presented here: A projective measurement $\mathbf{\Pi}_a$ on a state ρ reduces it to $\rho_a = |a\rangle\, \langle a|$.

$$\rho \xrightarrow{\qquad\quad \mathbf{\Pi}_a \qquad\quad} \frac{\mathbf{\Pi}_a\, \rho\, \mathbf{\Pi}_a}{Tr(\rho\, \mathbf{\Pi}_a)}.$$

Here, $\text{Tr}(\rho\mathbf{\Pi}_a)$ is the normalization factor which is the probability of obtaining the corresponding eigenvalue a, i.e, $p(a) = \text{Tr}(\rho\mathbf{\Pi}_a)$. A second consecutive measurement $\mathbf{\Pi}_b$ takes the state to $\rho_b = |b\rangle\langle b|$.

$$\rho \xrightarrow{\mathbf{\Pi}_a} \frac{\mathbf{\Pi}_a\,\rho\,\mathbf{\Pi}_a}{\text{Tr}(\rho\,\mathbf{\Pi}_a)} \xrightarrow{\mathbf{\Pi}_b} \frac{\mathbf{\Pi}_b\,\mathbf{\Pi}_a\,\rho\,\mathbf{\Pi}_a\,\mathbf{\Pi}_b}{Tr(\rho\,\mathbf{\Pi}_a)\frac{\text{Tr}(\mathbf{\Pi}_a\,\rho\,\mathbf{\Pi}_a\,\mathbf{\Pi}_b)}{\text{Tr}(\rho\,\mathbf{\Pi}_a)}}$$

The joint probability distribution of obtaining the values a and b is given by

$$\begin{aligned} p(a,b) &= \text{Tr}(\rho\,\mathbf{\Pi}_a)\frac{\text{Tr}(\mathbf{\Pi}_a\,\rho\,\mathbf{\Pi}_a\,\mathbf{\Pi}_b)}{Tr(\rho\,\mathbf{\Pi}_a)} \\ &= p(a)q(b|a) \end{aligned}$$

as is given by (A.1) $\Big)$

Substituting in Eq.(A.1), we obtain,

$$p(a,b) = p(a)\,\delta_{a,b} \tag{A.2}$$

It may be noted that the joint probabilities satisfy the required properties:

$$\begin{aligned} \sum_b p(a,b) &= \sum_b p(a)\,\delta_{a,b} = p(a), \\ \sum_{a,b} p(a,b) &= \sum_{a,b} p(a)\,\delta_{a,b} = \sum_a p(a) = 1, \\ \sum_a p(a,b) &= \sum_a p(a)\delta_{a,b} = p(b) \\ p(a,b) &= p(a)\,q(b|a) = p(b)\,q(a|b). \end{aligned}$$

Clearly, $p(a,b) \neq p(a)\,p(b)$ and so, the outcomes $a,\ b$ are correlated.

We may express the joint probabilities (A.1) as a convex sum of the product form,

$$p(a,b) = \sum_{a'} p(a')\,\delta_{a',a}\,\delta_{a',b} \tag{A.3}$$

where $p(a')$ takes the role of hidden variable probability and $\delta_{a',a}$ ($\delta_{a',b}$) are the individual probabilities for the outcomes a (b) in the statistical ensemble with $p(a')$ as the weight factor. (Note that $p(a') = \mathrm{Tr}[\rho\,\mathbf{\Pi}_{a'}] = \langle a'|\rho|a'\rangle$. If the density matrix is in a common eigenstate $|a'\rangle$ of $\mathbf{A}$, $\mathbf{B}$, then $p(a') = 1$ and the joint probability is then in a simple form $p(a,b) = \sum_{a'} \delta_{a',a}\,\delta_{a',b} = \delta_{ab}$.)

A.2 Joint probability distribution for a pair of non-commuting observables

Let us consider non-commuting operators $\mathbf{A}$ and $\mathbf{B}$. The joint probability $p(a,b)$ for measuring $\mathbf{A}$ first and then $\mathbf{B}$ is given by,

$$\begin{aligned} p(a,b) &= p(a)\,q(b|a) \\ \text{where}\;\; p(a) &= \mathrm{Tr}[\rho\,\mathbf{\Pi}_a], \quad q(b|a) = \mathrm{Tr}[\mathbf{\Pi}_a\,\rho\,\mathbf{\Pi}_a\,\mathbf{\Pi}_b]/p(a) = |\langle a|b\rangle|^2. \\ \text{Thus}\quad p(a,b) &= p(a)\,|\langle a|b\rangle|^2. \end{aligned} \tag{A.4}$$

On the other hand if we measure $\mathbf{B}$ first and then $\mathbf{A}$, we obtain,

$$\begin{aligned} p(b,a) &= p(b)\,q(a|b) \\ \text{where}\;\; p(b) &= \mathrm{Tr}[\rho\,\mathbf{\Pi}_b], \quad q(a|b) = \mathrm{Tr}[\mathbf{\Pi}_b\,\rho\,\mathbf{\Pi}_b\,\mathbf{\Pi}_a]/p(b) = |\langle a|b\rangle|^2. \\ \text{Thus}\quad p(b,a) &= p(b)\,|\langle a|b\rangle|^2. \end{aligned} \tag{A.5}$$

Unlike classical probabilities, here, $p(a,b) \neq p(b,a)$ in general. Only in the case $p(a) = p(b)$, we have both $p(a,b) = p(b,a)$.

According to Bayes rule, $q(a|b) = p(a,b)/p(b)$ and $q(b|a) = p(a,b)/p(a)$.

And notice from (A.4) and (A.5) that the conditional probabilities are equal: $q(b|a) = q(a|b)$. For Bayes rule to hold, we must have, $p(a) = p(b)$. In other words $p(a, b) = p(b, a)$. This is not true in general in quantum scenario!

Appendix B

Derivation of the pairwise and triplewise measurability bounds

Consider a set of N POVMs $\{E_k(x_k) = \frac{1}{2}(\mathbb{I} + \eta\, x_k\, \boldsymbol{\sigma}\cdot\mathbf{n}_k);\ k = 1, 2, \ldots N; x_k = \pm 1\}$ (where $0 \leq \eta \leq 1$ denotes unsharpness parameter; $0 \leq E_k(x_k) \leq \mathbb{I}$ and $\sum_{x_k} E_k(x_k) = \mathbb{I}$ for all k.

The Necessary condition for joint measurability of these POVMs is given in more detail in [145]. We only provide a statement of the theorem whose proof can be seen in [145].

Theorem: The qubit POVMs $\{E_k(x_k) = \frac{1}{2}(\mathbb{I}+\eta\, x_k\, \boldsymbol{\sigma}\cdot\mathbf{n}_k));\ k = 1, 2, \ldots N; x_k = \pm 1\}$ are compatible when

$$\eta \ \leq \ \frac{1}{N} \max_{x_1, x_2, \ldots, x_N} \ |\mathbf{m}_{x_1, x_2, \ldots, x_N}| \tag{B.1}$$

where

$$\mathbf{m}_{x_1, x_2, \ldots, x_N} = \sum_{k=1}^{N} \mathbf{n}_k\, x_k \tag{B.2}$$

and $|\mathbf{m}_{x_1, x_2, \ldots, x_N}|$ denotes the magnitude of the vector; in (B.1) 'maximum' is picked from the magnitudes of all 2^N vectors $\mathbf{m}_{x_1, x_2, \ldots, x_N}$.

In the example of two orthogonal orientations $\mathbf{n}_1,\ \mathbf{n}_2$ such that $\mathbf{n}_1 \cdot \mathbf{n}_2 = 0$ we find that

$$\begin{aligned} \eta &\le \frac{1}{2} \max_{x_1, x_2 = \pm 1} |(\mathbf{n}_1\, x_1 + \mathbf{n}_2\, x_2)| \\ &= \frac{1}{2} \max_{x_1, x_2 = \pm 1} \sqrt{2 + 2\, x_1\, x_2\, \mathbf{n}_1 \cdot \mathbf{n}_2} \\ i.e.,\ \eta &\le \frac{1}{\sqrt{2}}. \end{aligned}$$

In the example of three orthogonal orientations $\mathbf{n}_1,\ \mathbf{n}_2, \mathbf{n}_3$; $\mathbf{n}_1 \cdot \mathbf{n}_2 = 0 = \mathbf{n}_2 \cdot \mathbf{n}_3 = \mathbf{n}_1 \cdot \mathbf{n}_3$, we find that

$$\begin{aligned} \eta &\le \frac{1}{3} \max_{x_1, x_2, x_3 = \pm 1} |(\mathbf{n}_1\, x_1 + \mathbf{n}_2\, x_2 + \mathbf{n}_3\, x_3)| \\ &= \frac{1}{3} \times \sqrt{3} \\ i.e.,\ \eta &\le \frac{1}{\sqrt{3}}. \end{aligned}$$

For trine axes $\mathbf{n}_1,\ \mathbf{n}_2, \mathbf{n}_3$, $\mathbf{n}_1 \cdot \mathbf{n}_2 = \mathbf{n}_2 \cdot \mathbf{n}_3 = -\mathbf{n}_1 \cdot \mathbf{n}_3 = \cos(\pi/3)$, we obtain the compatiblity condition

$$\begin{aligned} \eta &\le \frac{1}{3} \max_{x_1, x_2, x_3 = \pm 1} |(\mathbf{n}_1\, x_1 + \mathbf{n}_2\, x_2 + \mathbf{n}_3\, x_3)| \\ &= \frac{1}{3} \max_{x_1, x_2, x_3 = \pm 1} \sqrt{3 + 2\, \cos(\pi/3)\, (x_1\, x_2 + x_2\, x_3 - x_1\, x_3)} \\ i.e.,\ \eta &\le \frac{2}{3}. \end{aligned}$$

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Alice measures $\mathbf{X}$ ($\mathbf{Z}$) conditioned by the outcome Bob obtains for $\mathbf{X}_0$ ($\mathbf{Z}_0$) on the state in his possession) is referred to as entropic Einstein-Podolsky-Rosen steering inequality. See [146]. 115

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[147] The first entropic criteria of steering was formulated for position and momentum by S. P. Walborn et.al, [155]. Entropic steering inequalities for discrete observables were developed more recently in Ref. [146]. 124, 130

[148] The roles played by Alice and Bob in non-local steering task (where conventionally Alice is an untrusted party and Bob needs to check violation/nonviolation of a steering inequality to verify if Alice's claim – that they share an entangled state – is true/false) is interchanged here so as to be consistent with the convention of Ref. [7]. 125

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[152] Note that $H(\mathbf{X}|\mathbf{X}') = -\sum_{x,x'} p(x|x') \log_2 p(x|x')$ – where $p(x,x') = \mathrm{Tr}[\rho_{AB}\mathbf{E}_{\mathbf{X}}(x) \otimes \mathbf{E}_{\mathbf{X}'}(x')]$, $p(x|x') = p(x,x')/p(x')$ – is the conditional Shannon entropy associated with the probabilities of Alice finding the outcome x of the observable $\mathbf{X}$, when Bob has obtained the outcome x' in the measurement of $\mathbf{X}'$ and $p(x') = \mathrm{Tr}[\rho_B\, \mathbf{E}_{\mathbf{X}'}(x')] = \sum_x p(x,x')$ is the probability of Bob's outcome x' in the measurement of $\mathbf{X}'$. 130, 132

[153] The entropic steering inequality (7.10) is violated when the unsharpness parameter $\eta > 0.78$ – whereas the POVMs of (7.7) are incompatible for $\eta > 1/\sqrt{2} \approx 0.707$. In order to obtain the necessary and sufficient condition that the POVMs of (7.7) are useful for steering in the entire range of incompatibility $1/\sqrt{2} < \eta \leq 1$, either one has to examine the set of all pure entangled states for the task of steering or to develop an appropriate steering inequality to capture the efficacy of the incompatible measurements [18, 19]. For instance, we find that the two qubit maximally entangled state shared between Alice and Bob violates a linear steering inequality with two measurement settings (Eq. (64) of [88]) for the *entire* range of incompatibility $1/\sqrt{2} < \eta \leq 1$ of the unsharpness parameter, when Bob (who claims to steer Alice's by measurements at his end) measures the pairs of POVMs of (7.7). 132

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