A Quantum version of coupling of Markov chains

Konrad Pawlikowski

4th Year Project Report
Computer Science and Mathematics
School of Informatics
University of Edinburgh

2024

Abstract

Many concepts in Quantum Theory are generalisations of concepts from Probability Theory, we aim to investigate potential generalisations of coupling, a concept from Probability Theory, in a Quantum Theoretic context with our investigation grounded by well-accepted generalisations to adjacent notions.

Research Ethics Approval

This project was planned in accordance with the Informatics Research Ethics policy. It did not involve any aspects that required approval from the Informatics Research Ethics committee.

Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

(*Konrad Pawlikowski*)

Table of Contents

Chapter 1

Introduction

1.1 Motivation

Quantum Computing and Quantum Information as fields have seen many advances in recent years, with near-term commercial prospects Bova, Francesco et al. (2021) such as in the development and/or discovery of medicines Cao et al. (2018); Zinner et al. (2022), quantum cryptography for secure modern systems Deutsch et al. (1996); Pirandola et al. (2020), and quantum machine learning promising speedup to the resource-intensive learning process Garros et al. (2023); Zhang and Ni (2020), to more theoretical endeavours such as quantum software verification for the understanding and guarantee on reliability and correctness of quantum algorithms Lewis et al. (2023); García de la Barrera Amo et al. (2022). Quantum Information, therefore, plays an important role in framing our understanding of the world and solutions to real-world problems of importance.

In the pursuit of understanding Quantum Information we note many approaches attempt to bridge the gap in understanding by introducing a classical analogue, indeed we expect classical theories to, at the very least, approximate Quantum Theory or provide partial solutions/insights. For example p-mechanics Kisil (2003), which sets out to understand quantum-classical systems, was used to show a relation within such mixed systems that was motivated in part by "the explicit similarity between the Hamiltonian descriptions of quantum and classical dynamics". Kisil (2005) Further, such classical analogues are also theoretically sound when Quantum Theory is understood to be a generalised probability theory Janotta and Hinrichsen (2014); Moyal (1949); Rédei and Summers (2007), for our goals a particularly relevant observation is that a collection of density operators, the fundamental objects in Quantum Theory that model the state of quantum systems (See Sec 2), which are diagonal in the same basis can be modelled as discrete probability spaces. This correspondence also allows us to model all problems in Discrete Probability Theory as problems in Quantum Theory, but beware that such a relation is certainly not an equivalence, as "entanglement and non-locality are known to be genuine non-classical features." Janotta and Hinrichsen (2014)

1.2 Why Coupling?

Markovian Coupling Levin and Peres (2017) is a well-studied concept in Probability Theory wherein the local properties of the marginals of a pair of stochastic processes are understood and studied in relation to one another, often this is realised in the form of a random process of interest and some other dependent process constructed, mathematically, to illuminate the behaviour of the process of interest over time. Markovian Coupling has numerous applications; An interesting application of Markovian Coupling is as a potential factor for noise reduction in gene regulation in sub-Fano regimes Ramos et al. (2015) allowing for a deeper understanding of basic biological processes, another important application is in the domain of adaptive learning/machine learning when it comes to understanding global properties of an adaptive Markov chain Monte Carlo and limiting behaviour Roberts and Rosenthal (2007) as well as compensating for the diffusive behaviour of Markov chain Monte Carlo and improving efficiency of sampling therewith Bou-Rabee et al. (2020) which has practical implications on the training time for ML models. And more generally, coupling is useful when understanding Mixing-Times, which represents the expected time until a stochastic process 'stabilizes' and when we expect samples from the process to look like they were taken from a particular fixed distribution known as a stationary distribution Levin and Peres (2017); Hunter (2009). Moreover, classical coupling already has applications in Quantum Mechanics such as Plasmon Emission Dynamics Kravtsov et al. (2014), given this we argue a specialised quantum coupling result could prove useful.

1.3 Background on Trace distance and Total Variation

Note that this section is meant to sketch out the concepts mentioned in table 1.1 but this section is by no means a replacement for chapter 2.

For probability measures absolutely continuous with respect to the Lebesgue measure, i.e. with probability density function $p : \mathbb{R} \to \mathbb{R}^+$, we can visualise the Total Variation distance (also known as the Earth Mover distance, Kantorovich distance, or the L^1 Wasserstein distance) as half the unsigned area between the two probability density functions, see fig. 1.1 for an example.

The trace distance can be formalised in terms of the eigenvalues of density operators (see chapter 2) however we will give an equivalent definition in terms of measurements and the total variation distance. What is a measurement? For quantum systems there exist measurement outcomes $i \in \mathcal{I}$ for some set $\mathcal{I}$ where the system can be measured with respect to this measurement irrespective of the state of the system (Note: we are using the Positive Operator Valued Measure (POVM) model of measurement), we will discuss measurements rigorously in chapter 2. For now we can think of the trace distance as

$$||\rho - \sigma||_{\text{TD}} = \max_{M} ||\mu_M - \nu_M||_{\text{TV}}$$

where ρ, σ are density operators, $||\cdot||_{\text{TV}}$ is the total variation distance as discussed above, and μ_M, ν_M are probability distributions induced by measurement of ρ, σ respectively, i.e. $\mu_M(i)$ is the probability that measurement outcome i was obtained when ρ was measured.

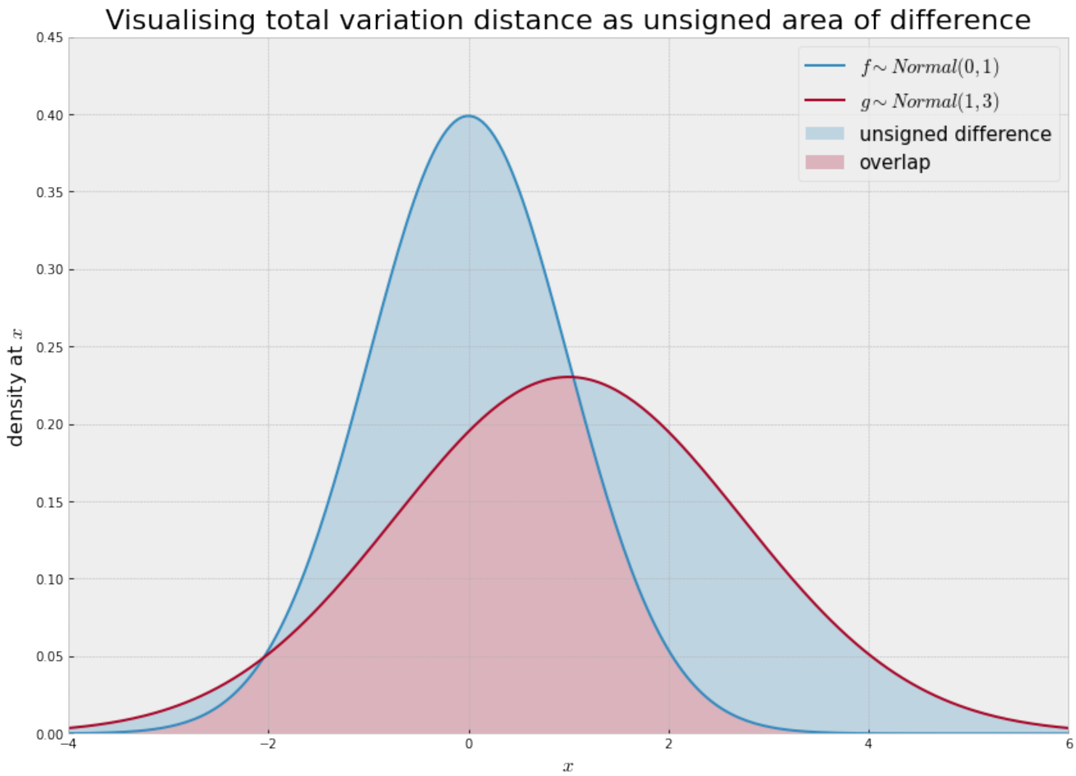


Figure 1.1: Visualisation of total variation distance ($\frac{1}{2}$ of the blue shaded area) between two normal/Gaussian distributions

This explains the second line in table 1.1 where equality holds given *optimisation* over the measurements.

1.4 Towards a quantum coupling & Problem Statement

Concept in Probability Theory	Analogue in Quantum Theory
Discrete probability spaces	Density operators
Total Variation distance	Trace distance
Coupling	?

Table 1.1: Quantum Theoretic analogues to concepts in Probability Theory

In section 1.1 we mentioned how a collection of density operators that are diagonal in a shared basis are analogous to discrete probability spaces, this explains the first line in table 1.1.

Now, the underpinning result for Markovian Coupling is an upper bound on the Total Variation Distance where optimisation over all possible Couplings of a pair of distributions leads to saturation of the bound, that is to say

$$\|\mu - \nu\|_{\text{TV}} = \inf_{(X,Y)\in\Gamma(\mu,\nu)} \mathbb{P}(X \neq Y)$$

where $\|\cdot\|_{\text{TV}}$ is the total variation, and $\Gamma(\mu,\nu)$ is the set of all couplings of the distributions μ and ν. Here $\inf_{(X,Y)\in\Gamma(\mu,\nu)}$ *optimises* the coupling. Returning back to trace distance, like in the above coupling equation, $\max_M$ *optimises* the measurement. Given these optimisations and table 1.1 we can understand the final row as a 'quantum coupling' analogue which looks like

$$\|\rho - \sigma\|_{\text{TD}} = \text{Opt}_{M \text{ and } C}\, \mathbb{P}(X \neq Y)$$

where Opt_M is an optimisation over measurements and Opt_C is an optimisation over entangled states, that we call quantum couplings, with reduced density operators ρ, σ.

1.5 Contributions

- General framework for understanding potential quantum couplings as a relation over collections of measurements indexed by bipartite (entangled) states.
- The infeasibility of arbitrary measurements for quantum coupling.
- Coupling bound for pairs of pure states in the 1-qubit system with restriction to Von Neumann measurements with saturation under measurement optimisation.
- Monotonicity of coupling function over the maximal Total Variation measurement scheme irrespective of restriction to states.
- Equality of coupling function over the maximal Total Variation measurement scheme under mild conditions.
- Negative result on saturation of coupling function over the maximal Variation measurement scheme.

1.6 Dissertation Structure

Background Chapter: This chapter introduces the main concepts of interest, the concepts from probability theory section motivate the maximal total variation measurement scheme and ground the project but are not critical to understanding any of the work done while the concepts from quantum theory section outlines foundational concepts that must be understood rigorously as they form the backbone of every result presented.

Measurement Systems and Understanding Quantum Couplings Chapter: This chapter introduces our framework, measurement systems, as motivated by problems that arise from other approaches towards a quantum coupling result and provides a practical application in the basics of the Von Neumann measurement scheme section.

Maximal Total Variation Measurement Scheme Chapter: This chapter applies all of the work done in the prior chapter towards the core quantum coupling problem and gives an extensive characterisation of any possible solution and general properties such as monotonicity, quantum coupling function, and saturation within an appropriate context.

Chapter 2

Background Chapter

2.1 Concepts from Probability Theory

The concepts of Total Variation Distance and Coupling are integral to our analogue and provide guiding principles for our study, we investigate their implications in Chapter 4. This section is based heavily on *Markov Chains and Mixing Times, second edition* Levin and Peres (2017) and aims to motivate the investigation of quantum couplings rigorously as well as provide some basic results as required in the main work.

2.1.1 Total Variation Distance

In the introductory chapter, we introduced the concept of Total Variation as 'the unsigned area between two probability densities', we now formalise this concept for discrete probability spaces, our probability spaces of interest, and give a few results relevant to us.

Definition 1 (Total Variation Distance)**.** Let $(\mu, \mathcal{F}, \Omega)$ and $(\nu, \mathcal{F}, \Omega)$ be probability spaces, then

$$\|\mu - \nu\|_{\text{TV}} = \max_{E \in \mathcal{F}} |\mu(E) - \nu(E)|$$

is the total variation distance (T.V).

Proposition 1. *$d(\mu, \nu) = \|\mu - \nu\|_{\text{TV}}$ is a metric.*

Proof. omitted. □

Lemma 2. *Let $(\mu, \mathcal{F}, \Omega)$ and $(\nu, \mathcal{F}, \Omega)$ be discrete probability spaces, then*

$$\|\mu - \nu\|_{\text{TV}} = \frac{1}{2} \sum_{\omega \in \Omega} |\mu(\omega) - \nu(\omega)|$$

Proof. We paraphrase from Markov Chains and Mixing Times Levin and Peres (2017) (pp. 48):

Let $B := \{\omega \in \Omega \,|\, \mu(\omega) \geq \nu(\omega)\}$ then clearly

$|\mu(B)-\nu(B)| = \max_{E\in\mathcal{F}} |\mu(E)-\nu(E)|$, and also
$|\mu(B^c)-\nu(B^c)| = |(1-\mu(B))-(1-\nu(B))| = |\nu(B)-\mu(B)| = \max_{E\in\mathcal{F}} |\mu(E)-\nu(E)|$
from which we find

$$
\begin{aligned}
&\sum_{\omega\in\Omega} |\mu(\omega)-\nu(\omega)| \\
&= \sum_{\omega\in B} |\mu(\omega)-\nu(\omega)| + \sum_{\omega\in B^c} |\mu(\omega)-\nu(\omega)| \\
&= \left|\sum_{\omega\in B} (\mu(\omega)-\nu(\omega))\right| + \sum_{\omega\in B^c} |\mu(\omega)-\nu(\omega)| && \text{since } \mu(\omega)\geq\nu(\omega) \text{ for all } \omega\in B \\
&= \left|\sum_{\omega\in B} (\mu(\omega)-\nu(\omega))\right| + \left|\sum_{\omega\in B^c} (\mu(\omega)-\nu(\omega))\right| && \text{since } \mu(\omega)<\nu(\omega) \text{ for all } \omega\in B^c \\
&= |\mu(B)-\nu(B)| + |\mu(B^c)+\nu(B^c)| && \text{by countable additivity} \\
&= 2\max_{E\in\mathcal{F}} |\mu(E)-\nu(E)|
\end{aligned}
$$

□

Remark. From the above we immediately see the relation between T.V and the unsigned area between the densities, in fact by approximating measures that are absolutely continuous w.r.t the Lebesgue measure with finite valued random variables (r.vs) we end up integrating the absolute value of the difference between the densities, i.e. calculating the unsigned area between the densities, for an illustration see fig. 1.1.

Lemma 2 is an integral component for proving the relation between the total variation distance and trace distance.

2.1.2 Coupling

We now introduce coupling alongside a simple example and introduce a key relation with T.V that motivates our investigation of a quantum analogue.

Definition 2. [Coupling] A *coupling* of the distributions μ,ν is a pair of r.vs (X,Y) such that $\mathbb{P}_X=\mu$ and $\mathbb{P}_Y=\nu$. (i.e. the marginal distributions of X,Y are μ and ν respectively.)

Example 1. Let $\mu=v$ be the distribution of a fair coin flip, i.e.

$$\mu(\text{heads}) = \nu(\text{heads}) = \frac{1}{2} = \mu(\text{tails}) = \nu(\text{tails})$$

then

$\mathbb{P}_{XY}$	$X=0$	$X=1$
$Y=0$	$\frac{1}{4}$	$\frac{1}{4}$
$Y=1$	$\frac{1}{4}$	$\frac{1}{4}$

(2.1)

and

$\mathbb{P}_{XY}$	$X=0$	$X=1$
$Y=0$	$\frac{1}{2}$	0
$Y=1$	0	$\frac{1}{2}$

(2.2)

describe two distinct couplings of μ, ν where in (2.1) the r.vs are independent and in (2.2) the r.vs are dependent and strongly correlated.

Lemma 3. *If (X,Y) is a coupling of μ and ν, then $\|\mu - \nu\|_{\text{TV}} \leq \mathbb{P}(X \neq Y)$*

Proof. We paraphrase from Markov Chains and Mixing Times Levin and Peres (2017) (pp. 50): Let (X,Y) be a coupling of the distributions μ and ν, then for any event E:

$$\begin{aligned}
\mu(E) - \nu(E) &= \mathbb{P}(X \in E) - \mathbb{P}(Y \in E) \\
&= \mathbb{P}(X \in E, Y \in E) + \mathbb{P}(X \in E, Y \notin E) - \mathbb{P}(Y \in E, X \in E) \\
&\quad - \mathbb{P}(Y \in E, X \notin E) \\
&= \mathbb{P}(X \in E, Y \notin E) - \mathbb{P}(Y \in E, X \notin E) \\
&\leq \mathbb{P}(X \in E, Y \notin E) \\
&\leq \mathbb{P}(X \neq Y)
\end{aligned}$$

Thus $\|\mu - \nu\|_{\text{TV}} = \max_{E \in \mathcal{F}} |\mu(E) - \nu(E)| \leq \max_{E \in \mathcal{F}} |\mathbb{P}(X \neq Y)| = \mathbb{P}(X \neq Y)$. □

Example 2. Recall the fair coin distributions μ and ν as in example 1, we find

$$\|\mu - \nu\|_{\text{TV}} = \|0\|_{\text{TV}} = 0$$

and, for the couplings (2.1) and (2.2) we find

$$\begin{aligned}
\mathbb{P}(X \neq Y) &= \mathbb{P}(X = 0, Y = 1) + \mathbb{P}(X = 1, Y = 0) = \frac{1}{2} && \text{For coupling (2.1)} \\
\mathbb{P}(X \neq Y) &= \mathbb{P}(X = 0, Y = 1) + \mathbb{P}(X = 1, Y = 0) = 0 && \text{For coupling (2.2)}
\end{aligned}$$

For the dependent fair coin joint distribution (2.2) we see that $\|\mu - \nu\|_{\text{TV}} = \mathbb{P}(X \neq Y)$, such a coupling is called *optimal*.

Proposition 4. *For any pair $(\mu, \mathcal{F}, \Omega)$, and $(\nu, \mathcal{F}, \Omega)$ of discrete probability spaces:*

$$\|\mu - \nu\|_{\text{TV}} = \min\{\mathbb{P}(X \neq Y) : \textit{For } (X,Y) \textit{ a coupling of } \mu \textit{ and } \nu\}$$

i.e. there exists an optimal coupling of μ and ν.

Proof. Note that inequality follows immediately from Lemma 3 thus this is more a statement about saturation of the inequality, proof omitted for brevity, see pp. 50-52 Levin and Peres (2017) (Proof of Proposition 4.7). □

Remark. The key properties to this relation are the monotone increasing bound $\mathbb{P}(X \neq Y)$ and saturation of the bound.

2.2 Concepts from Quantum Theory

To understand the existing quantum analogue to T.V, and also for all results that follow, we must understand density operators and positive operator valued measure (POVM) measurements, we will then be ready to introduce the trace distance (T.D) and show that it is indeed a quantum analogue to T.V. This section is based heavily on *Quantum Computation and Quantum Information* Nielsen and Chuang (2010). Note that it may be worthwhile to review section 2.3 (Nomenclature) first.

2.2.1 Hilbert Spaces and Density Operators

A Vector Space X is a Hilbert Space if it is an inner product space such that the norm induced by the inner product (formally $\langle\cdot,\cdot\rangle^{\frac{1}{2}}$) gives us a Banach Space $(X, \|\cdot\|)$, equivalently a Banach Space that satisfies the parallelogram identity is a Hilbert Space, we are concerned with complex Hilbert spaces over the base field $\mathbb{C}$ of dimension at least 2 equipped with the standard complex inner product. A common class of Hilbert Spaces are of the form $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$ which represent the n-qubit system.

Definition 3 (Density Operator)**.** For a given Hilbert space, $\mathcal{H}$, a density operator is an operator $\rho \in \mathcal{L}(\mathcal{H})$ such that

- ρ satisfies the trace condition: $\mathrm{tr}(\rho) = 1$
- ρ is positive semi-definite: $\forall |\varphi\rangle \in \mathcal{H} : \langle\varphi|\rho|\varphi\rangle \geq 0$

Remark. An important kind of density operator is one such that $\mathrm{tr}(\rho^2) = 1$, known as a *pure state*, for example, if $\rho = |\varphi\rangle\langle\varphi|$ is a density operator then it is pure, by spectral decomposition we can also show that the above representation is an iff characterisation.

2.2.2 POVM Measurements

Definition 4 (POVM Measurement)**.** A POVM element is a family of linear operators $\{M_i\}_{i\in\mathcal{I}} \subset \mathcal{L}(\mathcal{H})$ such that for every $i \in \mathcal{I}$ we have $M_i M_i^\dagger$ positive semi-definite and the completeness equation:

$$\sum_{i\in\mathcal{I}} M_i M_i^\dagger = \mathrm{id}$$

Definition 5 (POVM Elements)**.** Let $\{M_i\}_{i\in\mathcal{I}}$ be a POVM measurement, then $E_i = M_i M_i^\dagger$ is known as a POVM element, we will often refer to $\{E_i\}_{i\in\mathcal{I}}$ as a POVM measurement for convenience as often we do not care that $E_i = M_i M^\dagger$ just that E_i is positive semi-definite, in this case we also have the completeness equation:

$$\sum_{i\in\mathcal{I}} E_i = \mathrm{id}$$

Remark. Moreover since each E_i is positive semi-definite $\sqrt{E_i}$ exists and thus we have $E_i = \sqrt{E_i}\sqrt{E_i}^\dagger$ meaning that if all of E_i are positive semi-definite and the completeness equation is satisfied then there does indeed exist a corresponding POVM measurement.

Given this we are equipped to introduce the third postulate for Quantum Mechanics Nielsen and Chuang (2010):

- **Postulate 3**: For a POVM $\{E_i\}_{i\in\mathcal{I}}$, the index set, $\mathcal{I}$, describes the possible measurement outcomes of a quantum system. If the state of a quantum system is ρ (ρ a density operator) at the time of measurement then the probability of measurement outcome $i \in \mathcal{I}$ is

$$\mathbb{P}(X = i) = \mathrm{tr}(E_i \rho)$$

and more generally for $I \subseteq \mathcal{I}$ we have

$$\mathbb{P}(X \in I) = \operatorname{tr}((\sum_{i \in I} E_i)\rho)$$

This postulate is critical to our results and as such we verify that $\mathbb{P}$, as given above, is indeed a probability measure.

Proof. Non-negative:

$$\operatorname{tr}(M_i M_i^\dagger \rho) = \operatorname{tr}(M_i^\dagger \rho M_i) \qquad \text{by the cyclic property of the trace}$$

but for any vector $|\psi\rangle \in \mathcal{H}$ we have $|\psi'\rangle := M_i |\psi\rangle \in \mathcal{H}$ and by the positive semi-definite property of density operators we must have $\langle\psi'|\rho|\psi'\rangle \geq 0$ and thus $M_i^\dagger \rho M_i$ is positive semi-definite, hence the eigenvalues are non-negative reals and the trace, which is the sum of the eigenvalues, is non-negative, finally non-negativity follows in the general case by the linearity of the trace.

Distributive over countably many disjoint unions: Let $\{E_j\}_{j \in \mathcal{J}}$ be countably many disjoint events, then

$$\begin{aligned}
&\sum_{j \in \mathcal{J}} \mathbb{P}(X \in E_j) \\
&= \sum_{j \in \mathcal{J}} \mathbb{P}(X \in E_j) \\
&= \sum_{j \in \mathcal{J}} \operatorname{tr}(E_j^* \rho) && \text{where } E_j^* \text{ is the operator corresponding to the event } E_j \\
&= \operatorname{tr}(\sum_{j \in \mathcal{J}} E_j^* \rho) && \text{since tr is a linear operator} \\
&= \operatorname{tr}((\sum_{j \in \mathcal{J}} E_j^*)\rho) \\
&= \mathbb{P}(X \in \bigcup_{i \in \mathcal{J}} E_j) && \text{since } E_j \text{ are disjoint}
\end{aligned}$$

Completeness:

$$\begin{aligned}
\mathbb{P}(X \in \mathcal{I}) &= \operatorname{tr}((\sum_{i \in \mathcal{I}} E_i)\rho) \\
&= \operatorname{tr}(\mathrm{id}\,\rho) && \text{by the completeness equation} \\
&= \operatorname{tr}(\rho) = 1 && \text{since } \rho \text{ is a density operator}
\end{aligned}$$

Thus $\mathbb{P}$ is a probability measure. □

2.2.3 Spectral Decomposition and Q, S Matrices

Spectral Decomposition is a fundamental result in Algebra and is invaluable in the context of quantum information, we will rarely use the theorem directly but many relevant results are a direct consequence of this theorem.

Theorem 5 (Spectral Decomposition)**.** *If N is normal then N is diagonalizable, moreover N is diagonal in its eigenbasis with diagonalization*

$$N = \sum_{i \in \mathcal{I}} \lambda_i |\psi_i\rangle \langle \psi_i|$$

where λ_i are the eigenvalues counted with appropriate multiplicity and $|\psi_i\rangle$ the corresponding eigenvectors.

Proof. Ommited, see Nielsen and Chuang (2010) (pp. 73). □

Now, for density operators ρ, σ, recall that density operators are Hermitian from which we immediately see that $(\rho - \sigma)(\rho - \sigma)^\dagger = (\rho - \sigma)^\dagger(\rho - \sigma)$, i.e. $\rho - \sigma$ is normal, then by Thm. 5 (Spectral Decomposition) we have a diagonalization $\rho - \sigma = \sum_{i \in \mathcal{I}} \lambda_i |\psi_i\rangle \langle \psi_i|$, Let $Q = \sum \lambda_i |\psi_i\rangle \langle \psi_i|$ for the eigenvalues $\lambda_i > 0$ and $S = \sum -\lambda_i |\psi_i\rangle \langle \psi_i|$ for the eigenvalues $\lambda_i < 0$ (note that the eigenvalues are real since ρ and σ are positive semi-definite). These Q, S matrices have many nice properties and will be useful to us when aiming to understand the trace distance and our coupling results. One basic result is

Proposition 6. *For density operators $\rho, \sigma \in \mathcal{L}(\mathcal{H})$ with $\rho - \sigma = Q - S$ for positive semi-definite Q, S with $Q \perp S$ we have*

$$\rho \geq Q$$

Proof. For $|\psi\rangle$ in the null-space of S we get

$$\begin{aligned} \langle \psi| (\rho - \sigma) |\psi\rangle &= \langle \psi| (Q - S) |\psi\rangle \\ \langle \psi| \rho |\psi\rangle - \langle \psi| \sigma |\psi\rangle &= \langle \psi| Q |\psi\rangle \\ \langle \psi| \rho |\psi\rangle &\geq \langle \psi| Q |\psi\rangle \qquad \text{since } \langle \psi| \sigma |\psi\rangle \geq 0 \text{ as } \sigma \text{ is a density operator} \end{aligned}$$

then $\rho \geq Q$ follows by linearity from every other vector being the sum of a vector in the null-space of Q and $|\psi\rangle$ since $Q \perp S$ and since $\rho \geq 0$ is a density operator. □

2.2.4 Trace Distance

Definition 6 (Trace Distance)**.** Let $\rho, \sigma \in \mathcal{L}(\mathcal{H})$ be density operators, then the trace distance is

$$\|\rho - \sigma\|_{\text{TD}} = \frac{1}{2} \sum_i |\lambda_i| = \frac{1}{2} \operatorname{tr} |\rho - \sigma|$$

where λ_i are the eigenvalues of $\rho - \sigma$ counted with algebraic multiplicity.

Remark. Essentially the trace distance is the sum of the absolute values of the eigenvalues counted with multiplicity, formally the definition is $\frac{1}{2} \operatorname{tr} |\rho - \sigma|$ (hence the name trace distance, it is also (clearly) $\frac{1}{2}$ the trace norm), using S, Q matrices it can be shown that $|\rho - \sigma| = |Q - S| = Q + S$, intuitively $Q - S$ is diagonal in some basis and for a diagonal matrix we can explicitly find the matrix $|D|$ to be the matrix whose entries are $D'_{ij} = |D_{ij}|$, finally the trace is invariant w.r.t. the choice of orthonormal basis and hence the sum of unsigned eigenvalues counted with algebraic multiplicity follows.

While $\|\cdot\|$ can be viewed as a metric is a minor point, the proof introduces basic relations between the Q,S matrices and the T.D which are quite important for sections 4.2 and 4.3.

Proposition 7. $0 \leq d(\rho,\sigma) = \|\rho-\sigma\|_{\text{TD}} \leq 1$ *is a metric.*

Proof. We observe that

$$\begin{aligned} 0 = 1-1 = \text{tr}(\rho) - \text{tr}(\sigma) &= \text{tr}(\rho-\sigma) && \text{by the linearity of trace} \\ &= \text{tr}(Q-S) = \text{tr}(Q) - \text{tr}(S) \end{aligned}$$

hence $\text{tr}(Q) = \text{tr}(S)$, from which we find that the trace distance is also $\frac{1}{2}(\text{tr}(Q)+\text{tr}(S)) = \text{tr}(Q) = \text{tr}(S)$, then $0 \leq Q \leq \rho$ tells us that $\text{tr}(0) = 0 \leq \|\rho-\sigma\|_{\text{TD}} \leq 1 = \text{tr}(\rho)$ (giving us a stronger claim than just non-negativity).

Now, notice that $\|\rho-\sigma\|_{\text{TD}} = 0 \implies \text{tr}(Q) = \text{tr}(S) = 0$ but since Q,S are diagonalizable with non-negative eigenvalues we must find $Q = S = 0$ from which it follows $\rho - \sigma = Q - S = 0 \iff \rho = \sigma$, i.e. d is non-degenerate.

Note that symmetry follows immediately from $|\rho-\sigma| = Q+S = S+Q = |\sigma-\rho|$.

The triangle inequality follows from Jensen's trace inequality given the convexity of $|\cdot|$, this is not relevant to us and thus we omit it. □

The following proposition should be carefully understood as the key symmetry which underpins measurement systems.

Proposition 8. *Forall* $U \in \text{SL}(\mathcal{H})$ *and for all density operators* $\rho,\sigma \in \mathcal{L}(\mathcal{H})$ *we have* $\|\rho-\sigma\|_{\text{TD}} = \|U\rho U^\dagger - U\sigma U^\dagger\|_{\text{TD}}$*, i.e. the trace distance is invariant under unitary transform.*

Proof.

$$\begin{aligned} \|U\rho U^\dagger - U\sigma U^\dagger\|_{\text{TD}} &= \frac{1}{2}\text{tr}\,|U\rho U^\dagger - U\sigma U^\dagger| \\ &= \frac{1}{2}\text{tr}\,|U(\rho-\sigma)U^\dagger| \\ &= \frac{1}{2}\text{tr}\left|U(\sum_{i\in\mathcal{I}}\lambda_i\,|\psi_i\rangle\,\langle\psi_i|)U^\dagger\right| && \text{by Spectral Decomposition (Thm. 5)} \\ &= \frac{1}{2}\text{tr}\left|\sum_{i\in\mathcal{I}}\lambda_i U\,|\psi_i\rangle\,\langle\psi_i|\,U^\dagger\right| \\ &= \sum_{i\in\mathcal{I}}|\lambda_i| && \text{unitaries are a change of basis and} \\ &= \|\rho-\sigma\|_{\text{TD}} && \text{so the } \lambda_i\text{'s are still our eigenvalues} \end{aligned}$$

□

Remark. That is to say, the trace distance is invariant under a change of basis, intuitively this suggests that any quantum coupling result should likewise not depend on a choice of basis, indeed it would be strange to find our result dependent on a basis when the value we are interested in is not.

We are now ready to see how trace distance can be understood classically as maximisation through measurement optimisation of the total variation distance.

Proposition 9. *Let Γ be the set such that if $M = \{M_i\}_{i\in\mathcal{I}}$ is a POVM measurement over the Hilbert space $\mathcal{H}$ then $M \in \Gamma$, then for density operators $\rho, \sigma \in \mathcal{L}(\mathcal{H})$ we let $\mu_M(i) = \operatorname{tr}(M_i\rho)$ and $\nu_M(i) = \operatorname{tr}(M_i\sigma)$ be the distribution representing the probability of observing measurement outcome $i \in \mathcal{I}$ when measuring the operators ρ, σ respectively, then*

$$\|\rho-\sigma\|_{\mathrm{TD}} = \max_{M\in\Gamma} \|\mu_M - \nu_M\|_{\mathrm{TV}}$$

Proof. We first show that for every measurement $M = \{M_i\}_{i\in\mathcal{I}}$ we have $\|\mu_M - \nu_M\|_{\mathrm{TV}} \leq \|\rho-\sigma\|_{\mathrm{TD}}$.

$$\begin{aligned}
\|\mu_M - \nu_M\|_{\mathrm{TV}} &= \frac{1}{2}\sum_{i\in\mathcal{I}} |\mu_M(i) - \nu_M(i)| && \text{by Lemma 2} \\
&= \frac{1}{2}\sum_{i\in\mathcal{I}} |\operatorname{tr}(M_i\rho) - \operatorname{tr}(M_i\sigma)| \\
&= \frac{1}{2}\sum_{i\in\mathcal{I}} |\operatorname{tr}(M_i(\rho-\sigma))| && \text{by linearity of the trace} \\
&= \frac{1}{2}\sum_{i\in\mathcal{I}} |\operatorname{tr}(M_i(Q-S))| \\
&\leq \frac{1}{2}\sum_{i\in\mathcal{I}} \operatorname{tr}|M_i(Q-S)| && \text{since } |\cdot| \text{ is subadditive and } \operatorname{tr}|A| = \textstyle\sum|\lambda_i| \\
&\leq \frac{1}{2}\sum_{i\in\mathcal{I}} \operatorname{tr}(M_i|Q-S|) && \text{since } |\cdot| \text{ is submultiplicative} \\
&= \frac{1}{2}\sum_{i\in\mathcal{I}} \operatorname{tr}(M_i(Q+S)) && \text{since } Q \perp S \\
&= \frac{1}{2}\operatorname{tr}(\sum_{i\in\mathcal{I}} M_i(Q+S)) && \text{since tr is a linear map} \\
&= \frac{1}{2}\operatorname{tr}((Q+S)\sum_{i\in\mathcal{I}} M_i) \\
&= \frac{1}{2}\operatorname{tr}((Q+S)\,\mathrm{id}) && \text{by the completeness equation} \\
&= \|\rho-\sigma\|_{\mathrm{TD}}
\end{aligned}$$

Finally, saturation of the bound is a consequence of any POVM measurement $\{M_1, M_2\}$ with $M_1 \perp S$ and $M_2 \perp Q$ (e.g. M_1 the projection onto the eigenvectors with non-negative eigenvalues of $\rho - \sigma$ and M_2 the projection onto the eigenvectors with strictly negative eigenvalues of $\rho - \sigma$) as given this we find $M_1(Q-S) = Q$ and $M_2(Q-S) = -S$ from which the claim follows immediately. □

2.3 Nomenclature

We provide an extensive list for the readers' convenience, it should be noted that $f \vee g$, the piece-wise join is relevant to the addition of measurement systems (see appendix A) which provides a deeper understanding of what a measurement system represents and its behaviour, in particular addition gives a simple 'patchwork' approach to the investigation of potential quantum coupling functions but is not crucial to the question at hand.

Notation	Meaning
$\dagger$	adjoint/conjugate transpose
$\otimes$	tensor product
$\|\psi\rangle$	vector belonging to some complex Hilbert space
$\langle\psi\|$	dual to $\|\psi\rangle$, equivalently $\langle\psi\| = \|\psi\rangle^\dagger$
ρ^A	reduced density operator $\rho^A = \mathrm{tr}_B(\rho^{AB})$
$\mathcal{H}$	complex Hilbert space
μ_M/ν_M	distribution of outcome probabilities associated with POVM M
$\mathcal{L}(\mathcal{H})$	bounded linear operators over the Hilbert space $\mathcal{H}$
$\mathrm{SL}(\mathcal{H})$	special linear group over the Hilbert space $\mathcal{H}$
Π_A	least (orthogonal) projection such that $\Pi_A A = A$ for normal A
$A \perp B$	$AB = 0$, i.e. matrices A and B are orthogonal
$f \vee g$	piece-wise join function: $(f \vee g)(x) = \max\{f(x), g(x)\}$
$\mathrm{Mon}\, f$	least upper bound $f(x) \leq (\mathrm{Mon}\, f)(x)$ that is monotone non-decreasing

Table 2.1: Nomenclature

Chapter 3

Measurement Systems and Understanding Quantum Couplings

In this chapter, we will formally introduce the problem of coupling and justify requirements such as basis invariance and shared measurements. This will inform our definition of a measurement system and we will also see how measurement systems are a rigorous formalism for any reasonable quantum coupling candidate that are also specific enough for emergent behaviour. Further, we will classify measurement systems according to useful/insightful properties and briefly explore their interplay before moving on to quantum coupling functions. Finally, we will conclude with an extensive application of all the theory that we introduce and discuss the benefits provided by the framework. Please see appendix A for measurement system addition, a concept that helps illuminate the structure inherent to measurement systems and provides a 'patchwork' approach to quantum coupling results.

3.1 Arbitrary measurement schemes

Before going any further we must address so-called 'identity measurements', POVM measurements similar to $\{\frac{1}{2}\,\mathrm{id}, \frac{1}{2}\,\mathrm{id}\}$ or $\{\mathrm{id}, 0\}$ are often easy to analyse and help clarify certain results, however, from a physical perspective an 'identity measurement' corresponds to no measurement and thus results based on identity measurements might seem like they are arbitrary and non-informative. However we can 'emulate' such measurements with a multitude of meaningful and rich measurements, for example if we are measuring density operators $\rho, \sigma \in \mathcal{L}(\mathcal{H})$ which have both have support in the same proper subspace of $\mathcal{H}$ a binary measurement consisting of a projection onto said subspace and a projection on the difference subspace will give measurement outcomes identical to that of $\{\mathrm{id}, 0\}$, and this goes further in that changes to ρ, σ are permissible so long as the support is never the trivial subspace $\{0\}$, in fact pure states will almost always satisfy have support in a proper subspace with the only notable exception being when $\mathcal{H} = \mathbb{C}^2$ i.e. the 1-qubit system. One more method to 'emulate' 'identity measurements' is with limits, consider any binary POVM measurement $\{M_1, M_2\}$ then it is clear that for all $\varepsilon \in (0, 1]$ the POVM measurement $M_\varepsilon = \{(1-\varepsilon)M_1, \varepsilon M_2\}$ is an operationally meaningful POVM measurement but also as $\varepsilon \to 0$ our distribution $\mu_{M_\varepsilon} \to \mu_{\{\text{id},0\}}$ for any density operator by the linearity of the trace, this means we can get distributions ε close to a distribution given by an 'identity measurement' and in many of our applications this is sufficient. Do note that here we mainly focused on binary POVM measurements for simplicity, these arguments also apply to more general 'identity measurements' such as $\{\frac{1}{2}\,\text{id}, \frac{1}{4}\,\text{id}, \frac{1}{4}\,\text{id}\}$ and henceforth we will treat such measurements the same as any other POVM measurement.

3.1.1 Problem Statement

We understand the problem as follows: We have a shared resource $\rho^{AB} \in \mathcal{L}(\mathcal{H}^{\otimes 2})$, we provide Alice access to ρ^A and Bob gets ρ^B. Now, Alice performs some POVM measurement $\{M_i\}_{i\in\mathcal{I}}$ on her ρ^A and Bob performs some *possibly other* POVM measurement $\{M_j\}_{j\in\mathcal{J}}$ on his ρ^B, this process corresponds to measuring the shared resource ρ^{AB} using the POVM $\{M_i \otimes M_j\}_{(i,j)\in\mathcal{I}\times\mathcal{J}}$. After both parties have taken their measurements they 'compare the outcomes and determine if they are equal' and repeat until Alice and Bob know the odds of the two being different. Then coupling optimisation corresponds to a choice of shared resource $\sigma^{AB} \in \mathcal{L}(\mathcal{H}^{\otimes 2})$ with $\rho^A = \text{tr}_B(\sigma^{AB})$ and $\rho^B = \text{tr}_A(\sigma^{AB})$ that minimizes the probability of being different (denoted $\mathbb{P}(X \neq Y)$) and the final outcome is a bound $\|\rho^A - \rho^B\|_{\text{TD}} \leq \mathbb{P}(X \neq Y)$ with saturation for optimised couplings, we may also consider different functions for the odds of being different, i.e. $\|\rho^A - \rho^B\|_{\text{TD}} \leq Q(\mathbb{P}(X \neq Y))$ for some function Q, a particularly interesting pair of examples are the functions $\sqrt{2\mathbb{P}(X \neq Y)}$ and $\sqrt{2\mathbb{P}(X \neq Y) - 1}$ which we will see in a bit.

3.1.2 Why Should Alice and Bob Perform the Same Measurement?

Now, what does it mean to be equal? A simple definition is to choose a function $\iota : \mathcal{I} \to \mathcal{J}$ where we consider the outcome to be 'the same' whenever we find $\iota(i) = j$ and our measurement outcome is $M_i \otimes M_j$, but using this definition and considering the measurement $\{\text{id}, 0\}$ we can either find equality 100% of the time or inequality 100% of the time, instead considering the measurements $\{\text{id}, 0\}$ and $\{p\,\text{id}, (1-p)\,\text{id}\}$ for $p \in [0,1]$ we find $\mathbb{P}(X \neq Y) = p$ for any ρ^A, ρ^B which means, first and foremost, that the bound $\|\rho^A - \rho^B\|_{\text{TD}} \leq \mathbb{P}(X \neq Y)$ only holds for $\|\rho^A - \rho^B\|_{\text{TD}} = 1$, which isn't useful since we already know that $\|\rho^A - \rho^B\|_{\text{TD}} \leq 1$ in general, and the only function Q such that the bound $\|\rho^A - \rho^B\|_{\text{TD}} \leq Q(\mathbb{P}(X \neq Y))$ holds is the function $Q = 1$, i.e. $\|\rho^A - \rho^B\|_{\text{TD}} \leq 1$, again, this is not what we are looking for.

Well then, rather than choosing an arbitrary function $\iota : \mathcal{I} \to \mathcal{J}$ we can also choose one that 'minimizes the difference between the two measurements', it should be noted that this case has potential however it is beyond our scope, we will provide a short argument to persuade the reader that our choice is, if not required, practical. We choose the $\iota \in \text{HomSet}(\mathcal{I} \to \mathcal{J})$ such that the family of operators $(M_j, \sum_{i\in\iota^{-1}\{j\}} M_i)_{j\in\mathcal{J}}$ is minimized in some sense, for example, we could minimize by trying to minimize the trace norm of the operators, however:

Example 3. If M_1 and M_2 are mutually unbiased bases (MUBs) and we measure in these bases then an ι that minimizes the difference between the two measurements is any bijection, this is immediately concerning since we would like a canonical ι, but instead we just have ι a bijection meaning that there are $|M_1|!$ different choices of ι not only is this computationally expensive to compute all possibilities but each choice of bijection is meaningfully different as it corresponds to a permuation of the measurement outcome probabilities for ρ^B.

and if we take $|0\rangle, |1\rangle \in M_1$ then we find

$$\| |0\rangle\langle 0| - |0\rangle\langle 0| \|_{\mathrm{TD}} = 0$$
$$\| |0\rangle\langle 0| - |1\rangle\langle 1| \|_{\mathrm{TD}} = 1$$

now, note that since $|0\rangle\langle 0|$ is a pure state our shared resource must be $|0\rangle\langle 0|^{\otimes 2}$ or $|0\rangle\langle 0| \otimes |1\rangle\langle 1|$, given this we find

$$\begin{aligned}
&\mathbb{P}(X \neq Y) \\
&= \sum_{|\psi\rangle \in M_2 \setminus \iota(|0\rangle\langle 0|)} \mathrm{tr}(|0\rangle\langle 0| \otimes |\psi\rangle\langle\psi| \, |0\rangle\langle 0|^{\otimes 2}) \\
&= \sum_{|\psi\rangle \in M_2 \setminus \iota(|0\rangle\langle 0|)} \mathrm{tr}(|0\rangle\langle 0| \, |0\rangle\langle 0|) \, \mathrm{tr}(|\psi\rangle\langle\psi| \, |0\rangle\langle 0|) \\
&= \sum_{|\psi\rangle \in M_2 \setminus \iota(|0\rangle\langle 0|)} 1 \times \mathrm{tr}(|\psi\rangle\langle\psi| \, |0\rangle\langle 0|) \\
&= \sum_{|\psi\rangle \in M_2 \setminus \iota(|0\rangle\langle 0|)} \frac{1}{|M_2|} && \text{since } M_1 \text{ and } M_2 \text{ are MUBs} \\
&= \frac{|M_2| - 1}{|M_2|}
\end{aligned}$$

but notice that replacing $|0\rangle\langle 0|^{\otimes 2}$ with $|0\rangle\langle 0| \otimes |1\rangle\langle 1|$ does not change the above argument, and thus we also have $\mathbb{P}(X \neq Y) = \frac{|M_2|-1}{|M_2|}$ for the shared resource $|0\rangle\langle 0| \otimes |1\rangle\langle 1|$. For $\mathcal{H} = \mathbb{C}^2$ we know that $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$ and $\{|+\rangle\langle +|, |-\rangle\langle -|\}$ are MUBs meaning that $\mathbb{P}(X \neq Y) = \frac{1}{2}$ for both of the above cases and would imply that $\| |0\rangle\langle 0| - |1\rangle\langle 1| \|_{\mathrm{TD}} \leq \mathbb{P}(X \neq Y) = \frac{1}{2}$ but we already know that $\| |0\rangle\langle 0| - |1\rangle\langle 1| \|_{\mathrm{TD}} = 1$, this means that the basic inequality is falsified whenever there exist MUBs in the Hilbert Space (since clearly $\frac{|M_2|-1}{|M_2|} < 1$ for all $|M_2| \in \mathbb{N}$).

In the next subsection, we show that there is a need to restrict measurements, this (obviously) also applies to the general case wherein we permit Alice and Bob to perform different measurements and thus if such a path were to be pursued the question of what measurements are permissible is that much harder, especially from the algebraic side of things.

3.1.3 The Need for Restrictions for Measurements

Henceforth we will assume that Alice and Bob are performing the same measurements on their quantum states, we now show that it is not feasible to permit arbitrary measurements and thus demonstrate the need for restrictions to the measurements that Alice and Bob are permitted to perform.

Let ρ^{AB} be our shared resource, our measurements will be of the form $M_2 = \{\frac{1}{2}\,\mathrm{id}, \frac{1}{2}\,\mathrm{id}\}$, $M_3 = \{\frac{1}{3}\,\mathrm{id}, \frac{1}{3}\,\mathrm{id}, \frac{1}{3}\,\mathrm{id}\}, \ldots$, explicitly: $M_n = \bigsqcup_{k=1}^{n} \frac{1}{n}\,\mathrm{id}$ then the probability of inequality is

$$\begin{aligned}
\mathbb{P}(X_n \neq Y_n) &= \sum_{i=1}^{n} \sum_{j \neq i} \mathrm{tr}((\frac{1}{n}\,\mathrm{id})^{\otimes 2} \rho^{AB}) \\
&= \sum_{i=1}^{n} \sum_{j \neq i} \mathrm{tr}(\frac{1}{n}^2 \rho^{AB}) && \text{since } \mathrm{id}^{\otimes 2} \text{ is the identity of } \mathcal{H}^{\otimes 2} \\
&= \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j \neq i} \mathrm{tr}(\rho^{AB}) && \text{by the linearity of the trace} \\
&= \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j \neq i} 1 && \text{since } \rho^{AB} \text{ is a density operator} \\
&= \frac{1}{n^2} \sum_{i=1}^{n} (n-1) \\
&= \frac{n(n-1)}{n^2} = 1 - \frac{1}{n}
\end{aligned}$$

We now show that there exists a spectrum of measurements between every M_n and M_{n+1} such that $\mathbb{P}(X \neq Y)$ is continuous over spectrum, and since we start by performing the measurements M_n and end up performing the measurements M_{n+1} we must therefore have a measurement in the spectrum such that $\mathbb{P}(X \neq Y) = k$ for any $k \in [\frac{n-1}{n}, \frac{n}{n+1}]$. Let $\delta(x) = \frac{(n+1)-x}{n+1}$, then $(x, \delta(x))$ is the line that passes through $(0,1)$ and $(1, \frac{n}{n+1})$ (hence a continuous function) we define our spectrum of measurements by $\delta(x) M_n \sqcup (1-\delta(x))\,\mathrm{id}$, then each element of our spectrum is indeed a measurement since every operator is positive semi-definite (all of them are identity operators times some non-negative scalar) and as for the completeness equation:

$$\begin{aligned}
\sum_{E \in \delta(x) M_n} E + (1-\delta(x))\,\mathrm{id} &= \sum_{i=1}^{n} \delta(x) \frac{1}{n}\,\mathrm{id} + (1-\delta(x))\,\mathrm{id} \\
&= \delta(x)\,\mathrm{id} + (1-\delta(x))\,\mathrm{id} = \mathrm{id}
\end{aligned}$$

Thus indeed every set in our spectrum is a POVM measurement, moreover we can explicitly calculate

$$\begin{aligned}
\mathbb{P}(X_x = Y_x) &= \sum_{i=1}^{n} \sum_{j \neq i} \mathrm{tr}((\delta(x)\frac{1}{n}\,\mathrm{id})^{\otimes 2} \rho^{AB}) \\
&\quad + \sum_{i=1}^{n} \mathrm{tr}(\frac{\delta(x)}{n}\,\mathrm{id} \otimes (1-\delta(x))\,\mathrm{id}\, \rho^{AB}) \\
&\quad + \sum_{i=1}^{n} \mathrm{tr}((1-\delta(x))\,\mathrm{id} \otimes \frac{\delta(x)}{n}\,\mathrm{id}\, \rho^{AB}) \\
&= \delta(x)^2 \frac{n(n-1)}{n^2} + 2\frac{\delta(x)(1-\delta(x))}{n} \sum_{i=1}^{n} \mathrm{tr}(\mathrm{id}^{\otimes 2} \rho^{AB}) \\
&= \delta(x)^2 \frac{(n-1)}{n} + 2\delta(x)(1-\delta(x))
\end{aligned}$$

$$= \frac{n^2 - x^2 + 2x - 1}{n^2 + n}$$

which lets us find the measurement that gives said probability of inequality.

It should be noted that we can find a measurement such that $\mathbb{P}(X \neq Y) = k$ for any $k \in [0,1)$ but not for $k = 1$, one might think that $\mathbb{P}(X \neq Y) = 1$ iff $\rho^A \perp \rho^B$ however this is not the case.

Example 4. consider the shared resource $\rho^{AB} = \frac{1}{2} |0\rangle\langle 0| \otimes |1\rangle\langle 1| + \frac{1}{2} |1\rangle\langle 1| \otimes |0\rangle\langle 0|$, then we find $\rho^A = \frac{1}{2}\,\mathrm{id} = \rho^B$ and since the trace distance is a metric we must have $\|\rho^A - \rho^B\|_{\mathrm{TD}} = 0$, clearly our states are not orthogonal, but consider the measurement $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$, i.e. measurement in the 0/1 basis, here we find

$$\begin{aligned}\mathbb{P}(X \neq Y) &= \mathrm{tr}(|0\rangle\langle 0| \otimes |1\rangle\langle 1| \rho^{AB}) \\ &\quad + \mathrm{tr}(|1\rangle\langle 1| \otimes |0\rangle\langle 0| \rho^{AB}) \\ &= \frac{1}{2} + \frac{1}{2} = 1\end{aligned}$$

In other words to find a measurement such that $\mathbb{P}(X \neq Y) = 1$ we need to find POVM measurements $\{M_i\}_{i\in\mathcal{I}}$ such that $\mathrm{tr}_A(\mathrm{id} \otimes M_i \rho^{AB}) \perp \mathrm{tr}_B(M_i \otimes \mathrm{id}\, \rho^{AB})$ meaning that, when observed the reduced density operators look orthogonal, from the above it is also clear that this is an iff statement since whenever $M_i^{\otimes}2\rho^{AB} \neq 0$ we have some chance $p > 0$ such that $X = i$ and $Y = i$, i.e. $\mathbb{P}(X = Y) > 0 \implies \mathbb{P}(X \neq Y) < 1$. This does mean that if our shared resource is e.g. $|0\rangle\langle 0|^{\otimes 2}$ there is no measurement such that $\mathbb{P}(X \neq Y) = 1$.

3.2 Measurement Systems

This section introduces measurement systems, we will be developing our understanding of these mathematical structures and giving results on quantum coupling in the language of measurement systems from here on out.

Definition 7 (M-System)**.** Let $\mathcal{H}$ be a Hilbert space and $\mathcal{D} \subset \mathcal{L}(\mathcal{H}^{\otimes 2})$ a set of density operators, then a measurement system (M-System) over $\mathcal{D}$ is a collection $\{M_\rho\}_{\rho\in\mathcal{D}}$ where each M_ρ is a non-empty set of POVMs on $\mathcal{H}$ and we satisfy

- Trivial Motion: For $\rho \in \mathcal{D}$ if $\rho' := U^{\otimes 2}\rho U^{\otimes 2\dagger} \in \mathcal{D}$ for some unitary $U \in \mathrm{SL}(\mathcal{H})$ then

$$M_{\rho'} = \{\{U M_i U^\dagger\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in M_\rho\}$$

Remark. For clarification: $\{M_\rho\}_{\rho\in\mathcal{D}}$ is a family of sets, i.e. given a density operator $\rho \in \mathcal{D}$ (corresponding with a global state) we find an associated **set** M_ρ where all of $\{M_i\}_{i\in\mathcal{I}} \in M_\rho$ are POVM measurements over a local system $\mathcal{H}$. Explicitly $\mathcal{D} \subset \mathcal{L}(\mathcal{H}^{\otimes 2})$ where $\rho \in \mathcal{D}$ is a density operator and $\{M_i\}_{i\in\mathcal{I}} \subset \mathcal{P}(\mathcal{L}(\mathcal{H}))$ such that $\{M_i\}_{i\in\mathcal{I}}$ is a POVM measurement.

Remark. A key aspect is that the set $\mathcal{D}$ is not determined, we may thus consider a quantum coupling of $\rho, \sigma \in \mathcal{H}$ to be any $\rho^{AB} \in \mathcal{D}$ such that $\mathrm{tr}_B(\rho^{AB}) = \rho^A = \rho$ and

$\mathrm{tr}_A(\rho^{AB}) = \rho^B = \sigma$ and so part of our investigation is to understand which sets $\mathcal{D}$ are 'well-behaved' with respect to some analogue to the classical coupling bound.

The trivial motion condition is meant to capture the fact that the trace distance is invariant under unitary transforms (see Prop. 8), i.e. an M-System isn't tied to a particular choice of basis. The name comes from Geometric Rigidity theory as M-Systems happen to share some key similarities, in particular the factoring of isomorphisms, we however, do not factor out all isomorphisms since an attempt to do so leads to complications in both proofs and also does not admit an intuitive notion of M-System addition.

Definition 8. Let $\mathcal{D} \subset \mathcal{L}(\mathcal{H})$ be a set of density operators, then $\mathcal{D}$ is *full* if for every pair of density operators $\rho, \sigma \in \mathcal{L}(\mathcal{H})$ there exists an operator $\rho^{AB} \in \mathcal{D}$ such that $\rho^A = \rho$ and $\rho^B = \sigma$.

Remark. Ultimately we want to understand and work with full sets of density operators $\mathcal{D}$, and if such is the case we speak of the M-System over $\mathcal{D}$ as being full.

Though not particularly insightful, all of our key M-Systems satisfy a symmetry condition, hence we will spell it out:

Definition 9 (Symmetric M-System)**.** An M-System $\{M_\rho\}_{\rho\in\mathcal{D}}$ is regular if it satisfies the symmetry condition.

- Symmetry: If $\rho \in \mathcal{D}$ and $U_{\text{SWAP}}\rho U_{\text{SWAP}}^\dagger \in \mathcal{D}$ where $U_{\text{SWAP}} \in \mathrm{SL}(\mathcal{H}^{\otimes 2})$ is the unitary that maps $a \otimes b \mapsto b \otimes a$ for $a, b \in \mathscr{B}$, $\mathscr{B}$ an orthonormal basis of $\mathcal{H}$ then

$$M_\rho = M_{U_{\text{SWAP}}\rho U_{\text{SWAP}}^\dagger}$$

Definition 10 (Simple M-System)**.** An M-System $\{M_\rho\}_{\rho\in\mathcal{D}}$ is simple if forall $\rho, \sigma \in \mathcal{D} : M_\rho = M_\sigma$.

Definition 11 (Regular M-System)**.** An M-System $\{M_\rho\}_{\rho\in\mathcal{D}}$ is regular if

$$(\forall \rho \in \mathcal{D})(\forall U \in \mathrm{SL}(\mathcal{H}))(M_\rho = \{\{UM_iU^\dagger\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in M_\rho\})$$

i.e. if $M \in M_\rho$ then applying a change of basis to the measurement operators gives us another measurement $M' \in M_\rho$.

Remark. It should be noted that being regular is not implied by trivial motion, trivial motion gives us the same behaviour as regularity whenever $U \in \mathrm{SL}(\mathcal{H})$ is such that $U^{\otimes 2}\rho U^{\otimes 2\dagger} = \rho$ but this only holds for a subgroup of $\mathrm{SL}(\mathcal{H})$.

Remark. It should be immediately clear that being simple is a stricter condition than being symmetric, indeed simple $\implies$ symmetric but one of our core M-Systems of interest, those that fall under a maximal total variation measurement scheme, are not simple or regular but are symmetric. Finally regular and simple are distinct, there are clear examples of regular M-Systems that aren't simple and M-Systems that are simple but not regular, this is a direct consequence of the fact that there exists no unitary U such that $U|0\rangle\langle 0|U^\dagger = \frac{1}{2}\,\mathrm{id}$ (there is no such unitary since if there were then

$$\frac{1}{2} = \mathrm{tr}((\frac{1}{2}\,\mathrm{id})^2)$$

$$= \mathrm{tr}(U\,|0\rangle\,\langle 0|\,U^{\dagger}U\,|0\rangle\,\langle 0|\,U^{\dagger})$$
$$= \mathrm{tr}(U(|0\rangle\,\langle 0|)^{2}U^{\dagger})$$
$$= \mathrm{tr}(U^{\dagger}U(|0\rangle\,\langle 0|)^{2})$$
$$= 1$$

but clearly $\frac{1}{2} \neq 1$)

Before going any further we introduce the notion of a measurement scheme. For example the arbitrary measurement scheme is simply the collection of all M-Systems with $M_\rho = \Gamma(\mathcal{H})$ for all $\rho \in \mathcal{D}$ where $\{M_i\}_{i\in\mathcal{I}} \in \Gamma(\mathcal{H})$ iff $\{M_i\}_{i\in\mathcal{I}}$ is a POVM measurement over $\mathcal{H}$. That is to say, measurement schemes are just swathes of M-Systems that we group together due to shared properties.

Remark. It should be noted that every M-System in the arbitrary measurement scheme is simple and regular.

We will now introduce some basic results surrounding M-Systems before moving on to the core problem: quantum coupling functions.

Definition 12 (unital closure)**.** A set $\mathcal{D} \subset \mathcal{L}(\mathcal{H}^{\otimes 2})$ of density operators is closed under unitaries if forall $U \in \mathrm{SL}(\mathcal{H})$, $\rho \in \mathcal{D}$ implies that $U^{\otimes 2}\rho U^{\otimes 2\dagger} \in \mathcal{D}$, if $\mathcal{D}$ is a set of density operators we denote its closure by $\overline{D}$ (where $\overline{D} = \{U^{\otimes 2}\rho U^{\otimes 2\dagger} : \rho \in \mathcal{D}, U \in U(\mathcal{H})\}$).

Proposition 10. $\overline{\overline{\mathcal{D}}} = \overline{\mathcal{D}}$.

Proof. Immediate from the composition of unitaries being a unitary. □

Definition 13 (unital closure)**.** Let $\mathcal{M}$ be a M-System over $\mathcal{D}$ then the unital closure of $\mathcal{M}$ is an M-System over $\overline{\mathcal{D}}$, denoted $\overline{\mathcal{M}}$, that agrees with $\mathcal{M}$ on $\rho \in \mathcal{D}$, i.e. for $\rho \in \mathcal{D}$: $M_\rho \in \mathcal{M}$ and $\overline{M_\rho} \in \overline{\mathcal{M}}$ are equal ($M_\rho = \overline{M_\rho}$).

Lemma 11. *For any M-System, $\mathcal{M}$, there exists a unique unital closure of $\mathcal{M}$.*

Proof. Let $(M_\rho)_{\rho\in\mathcal{D}}$ be an M-System, then the unital closure is $(\overline{M_\rho})_{\rho\in\overline{\mathcal{D}}}$ where $\overline{M_\rho} = M_\rho$ for $\rho \in \mathcal{D}$ and for $\rho' \in \overline{\mathcal{D}}\backslash\mathcal{D}$ there exists a $\rho \in \mathcal{D}$ and a unitary $U \in U(\mathcal{H})$ s.t. $U^{\otimes 2}\rho U^{\dagger\otimes 2} = \rho' \in \overline{\mathcal{D}}$ (see Defn. 12) thus to satisfy trivial motion (see Defn. 7) we must have $M_{\rho'} = \{\{UM_iU^{\dagger}\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in M_\rho\}$.

Now for the sake of a contradiction suppose we find conflicting $\rho, \sigma \in \mathcal{D}$ such that $\{\{U_1M_iU_1^{\dagger}\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in M_\rho\}$ induced by ρ does not equal $\{\{U_2M_iU_2^{\dagger}\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in M_\sigma\}$ induced by σ. Here we have $U_1^{\otimes 2}\rho U_1^{\dagger\otimes 2} = \rho' = U_2^{\otimes 2}\sigma U_2^{\dagger\otimes 2}$ for some unitaries U_1, U_2 and thus $(U_2^{\dagger}U_1)^{\otimes 2}\rho(U_2^{\dagger}U_1)^{\dagger\otimes 2} = \sigma$, thus by trivial motion we get $M_\sigma = \{\{U_2^{\dagger}U_1M_i(U_2^{\dagger}U_1)^{\dagger}\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in M_\rho\}$, since unitaries are isomorphisms this induces a bijection $F = G \circ H : M_\rho \to M_\sigma$ where both $G : M_{\rho'} \to M_\sigma$ and $H : M_\rho \to M_{\rho'}$. Again, G and H are bijections since unitaries are isomorphisms whose existence is a contradiction (we would no longer have the conflict between $M_{\rho'}$ as induced by ρ in comparison to σ) thus we assume there does not exist a bijection F, i.e. either the unitary U_1 or the unitary U_2 do not exist, thus $M_{\rho'}$ is well-defined. Note that the above is sufficient for uniqueness while for existence we must finish off by showing that there exist no contradictions as described above for the cases of $\rho \in \mathcal{D}$ and $\sigma \in \overline{\mathcal{D}} \setminus \mathcal{D}$, or $\rho, \sigma \in \overline{\mathcal{D}} \setminus \mathcal{D}$. This follows immediately by considering $\rho_1, \sigma_1 \in \mathcal{D}$ with $U_1^{\otimes 2} \rho_1 U_1^{\otimes 2\dagger} = \rho$ and $U_2^{\otimes 2} \sigma_1 U_2^{\otimes 2\dagger} = \sigma$ (which exist directly from Defn. 12 and considering the identity unitary for $\rho \in \mathcal{D}$) then $M_{\rho'}$ is an M-System as:

- We have already shown that $\rho, \sigma \in \mathcal{D}$ lead to a consistent $M_{\rho'}$.
- If at least one of $\rho, \sigma \notin \mathcal{D}$ then there exist $\rho_1, \sigma_1 \in \mathcal{D}$ as described above and if ρ, ρ', σ do not satisfy trivial motion then we have $U^{\otimes 2} U \rho_1 U^{\otimes 2\dagger} = \sigma_1$ but $M_{\sigma_1} \neq \{\{U M_i U^\dagger\}_{i \in \mathcal{I}} : (M_i)_{i \in \mathcal{I}} \in M_{\rho_1}\}$ (as in the initial case, this follows as unitaries are isomorphisms to we have a chain of bijections), i.e. $\rho_1, \sigma_1 \in \mathcal{D}$ do not satisfy trivial motion and $\mathcal{M}$ is not an M-System, but $\mathcal{M}$ is an M-System and thus $\overline{\mathcal{M}}$ satisfies trivial motion.

□

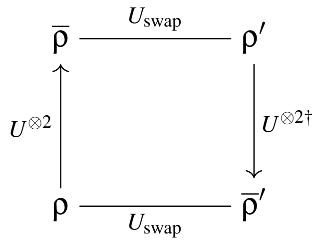
Proposition 12. *We have the following implications*

- *$\overline{\mathcal{M}}$ is simple (symmetric) $\implies$ $\mathcal{M}$ is simple (symmetric).*
- *$\mathcal{M}$ is regular iff $\overline{\mathcal{M}}$ is regular.*
- *$\mathcal{M}$ is regular and simple iff $\overline{\mathcal{M}}$ is regular and simple.*

Proof. For every $\rho \in \mathcal{D}$ we have $M_\rho = \overline{M}_\rho$, thus if $\overline{\mathcal{M}}$ is symmetric then clearly $\mathcal{M}$ is symmetric, if $\overline{\mathcal{M}}$ is simple then clearly $\mathcal{M}$ is simple, and likewise if $\overline{\mathcal{M}}$ is regular then by the same argument we get that $\mathcal{M}$ is regular, however if $\mathcal{M}$ has $\mathcal{D} = \{|0\rangle\langle 0|\}$ over $\mathcal{H}$ the 1-qubit system then letting $M_{|0\rangle\langle 0|} = \{\{|0\rangle\langle 0|, |1\rangle\langle 1|\}\}$ we can easily verify that $\mathcal{M}$ is an M-System, clearly it is simple but $\overline{M}$ is not simple, since $|+\rangle\langle +| \in \overline{\mathcal{D}}$ but by direct calculation we find $M_{|+\rangle\langle +|} = \{|+\rangle\langle +|, |-\rangle\langle -|\} \neq M_{|0\rangle\langle 0|}$. Thus we have shown that $\overline{\mathcal{M}}$ is simple/regular $\implies$ $\mathcal{M}$ is simple/regular respectively and that $\mathcal{M}$ is simple $\not\Longrightarrow$ $\overline{\mathcal{M}}$ is simple, we now suppose that $\mathcal{M}$ is regular, then for every $\rho \in \overline{D}$ we have some $\rho' \in \mathcal{D}$ and some unitary $U \in \mathrm{SL}(\mathcal{H})$ such that $U^{\otimes 2} \rho' U^{\otimes 2\dagger} = \rho$, in the proof of existence and uniqueness of the unital closure (Lemma 11) we've shown that $M_\rho = \{\{U M_i U^\dagger\}_{i \in \mathcal{I}} : \{M_i\}_{i \in \mathcal{I}} \in M_{\rho'}\}$ but since $\mathcal{M}$ is regular we know that every $\{U M_i U^\dagger\}_{i \in \mathcal{I}} \in M_{\rho'}$ and infact the two sets are equal, thus $M_\rho = M_{\rho'}$ but then M_ρ satisfies the regularity condition and so $\overline{\mathcal{M}}$ is regular, finally notice that if $\mathcal{M}$ is simple then since we have $M_\rho = M_{\rho'}$ for every $\rho \in \overline{D}$ and we must have $\overline{\mathcal{M}}$ be simple. □

Remark. We can see visualise why $\mathcal{M}$ being symmetric does not imply that $\overline{\mathcal{M}}$ is symmetric even when $\mathcal{M}$ is regular by considering $\mathcal{D} = \{\rho, \rho'\}$ with $U \neq \mathrm{id}$ and

$\rho' = U_{\text{swap}} U^{\otimes 2\dagger} \rho U^{\otimes 2} U_{\text{swap}}^{\dagger}$ then we simply pick $M_\rho \neq M_{\rho'}$ and the diagram



clearly shows the issue, note that this could be amended by requiring symmetric M-Systems to satisfy a stronger symmetry condition, one such that symmetry holds after composition with any unitary $U^{\otimes 2} \cdot U^{\otimes 2\dagger}$.

Remark. In the above we've show that $\mathcal{M}$ is simple $\not\Longrightarrow$ $\overline{\mathcal{M}}$ is simple using a contrived example, fig. 4.2 and the corresponding representative set is a meaningful instance of this fact and demonstrates how simplicity can be induced by choosing 'good' representations (see Defn. 17).

See section 3.4, Von Neumann measurement scheme, for a practical application of the above to quantum coupling functions (Defn. 14), in particular to derive the initial quantum coupling (Defn. 15).

3.3 Quantum Coupling Functions

Quantum coupling functions are the generalised analogue to the classical coupling function and our success in constructing these bounds is exactly the aim of the project.

Definition 14 (Quantum Coupling Function)**.** Let $A = B = \mathcal{H}$, $\mathcal{H}$ a Hilbert space, let $\mathcal{D} \subset \mathcal{L}(A \otimes B)$, $\mathcal{D}$ consisting of density operators, then a quantum coupling function (q.c) is a function $Q : [0,1] \to \mathbb{R}^+$ (non-negative reals, including 0) and an M-System $(M_{\rho^{AB}})_{\rho^{AB} \in \mathcal{D}}$ such that for every $\rho^{AB} \in \mathcal{D}$ and every POVM $\{M_i\}_{i \in \mathcal{I}} \in M_{\rho^{AB}}$ we have

$$\|\rho^A - \rho^B\|_{\text{TD}} \leq Q(\mathbb{P}(X \neq Y))$$

where X represents measurement of ρ^A w.r.t. $\{M_i\}_{i \in \mathcal{I}}$ and Y represents measurement of ρ^B w.r.t. $\{M_i\}_{i \in \mathcal{I}}$. Explicitly:

$$\begin{aligned}
\mathbb{P}(X \neq Y) &= \sum_{i \in \mathcal{I}} \operatorname{tr}(M_i \otimes (\text{id} - M_i) \rho^{AB}) \\
&= 1 - \sum_{i \in \mathcal{I}} \operatorname{tr}(M_i^{\otimes 2} \rho^{AB}) \\
&= 1 - \mathbb{P}(X = Y)
\end{aligned}$$

Definition 15 (Initial Quantum Coupling)**.** A q.c $\overline{Q}$ is initial if for any other q.c Q over the same M-System we have $\overline{Q} \leq Q$, we use the bar to indicate that a q.c is initial.

Remark. The name initial comes from category theory Leinster (2016), wherein $\overline{Q}$ is the initial object of the category of quantum couplings with an arrow $A \to B$ whenever $A \leq B$ for objects A, B.

Lemma 13. *For any M-System there exists a unique initial q.c.*

Proof. Uniqueness: if $\overline{Q_1}$ and $\overline{Q_2}$ are both initial then by Defn. 15: $\overline{Q_1} \leq \overline{Q_2} \leq \overline{Q_1}$, and thus $\overline{Q_1} = \overline{Q_2}$.

Existence: for $x \in [0,1]$ let $B_x = \{\rho^{AB} : (\exists (M_i)_{i\in\mathcal{I}} \in M_{\rho^{AB}})(\mathbb{P}(X \neq Y) = x)\}$ then define

$$\overline{Q}(x) = \begin{cases} \sup_{\rho^{AB}\in B_x} \|\rho^A - \rho^B\|_{\text{TD}} & \text{for } B_x \neq \emptyset \\ 0 & \text{otherwise} \end{cases}$$

for any $\rho^{AB} \in \mathcal{D}$ and any $(M_i)_{i\in\mathcal{I}} \in M_{\rho^{AB}}$ let $x = \mathbb{P}(X \neq Y)$, then $\rho^{AB} \in B_x$ and so

$$\begin{aligned} \|\rho^A - \rho^B\|_{\text{TD}} &\leq \sup_{\sigma^{AB}\in B_x} \|\sigma^A - \sigma^B\|_{\text{TD}} \\ &= \overline{Q}(x) = \overline{Q}(\mathbb{P}(X \neq Y)) \end{aligned}$$

thus $\overline{Q}$ is a q.c.

Now suppose there exists a q.c such that $Q(x) < \overline{Q}(x)$ for some $x \in [0,1]$, then for said x there exists a sequence $\rho_n^{AB} \in B_x$ for $n \in \mathbb{N}$ such that
$\|\rho_n^A - \rho_n^B\|_{\text{TV}} \to \sup_{\rho^{AB}\in B_x} \|\rho^A - \rho^B\|_{\text{TV}}$ as $n \to \infty$, thus eventually $\|\rho_n^A - \rho_n^B\| > Q(x)$ (or alternatively if $B_x = \emptyset$ then $\overline{Q}(x) = 0$ and Q is negative, hence not a q.c) and thus $Q(x)$ is not a q.c, hence $\overline{Q}$ is initial. □

Remark. We may therefore speak of *the* initial/optimal quantum coupling of some M-System.

Example 5. We now take a small break to apply what we have introduced to M-Systems in the arbitrary measurement scheme, based on our results in subsection 3.1.3, the need for restrictions for measurements, we've shown that for any shared resource, i.e. $\rho^{AB} \in \mathcal{D}$, we can find measurements such that $\mathbb{P}(X \neq Y) = k$ for $k \in [0,1)$ then let us take $c = \sup_{\rho^{AB}\in\mathcal{D}} \|\rho^A - \rho^B\|_{\text{TD}}$, then there must also exist a sequence $(\rho_n^{AB})_{n\in\mathbb{N}} \subseteq \mathcal{D}$ such that $\lim_{n\to\infty} \|\rho^A - \rho^B\|_{\text{TD}} = c$, now for each $k \in [0,1)$ there exists a measurement, M_n, such that $\mathbb{P}(X_n \neq Y_n) = k$ which means that $\lim_{n\to\infty} \overline{Q}(\mathbb{P}(X_n \neq Y_n)) = \overline{Q}(k) \geq \lim_{n\to\infty} \|\rho_n^A - \rho_n^B\|_{\text{TD}} = c$, moreover there does not exist ρ^{AB} with $\|\rho^A - \rho^B\|_{\text{TD}} > c$ and thus $\overline{Q}(k) = C$ for all $k \in [0,1)$, this means that the initial coupling over any M-System in the arbitrary measurement scheme is finite-valued, taking at-most 2 values, if the q.c is continuous, a desireable property to have, then it is constant and in the case that there exists $\rho^{AB} \in \mathcal{D}$ such that $\rho^A \perp \rho^B$ then clearly $\|\rho^A - \rho^B\|_{\text{TD}} = 1$ and by performing a measurement $\{M_1, M_2\}$ with $M_1 \perp \rho^B$ and $M_2 \perp \rho^A$ (e.g. the measurement consisting of a projection onto the support of ρ^A and a projection onto the support of ρ^B) we find $\mathbb{P}(X \neq Y) = 1$ and thus $\overline{Q} = 1$. Clearly, the arbitrary measurement scheme is uninformative, and thus we can conclude, using the language of M-Systems, that there is a need for measurement restriction.

The final key ingredient is a notion of saturation:

Definition 16 (Saturated in State)**.** A q.c, Q, is saturated in state-space/saturated in state/saturated if for all $\rho^{AB} \in \mathcal{D}$ there exists some σ^{AB} with $\rho^A = \sigma^A$ and $\rho^B = \sigma^B$ and there exists a measurement $(M_i)_{i\in\mathcal{I}} \in M_{\sigma^{AB}}$ such that

$$\|\sigma^A - \sigma^B\|_{\text{TD}} = Q(\mathbb{P}(X \neq Y))$$

i.e.

$$(\forall\rho^{AB} \in \mathcal{D})(\exists\sigma^{AB} \in \mathcal{D})(\exists(M_i)_{i\in\mathcal{I}} \in M_{\sigma^{AB}})(\rho^A = \sigma^A)(\rho^B = \sigma^B)$$
$$(\|\sigma^A - \sigma^B\|_{\text{TD}} = Q(\mathbb{P}(X \neq Y)))$$

Lemma 14. *There exists a saturated q.c, Q, if and only if $\overline{Q}$ is saturated in state.*

Proof. the $\Longleftarrow$ case is trivial thus we show $\Longrightarrow$:

If Q is saturated in state then for all $\rho^{AB} \in \mathcal{D}$ there exists $\sigma^{AB} \in \mathcal{D}$ with $\rho^A = \sigma^A$, $\rho^B = \sigma^B$, and a measurement $(M_i)_{i\in\mathcal{I}} \in M_{\sigma^{AB}}$ such that for $x = \mathbb{P}(X \neq Y)$ we have $\|\sigma^A - \sigma^B\|_{\text{TD}} = Q(x)$, but then $\overline{Q}(x) \leq Q(x)$ by Defn. 15 but $\|\sigma^A - \sigma^B\|_{\text{TD}} \leq \overline{Q}(x)$ (since $\overline{Q}$ is a q.c, see Defn. 14) thus $\overline{Q}(x) = \|\sigma^A - \sigma^B\|_{\text{TD}}$ and so $\overline{Q}$ is saturated in state. □

Remark. Given this, we are intimately interested in initial couplings when derivable since they naturally give us saturation, if at all possible, within the M-System we are considering.

3.3.1 Representative Sets

Representative sets give us a clever way to exploit symmetries and parameterise our coupling bound in a way that admits direct computation, this will be and integral to the result given in section 3.4.

Let $\mathcal{D} \subset \mathcal{L}(\mathcal{H}^{\otimes 2})$ be a set of density operators and consider the binary relation $\sim$: $\mathcal{D} \times \mathcal{D} \to \{\text{True}, \text{False}\}$ s.t. for $\rho, \sigma \in \mathcal{D}$ we have $\rho \sim \sigma$ if and only if there exists a unitary, $U \in U(\mathcal{H})$, such that $U^{\otimes 2}\rho U^{\dagger\otimes 2} = \sigma$.

We show this relation is an equivalence:

- Reflexive: $U = \text{id}$ is a unitary, thus $\text{id}^{\otimes 2}\,\rho\,\text{id}^{\otimes 2\dagger} = \rho$ thus $\rho \sim \rho$.
- Symmetric: If $\rho \sim \sigma$ then there exists a unitary, U, s.t. $U^{\otimes 2}\rho U^{\otimes 2\dagger} = \sigma$ then $U^\dagger$ is also a unitary and $U^{\dagger\otimes 2}\sigma U^{\otimes 2} = \rho$, thus $\sigma \sim \rho$.
- Transitive: If $\rho \sim \rho'$ and $\rho' \sim \sigma$ then there exist unitaries U_1, U_2 such that we have

$$\begin{aligned}\sigma &= U_2^{\otimes 2}\rho' U_2^{\dagger\otimes 2}\\ &= U_2^{\otimes 2}U_1^{\otimes 2}\rho U_1^{\dagger\otimes 2}U_2^{\dagger\otimes 2}\\ &= (U_2U_1)^{\otimes 2}\rho(U_2U_1)^{\dagger\otimes 2}\end{aligned}$$

  and thus $\rho \sim \sigma$.

Thus $\sim$ is an equivalence and we define a representative set as a choice of representation of the equivalence classes induced by $\sim$.

Definition 17 (Representative Set)**.** For a set of density operators $\mathcal{D} \subset \mathcal{L}(\mathcal{H}^{\otimes 2})$ a representative set/representation of $\mathcal{D}$ is a set $S \subseteq \mathcal{D}$ such that forall $\rho \in \mathcal{D}$ there exists exactly one $\rho' \in S$ such that for some unitary $U^{\otimes 2}\rho U^{\dagger\otimes 2} = \rho'$.

As shown above, this notion is well-defined and we will now show that the behaviour of a representation of $\mathcal{D}$ w.r.t. a q.c, Q, determines the behaviour of Q over $\mathcal{D}$ and as such a representation of $\mathcal{D}$ is the least amount of states one must consider to understand q.cs over $\mathcal{D}$, we also explore the relation with the unital closure $\overline{D}$.

Proposition 15. *If S is a representation of $\mathcal{D}$ then:*

1. *S is the representation of S.*
2. *$\overline{S} = \overline{\mathcal{D}}$.*
3. *S is a representation of $\overline{\mathcal{D}}$.*
4. *If S is a representation of $\mathcal{D}, \mathcal{D}'$ then $\overline{\mathcal{D}} = \overline{\mathcal{D}'}$.*

Proof. We handle the claims as follows:

1. If there exists a unitary $U \in U(\mathcal{H})$ s.t. for $s_1, s_2 \in S$ with $s_1 \neq s_2$ we have $U^{\otimes 2}s_1U^{\dagger\otimes 2} = s_2$ then s_1 and s_2 belong to the same equivalence class and thus S is not a representative set, thus no such unitaries exist from which it is immediately clear that a representation of S is S and since representations are subsets, for any $S' \subset S$ if S' were a representative set we would have a unitary U for $s \in S \backslash S' \neq \emptyset$ with $U^{\otimes 2}sU^{\dagger\otimes 2} = s' \in S'$, but we have shown no such unitaries exist, thus S is the only representation.
2. Forall $\rho \in \overline{D}$ we have $\rho' \in \mathcal{D}$ and some unitary, $U_1 \in U(\mathcal{H})$, s.t. $U_1^{\otimes 2}\rho' U_1^{\dagger\otimes 2} = \rho$ (see Defn. 12) while by Defn. 17 we have some representative, $\sigma \in S$, such that $U_2^{\otimes 2}\sigma U_2^{\dagger\otimes 2} = \rho'$ and thus we have
$$\begin{aligned}\rho &= U_1^{\otimes 2}U_2^{\otimes 2}\sigma U_2^{\otimes 2\dagger}U_1^{\otimes 2\dagger}\\ &= (U_1U_2)^{\otimes 2}\sigma(U_1U_2)^{\otimes 2\dagger}\end{aligned}$$
thus $\rho \in \overline{S}$, i.e. $\overline{D} \subseteq \overline{S}$ but since $S \subseteq \mathcal{D}$ it is obvious that $\overline{S} \subseteq \overline{\mathcal{D}}$ and thus $\overline{S} = \overline{\mathcal{D}}$.
3. As argued in 2, we know that forall $\rho \in \overline{D}$ we have some $\sigma \in S$ s.t. $\rho = U^{\otimes 2}\sigma U^{\dagger\otimes 2}$, as argued in 1, we know that for any $\sigma, \sigma' \in S$ we have no unitaries $U^{\otimes 2}\sigma U^{\otimes 2\dagger} = \sigma'$, thus the σ in question is unique and the representative of $\rho \in \overline{D}$ and thus the claim holds.
4. Immediately from 2. we have $\overline{\mathcal{D}} = \overline{S} = \overline{\mathcal{D}'}$.

□

Lemma 16. *If S is a representation of $\mathcal{D}$ with M-System $\mathcal{M} = (M_\rho)_{\rho\in\mathcal{D}}$, then Q is a q.c on $\mathcal{M}$ if and only if Q is a q.c on $(M_\sigma)_{\sigma\in S}$ moreover Q is initial on $\mathcal{M}$ if and only if it is the initial coupling over $(M_\sigma)_{\sigma\in S}$.*

Proof. If Q is a q.c on $\mathcal{M}$ then it is clearly a q.c on $(M_\rho)_{\rho\in\mathcal{S}}$, suppose Q is initial on $\mathcal{M}$, since Q is initial we have a sequence of density operators $\rho_n^{AB} \in B_x := \{\rho^{AB} : (\exists (M_i)_{i\in\mathcal{I}} \in M_{\rho^{AB}})(\mathbb{P}(X \neq Y) = x)\}$ for $n \in \mathbb{N}$ such that $\|\rho_n^A - \rho_n^B\|_{\text{TD}} \to Q(x)$ as $n \to \infty$. Now let σ_n^{AB} be the representative of ρ_n^{AB} for all $n \in \mathbb{N}$, then by trivial motion we have $\sigma_n^{AB} \in B_x$ for all $n \in \mathbb{N}$ and since the trace distance is invariant under unitary transform we conclude that $\|\sigma_n^A - \sigma_n^B\| = \|\rho_n^A - \rho_n^B\| \to Q(x)$ as $n \to \infty$ thus Q is initial over $\mathcal{S}$.

Now suppose that Q is a q.c over $(M_\rho)_{\rho\in\mathcal{S}}$, for any $\rho^{AB} \in \mathcal{D}$ and measurement $(M_i)_{i\in\mathcal{I}} \in M_{\rho^{AB}}$, let σ^{AB} be the representative of ρ^{AB}, then there exists a unitary U s.t. $U^{\otimes 2}\rho^{AB}U^{\dagger\otimes 2} = \sigma^{AB}$ and by trivial motion we have $\{UM_iU^\dagger\}_{i\in\mathcal{I}} \in M_{\sigma^{AB}}$, now observe that

$$
\begin{aligned}
\|\rho^A - \rho^B\|_{\text{TD}} &= \|\sigma^A - \sigma^B\|_{\text{TD}} \\
&\leq Q(\mathbb{P}(X_\sigma \neq Y_\sigma)) && \text{since } Q \text{ is a q.c over } \mathcal{S} \\
&= Q(1 - \sum_{i\in\mathcal{I}} \operatorname{tr}((UM_iU^\dagger)^{\otimes 2}\sigma^{AB})) \\
&= Q(1 - \sum_{i\in\mathcal{I}} \operatorname{tr}(M_i^{\otimes 2}(U^{\dagger\otimes 2}\sigma^{AB}U^{\otimes 2}))) && \text{by cyclic property of the trace} \\
&= Q(1 - \sum_{i\in\mathcal{I}} \operatorname{tr}(M_i^{\otimes 2}\rho^{AB})) \\
&= Q(\mathbb{P}(X_\rho \neq Y_\rho))
\end{aligned}
$$

and thus Q is also a q.c over $\mathcal{M}$.

Finally for Q initial over $(M_\rho)_{\rho\in\mathcal{S}}$, let $\overline{Q}$ be initial over $\mathcal{M}$, for any sequence $\rho_n^{AB} \in B_x$ s.t. $\|\rho_n^A - \rho_n^B\|_{\text{TD}} \to \overline{Q}(x)$ as $n \to \infty$ (which must exist since $\overline{Q}$ is initial, except for $B_x = \emptyset$ in which case $\overline{Q}(x) = 0 = Q(x)$) we take the representative σ_n^{AB} of ρ_n^{AB} which gives $\|\sigma_n^A - \sigma_n^B\|_{\text{TD}} \to \overline{Q}(x)$ and thus since Q is a q.c we have $\overline{Q}(x) \leq Q(x)$ but trivially $Q(x) \leq \overline{Q}(x)$ and thus $Q \leq \overline{Q} \leq Q$ and thus $Q = \overline{Q}$ and the initial q.c over $(M_\rho)_{\rho\in\mathcal{S}}$ is the initial q.c over $\mathcal{M}$. □

Proposition 17. *Let $\mathcal{M}$ be an M-System, if Q is a q.c over $\mathcal{M}$ then Q is a q.c over $\overline{\mathcal{M}}$, moreover if Q is initial over $\mathcal{M}$ then it is initial over $\overline{\mathcal{M}}$.*

Proof. Let S be a representation of $\mathcal{D}$ where $\mathcal{M}$ is over $\mathcal{D}$, then by Prop. 15 (part 3) S is also a representation of $\overline{D}$, and the claim follows immediately by Lemma 16. □

Proposition 18. *Let $S \subseteq \mathcal{D}_{pure} = \{\rho\otimes\sigma : \rho,\sigma \in \mathcal{L}(\mathcal{H}) : \rho,\sigma$ are pure states$\}$, then S is a representation of $\mathcal{D}_{pure}$ if and only if the map $\|\operatorname{tr}_B(\cdot) - \operatorname{tr}_A(\cdot)\|_{\text{TD}} : S \to [0,1]$ is a bijection.*

Proof. Since the representation of ρ has the same trace distance as ρ we know that S must induce a surjection immediately. Now suppose that for $s_1^{AB}, s_2^{AB} \in S$ we have $\|s_1^A - s_1^B\|_{\text{TD}} = \|s_2^A - s_2^B\|_{\text{TD}}$, since $s_1^{AB}, s_2^{AB} \in \mathcal{D}_{\text{locally pure}}$ we know that the relevant density operators are pure and thus we know that $1 \leq \dim\operatorname{span}\{s_1^A, s_1^B\} \leq 2$ (and likewise for s_2^{AB}), if $\dim\operatorname{span}\{s_1^A, s_1^B\} = 1$ then since s_1^A and s_1^B are colinear density operators we must have $s_1^A = s_1^B$, thus $\|s_1^A - s_1^B\|_{\text{TD}} = 0 = \|s_2^A - s_2^B\|_{\text{TD}}$, since the trace distance is a norm we have $s_2^A = s_2^B$ by the non-degenerate property of a norm. But then S is not a representation as for any pair of pure density operators we have a unitary s.t. $Us_1^AU^\dagger = s_2^A$, i.e. s_1^{AB} and s_2^{AB} belong to the same equivalence class and thus S is not a representative set. Otherwise if $\dim\operatorname{span}\{s_1^A, s_1^B\} = 2$ we can immediately see that $\dim\operatorname{span}\{s_2^A, s_2^B\} = 2$ (we've already shown that $\dim\operatorname{span}\{s_2^A, s_2^B\} = 1 \iff \dim\operatorname{span}\{s_1^A, s_1^B\} = 1$) Notice that since s_1^A, s_1^B are pure states they exist in a subspace isomorphic to the one qubit system $\mathbb{C}^2$, call the elements of an orthonormal basis of this subspace $|0\rangle\langle 0|$ and $|1\rangle\langle 1|$. Let U be a unitary such that $Us_1^AU^\dagger = |0\rangle\langle 0|$ and U' be a unitary such that $U's_1s_2^AU'^\dagger = |0\rangle\langle 0|$. Finally, if $\|s_1 - s_2\|_{\mathrm{TD}} = p$ then $Us_1^BU^\dagger$ and $U's_2^BU'^\dagger$ are one of $((1-p^2)|0\rangle + e^{i\theta}p^2|0\rangle)((1-p^2)\langle 0| + e^{i\theta}p^2\langle 0|)$ (these are the only states in the subspace that satisfy the trace distance condition, that are also pure states) for some (possibly distinct) phases θ, but then rotating around $|0\rangle$ gives an isomorphism, and thus s_1^{AB} and s_2^{AB} belong to the same equivalence class.

Finally, if S induces the bijection described above then for any ρ^{AB} we will show that $\sigma^{AB} \in \{\rho'^{AB} \in S : \|\rho'^A - \rho'^B\|_{\mathrm{TD}} = \|\rho^A - \rho^B\|_{\mathrm{TD}}\}$ belongs to the same equivalence class thus completing the proof.

Note that this follows exactly as above, if $\|\rho^A - \rho^B\|_{\mathrm{TD}} = 0$ then $\rho^A = \rho^B$ (and also $\sigma^A = \sigma^B$ since $\|\cdot\|_{\mathrm{TD}}$ is a norm), we have an isomorphism $U\rho^AU^\dagger = \sigma^A$ and thus σ^{AB} and ρ^{AB} belong to the same equivalence class. While for $\rho^A \neq \rho^B$ we again map the 2-dimensional subspace containing ρ^A, ρ^B to the 2-dimensional subspace containing σ^A, σ^B, take an orthonormal basis of this subspace and call the first element $|0\rangle\langle 0|$ and the second element $|1\rangle\langle 1|$, again map $U\sigma^AU^\dagger = |0\rangle\langle 0|$ and $U'\rho^AU'^\dagger = |0\rangle\langle 0|$, then as before $U\sigma^BU^\dagger$ and $U'\rho^BU'^\dagger$ are isomorphic up to rotation around the $|0\rangle\langle 0|$ and thus σ^{AB} and ρ^{AB} belong to the same equivalence class, as desired. □

3.4 basics of the Von Neumann Measurement scheme

As teased at the start of subsection 3.3.1, representative sets, we now apply our tools to the following M-System in the Von Neumann measurement scheme (in the Von Neumann measurement scheme exactly the Von Neumann measurements are permitted): our set $\mathcal{D}$ is the set of pure states of the 1-qubit system, explicitly

$$\mathcal{D} = \{\rho \otimes \sigma \in \mathcal{L}((\mathbb{C}^2)^{\otimes 2}) : \operatorname{tr}(\rho^2) = \operatorname{tr}(\sigma^2) = 1, \text{ and } \rho \text{ and } \sigma \text{ are density operators}\}$$

and

$$M_\rho = \{(E_i)_{i\in\{1,2\}} : E_1 \in \mathcal{L}(\mathcal{H}) \text{ and } E_2 \in \mathcal{L}(\mathcal{H}) \text{ are idempotent rank 1 projectors}\}$$

Clearly this M-System, $\mathcal{M}$, is simple and a change of basis does not change the rank of a matrix (and the resulting matrix will still be idempotent since $(U\Pi U^\dagger)^2 = U\Pi UU^\dagger\Pi U^\dagger = U\Pi^2U^\dagger = U\Pi U^\dagger$) thus the M-System is also regular. Now, by the completeness equation, we know that $E_1 + E_2 = \mathrm{id} \implies E_2 = \mathrm{id} - E_1$ and every rank 1 idempotent projector is of the form $|\psi\rangle\langle\psi|$ by spectral decomposition, now every $|\psi\rangle \in \mathbb{C}^2$ is a linear combination of $a|0\rangle + b|1\rangle$ with $a\bar{a} + b\bar{b} = 1$ (since an idempotent operator can only have 1 or 0 as its eigenvalues thus $|\psi\rangle$ must be normal w.r.t. the standard complex inner product). Thus we let $q \in [0,1]$ and $\theta, \theta' \in \mathbb{R}$ to parameterise our measurements by using the polar form as $e^{i\theta'}(\sqrt{1-q}\,|0\rangle + \sqrt{q}e^{i\theta}\,|1\rangle)$ (here $e^{i\theta}$ is the global phase) and thus our measurement operators are

$$\begin{aligned} E_1 &= e^{i\theta'}(\sqrt{1-q}\,|0\rangle + \sqrt{q}e^{i\theta}\,|1\rangle)(e^{i\theta'}(\sqrt{1-q}\,|0\rangle + \sqrt{q}e^{i\theta}\,|1\rangle))^\dagger \\ &= (\sqrt{1-q}\,|0\rangle + \sqrt{q}e^{i\theta}\,|1\rangle)(\sqrt{1-q}\,\langle 0| + \sqrt{q}e^{-i\theta}\,\langle 1|) \\ &= \begin{pmatrix} 1-q & \sqrt{q(1-q)}e^{-i\theta} \\ \sqrt{q(1-q)}e^{i\theta} & q \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} E_2 &= \mathrm{id} - E_1 \\ &= \begin{pmatrix} q & -\sqrt{q(1-q)}e^{-i\theta} \\ -\sqrt{q(1-q)}e^{i\theta} & 1-q \end{pmatrix} \end{aligned}$$

Now, since $e^{i\theta}$ is 2π periodic we can take $\theta \in (-\pi, \pi]$ and for normalization we require $q \in [0,1]$ thus every measurement corresponds with some point (q,θ). Let $\rho_p = \begin{pmatrix} 1-p & \sqrt{p(1-p)} \\ \sqrt{p(1-p)} & p \end{pmatrix}$ for $p \in [0,1]$, then we have $S = \{|0\rangle\langle 0| \otimes \rho_p : p \in [0,1]\}$ a representation of $\mathcal{D}$ by Prop. 18 since

$$\begin{aligned} \| \, |0\rangle\langle 0| - \rho_p \|_{\mathrm{TD}} &= \| \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 1-p & \sqrt{p(1-p)} \\ \sqrt{p(1-p)} & p \end{pmatrix} \|_{\mathrm{TD}} \\ &= \| \begin{pmatrix} p & -\sqrt{p(1-p)} \\ -\sqrt{p(1-p)} & -p \end{pmatrix} \|_{\mathrm{TD}} \\ &= \frac{1}{2}(|\sqrt{p}| + |-\sqrt{p}|) && \text{the eigenvalues} \\ &= \sqrt{p} && \text{are } \pm\sqrt{p} \end{aligned}$$

meaning that the map given in Prop. 18 is a bijection and thus S is a representation, now we simply pick some $\rho \in S$ and $M \in M_\rho$, then using our parameterisations we can calculate the probability of inequality directly and get the equation

$$\mathbb{P}(X \neq Y) = 2(2q^2p - q^2 - 2qp + 1) + 2(2q-1)\sqrt{q(1-q)}\sqrt{p(1-p)}\cos\theta$$

Now, for our q.c we need to find the global minima, we will do this by finding the critical points:

$$\frac{\partial}{\partial\theta}\mathbb{P}(X \neq Y) = -2\sin\theta(2q-1)\sqrt{q(1-q)}\sqrt{p(1-p)}$$

The above is 0 exactly when

1. $\sqrt{q(1-q)} = 0$, this holds for $q = 0,1$ and any $\theta \in (-\pi, \pi]$.
2. $2q - 1 = 0$, this holds for $q = \frac{1}{2}$ and any $\theta \in (-\pi, \pi]$.
3. $\sqrt{p(1-p)} = 0$, this holds if and only if $p = 0,1$ which gives us some boundary conditions.

4. $\sin\theta = 0$, this holds for any $q \in [0,1]$ and $\theta = 0, \pi$.

$$\frac{\partial\mathbb{P}(X \neq Y)}{\partial q} = \frac{2q(1-q)(2q-1)(2p-1) - \cos\theta(8q^2-8q+1)\sqrt{q(1-q)}\sqrt{p(1-p)}}{q(1-q)}$$

Recall we must find both $\frac{\partial}{\partial Q}\mathbb{P}(X \neq Y) = \frac{\partial}{\partial c}\mathbb{P}(X \neq Y) = 0$ for the point to be a critical point:

1. when $q = 0, 1$ the denominator $q(q-1) = 0$ and the partial derivative is undefined.
2. when $q = \frac{1}{2}$ the partial derivative is $2\cos\theta\sqrt{p(1-p)}$, thus 0 whenever $p = 0, p = 1$, and $\theta \in (-\pi, \pi]$ or $\cos\theta = 0$, i.e. $\phi = -\frac{\pi}{2}, \frac{\pi}{2}$ for all $p \in [0,1]$.
3. when $p = 0, 1$ the singularities at $q = 0, 1$ are removable and the analytic continuation is $\mp 2(2q-1)$ which is zero only for $q = \frac{1}{2}$ (and any $\theta \in (-\pi, \pi]$).
4. finally, whenever $\sin\theta = 0$ (i.e. $\theta = 0, \pi$ and $\cos\theta = \pm 1$) the partial derivative is zero when
$$2\frac{2p-1}{\sqrt{p(1-p)}} = \pm\frac{8q^2-8q+1}{\sqrt{q(1-q)}(2q-1)}$$
squaring both sides and turning into simple fractions gives us
$$\frac{4}{p(1-p)} = \frac{1}{q(1-q)(2q-1)^2}$$
for $p \neq 0, 1$ and $q \neq 0, \frac{1}{2}, 1$ (which we may disregard wholesale as these cases have already been handled) the solutions of the corresponding diophantine equation (which are also solutions to the given equation for $p \neq 0, 1$ and $q \neq 0, 1, \frac{1}{2}$) are $q = \frac{1 \pm \sqrt{p}}{2}, \frac{1 \pm \sqrt{1-p}}{2}$.

Evaluating our original expression for $\mathbb{P}(X \neq Y)$ at these critical points gives us the following equations

$$\begin{aligned}
\text{at } q = 0, 1 &: \mathbb{P}(X \neq Y) = p \\
\text{at } q = \frac{1}{2} &: \mathbb{P}(X \neq Y) = \frac{1}{2} \\
\text{at } q = \frac{1-\sqrt{p}}{2} &: \mathbb{P}(X \neq Y) = \frac{p+1}{2} - 2p(1-p) \\
\text{at } q = \frac{1+\sqrt{p}}{2} &: \mathbb{P}(X \neq Y) = \frac{p+1}{2} \\
\text{at } q = \frac{1-\sqrt{1-p}}{2} &: \mathbb{P}(X \neq Y) = \frac{p}{2} \\
\text{and at } q = \frac{1+\sqrt{1-p}}{2} &: \mathbb{P}(X \neq Y) = \frac{p}{2} + 2p(1-p)
\end{aligned}$$

The easiest way to find the global minima is to plot the equations, fig. 3.1 shows us that the global minima is the line at $q = \frac{1-\sqrt{1-p}}{2}$ which gives us $\mathbb{P}(X \neq Y) = \frac{p}{2}$, we know that this is the global minima since we have already handled the boundary conditions and thus we conclude that $Q(\mathbb{P}(X \neq Y)) = \sqrt{2\mathbb{P}(X \neq Y)}$ is the initial q.c, moreover the

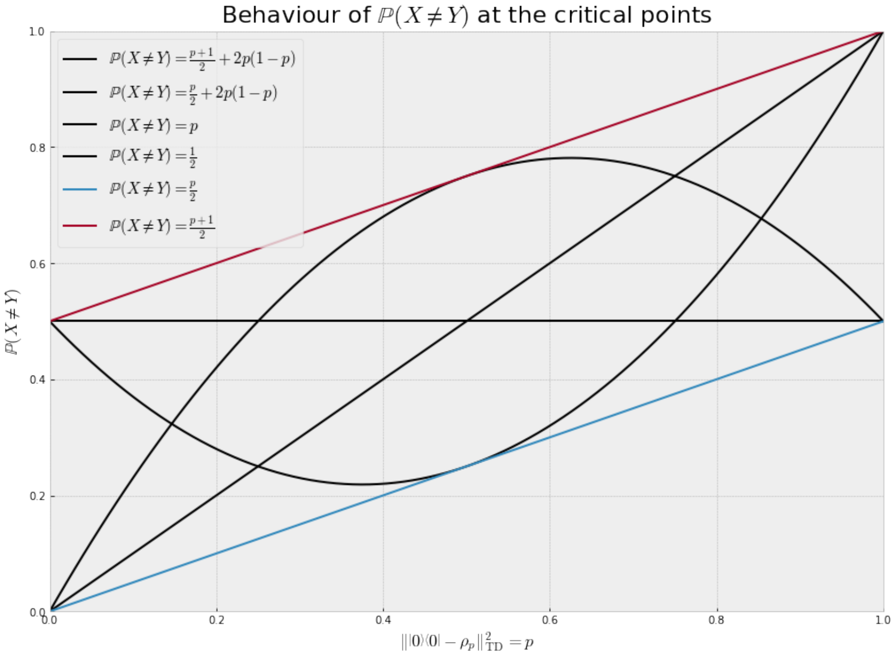


Figure 3.1: Plot of $\mathbb{P}(X \neq Y)$ vs. the square of the trace distance at the critical POVM measurements.

bound is saturated since we have equality when measuring at the critical measurements for which $q = \frac{1-\sqrt{1-p}}{2}$. Explicitly this means that we have the inequality

$$\|\rho^A - \rho^B\|_{\mathrm{TD}} \leq \sqrt{2\mathbb{P}(X \neq Y)}$$

for all pure states ρ^A, ρ^B in the 1-qubit system. Now, how do the tools of M-Systems that we've introduced make the problem that we've solved above tractable? Firstly Prop. 18 let us parameterise our collection of states S with only one parameter, $p \in [0,1]$ rather than the 4 parameters (p_1, θ_1 for the first qubit and p_2, θ_2 for the second) required to parameterise $\mathcal{D}$ and this reduction in dimension had no cost to the applicability of our results, furthermore since our M-System is simple we could parameterise our measurements independently of our state, i.e. with $q \in [0,1]$ and $\theta \in (-\pi, \pi]$ giving us a parameterisation $M(q,\theta)$ rather than a collection of parameterisations $\{M_\rho(q,\theta)\}_{\rho \in \mathcal{D}}$, in chapter 4, maximal total variation measurement schemes, we will work with M-Systems that are not simple or regular and we will have to rely on algebraic arguments rather than a direct computation of the criticial points, and evaluation. Now, this result generalises if

conjecture 1. Fix a subspace $V \subset \mathcal{H}$ of dimension 2, for every $\{E_i\}_{i \in \mathcal{I}} \in M_\rho \in \mathcal{M}$ where $\mathcal{M}$ is a M-System over $\mathcal{D} = \mathcal{D}_{\text{pure}}$ in the Von Neumann measurement scheme there exists a binary dilution of $\{E_i\}_{i \in \mathcal{I}}$ (see Defn. 18) $\{E_1, E_2\}$ such that the dilution understood as a measurement of the local system V is a Von Neumann measurement of the system.

The existence of the aforementioned dilution immediately gives us the desired inequality due to Prop. 19, it should be noted that this is not an iff statement, that is to say the claim may be false while the bound holds.

Chapter 4

Maximal Total Variation Measurement Scheme

We are finally ready to tackle the coupling problem: M-Systems part of the maximal total variation measurement scheme.

Fix some $\mathcal{D} \subset \mathcal{L}(\mathcal{H}^{\otimes 2})$, a set of density operators. For $\rho^{AB} \in \mathcal{D}$ we let μ_E be the distribution given by performing the POVM measurement E on the system ρ^A and ν_E be the distribution given by performing the POVM E on the system ρ^B, then we let

$$M_{\rho^{AB}} = \{E : \|\rho^A - \rho^B\|_{\text{TD}} = \|\mu_E - \nu_E\|_{\text{TV}} \text{ for } E \text{ a POVM measurement}\}$$

Then $\{M_\rho\}_{\rho \in \mathcal{D}} \coloneqq \mathcal{M}^\infty$ is an M-System since:

We let μ'_E and ν'_E be the distrubution obtained when measuring σ^A and σ^B with the POVM measurement E respectively, then if $U^{\otimes 2}\rho^{AB}U^{\otimes 2\dagger} := \sigma^{AB} \in \mathcal{D}$ for $\rho^{AB} \in \mathcal{D}$ and some unitary U we take $E = (E_i)_{i \in \mathcal{I}} \in M_{\rho^{AB}}$ and let $UEU^\dagger = (UE_iU^\dagger)_{i \in \mathcal{I}}$. We will now show that $UEU^\dagger \in M_{\sigma^{AB}}$ which will be sufficient to satisfy trivial motion.

$$\begin{aligned}
&\|\mu'_{UEU^\dagger} - \nu'_{UEU^\dagger}\|_{\text{TV}} \\
&\quad = \frac{1}{2}\sum_{i \in \mathcal{I}} |\mu'_{UEU^\dagger}(i) - \nu'_{UEU^\dagger}(i)| && \text{by Lemma 2} \\
&\quad = \frac{1}{2}\sum_{i \in \mathcal{I}} |\operatorname{tr}(UE_iU^\dagger\sigma^A) - \operatorname{tr}(UE_iU^\dagger\sigma^B)| && \text{by postulate 3} \\
&\quad = \frac{1}{2}\sum_{i \in \mathcal{I}} |\operatorname{tr}(E_iU^\dagger\sigma^A U) - \operatorname{tr}(E_iU^\dagger\sigma^B U)| && \text{by the cyclic property} \\
&\quad = \frac{1}{2}\sum_{i \in \mathcal{I}} |\operatorname{tr}(E_i\rho^A) - \operatorname{tr}(E_i\rho^B)| && \text{since } U^{\otimes 2}\rho^{AB}U^{\otimes 2\dagger} = \sigma^{AB} \\
&\quad = \frac{1}{2}\sum_{i \in \mathcal{I}} |\mu_E(i) - \nu_E(i)| && \text{by postulate 3} \\
&\quad = \|\mu_E - \nu_E\|_{\text{TV}} && \text{by Lemma 2}
\end{aligned}$$

and thus we have a map $M_U : M_{\rho^{AB}} \to M_{\sigma^{AB}}$ given by $(E_i)_{i\in\mathcal{I}} \mapsto (UE_iU^\dagger)_{i\in\mathcal{I}}$ an injection (since unitaries are isomorphisms) and by analogous argument the inverse map $M_{U^\dagger}$: $M_{\sigma^{AB}} \to M_{\rho^{AB}}$ is an injection, but then M_U must be surjective, and we know M_U to be an injection, thus M_U is a bijection and thus $\mathcal{M}^\infty$ satisfies trivial motion.

We also have symmetry:

If $\rho^{AB} \in \mathcal{D}$ and $U_{\text{SWAP}}\rho^{AB}U_{\text{SWAP}}^\dagger \in \mathcal{D}$ then for every POVM measurement E we have

$$\|\mu_E - \nu_E\|_{\text{TV}} = \|\mu_E - \nu_E\|_{\text{TV}}$$
$$\|\rho^A - \rho^B\|_{\text{TD}} = \|\rho^B - \rho^A\|_{\text{TD}}$$

since $\|\cdot\|_{\text{TV}}$ and $\|\cdot\|_{\text{TD}}$ are metrics, but then for any measurement $E \in M_{\rho^{AB}}$ we have

$$\|\rho^B - \rho^A\|_{\text{TD}} = \|\rho^A - \rho^B\|_{\text{TD}} = \|\mu_E - \nu_E\|_{\text{TV}} = \|\nu_E - \mu_E\|_{\text{TV}}$$

thus $(M_i)_{i\in\mathcal{I}} \in M_{U_{\text{SWAP}}\rho^{AB}U_{\text{SWAP}}^\dagger}$, i.e. $\iota : M_{\rho^{AB}} \to M_{U_{\text{SWAP}}\rho^{AB}U_{\text{SWAP}}^\dagger}$ for ι the identity map (which is an injection since unitaries are isomorphisms), and by an analogous argument to above, by starting with $U_{\text{SWAP}}\rho^{AB}U_{\text{SWAP}}^\dagger$ instead of ρ^{AB}, gives $\iota' : M_{U_{\text{SWAP}}\rho^{AB}U_{\text{SWAP}}^\dagger} \to M_{\rho^{AB}}$ for ι' the identity map (again, ι' is an injection as unitaries are isomorphisms), but clearly ι' is the inverse to ι, thus ι is a surjection, and we know ι to be an injection, thus ι is a bijection, and as required for symmetry we have $M_{\rho^{AB}} = M_{U_{\text{SWAP}}\rho^{AB}U_{\text{SWAP}}^\dagger}$.

We also consider $\mathcal{M}^n$ for $n \in \mathbb{N}$ to be defined as above but with the additional restriction that every POVM $(M_i)_{i\in\mathcal{I}} \in M_\rho$ has index set $\emptyset \subset \mathcal{I} \subseteq \{1,2,\ldots,n\}$, i.e. the measurement has $\leq n$ outcomes. Notice that the same argument as above applies to every $\mathcal{M}^n$ to show that $\mathcal{M}^n$ is an M-System and it also partially justifies the name $\mathcal{M}^\infty$, the main reason we do not care much for large cardinals, and thus group all of that structure under $\mathcal{M}^\infty$ is because the structural properties we are concerned with, such as monotonicity of the q.c, emerge when just considering numerable index sets. Now, the measurements in $\mathcal{M}^2$ have a very useful algebraic structure, they are all of the form $\{E_1, E_2\}$ with $E_1 \perp S$ and $E_2 \perp Q$ where $\rho^A - \rho^B = Q - S$ for positive semi-definite Q, S for this reason we need one final tool, the notion of a measurement dilation which will allow us to develop and understand q.c's in $\mathcal{M}^2$ and then transfer these results to our main M-Systems of interest, $\mathcal{M}^\infty$.

Definition 18 (Measurement Dilation)**.** A measurement $(E_i)_{i\in\mathcal{I}}$ is a dilution of $(E_i')_{i\in\mathcal{I}'}$ if there exists a partition of $\mathcal{I}$ into $\{P_i\}_{i\in\mathcal{I}'}$ such that $\sum_{E\in P_i} E = E_i'$

Proposition 19. *If E is a dilution of E' then for all $\rho \in \mathcal{D}$ we have $\mathbb{P}(X_E \neq Y_E) \geq \mathbb{P}(X_{E'} \neq Y_{E'})$.*

Proof. Let $E = (E_i)_{i\in\mathcal{I}}$ be a dilation of $E' = (E_i')_{i\in\mathcal{I}'}$, then by Defn. 18 there exists a partition of $\mathcal{I}$ into $\{P_i\}_{i\in\mathcal{I}'}$ such that $\sum_{E\in P_i} E = E_i'$. Notice that

$$\begin{aligned}\{X_{E'} \neq Y_{E'}\} &= \bigcup_{i\in\mathcal{I}'} \{X_{E'} = i \text{ and } Y_{E'} \neq i\} \\ &= \bigcup_{i\in\mathcal{I}'} \{X_E \in P_i \text{ and } Y_E \notin P_i\}\end{aligned}$$

$$\subseteq \{X_E \neq Y_E\}$$

and thus the claim holds by the monotonicity of the probability measure $\mathbb{P}$. □

Proposition 20. *Every measurement in $M_{\rho^{AB}} \in \mathcal{M}^n$ for $n \in \mathbb{N}$ or $M_{\rho^{AB}} \in \mathcal{M}^\infty$ is a dilution of some measurement in $M'_{\rho^{AB}} \in \mathcal{M}^2$.*

Proof. Let $E = (E_i)_{i \in \mathcal{I}} \in M_{\rho^{AB}}$, and let $\rho^A - \rho^B = Q - S$ for Q, S positive semi-definite.

Then for each $i \in \mathcal{I}$ either $E_i \perp Q$ or $E_i \perp S$ as if neither holds then $(E_i)_{i \in \mathcal{I}}$ does not maximise the total variation distance $\|\mu_E - \nu_E\|_{\mathrm{TV}}$. Let $P_Q = \{E_i : E_i \perp S\}$ and $P_S = \{E_i : E_i \perp Q\}$, then clearly $P_Q \geq \Pi_Q$ and $P_S \geq \Pi_S$ thus $\{P_Q, P_S\} \in M'_{\rho^{AB}}$ as $\{P_Q, P_S\}$ maximises the total variation distance, finally the only exception is a measurement of cardinality 1, and by the completeness equation we must have $\sum_{i \in \{1\}} M_i = \mathrm{id} \implies M_i = \mathrm{id}$ and $\mathrm{id} \in M_\rho \implies \mathrm{id} \in M'_\rho$, thus the claim holds. □

4.1 Monotonicity of the Quantum Coupling Function

Lemma 21. *The initial q.c over $\mathcal{M}^\infty$ (over $\mathcal{D}$) is monotone non-decreasing on $[0,1)$, moreover if there exists $\rho^{AB} \in \mathcal{D}$ s.t. $\|\rho^A - \rho^B\|_{\mathrm{TD}} = 1$ then $\overline{Q}(x) = 1$ for $x = 1$ and $\overline{Q}$ is monotone non-decreasing on $[0,1]$.*

Proof. Since measurements in $\mathcal{M}^\infty$ are dilutions of measurements in $\mathcal{M}^2$ by Prop. 20 (and $\mathcal{M}^2 \subset \mathcal{M}^\infty$) we know there exists a sequence of measurements $E_n := \{E_{1n}, E_{2n}\} \in M_{\rho^{AB}} \in \mathcal{M}^2 \subset \mathcal{M}^\infty$ such that $\lim_{n\to\infty} \mathbb{P}(X_{E_n} \neq Y_{E_n}) \leq \mathbb{P}(X_E \neq Y_E)$ with $\lim_{n\to\infty} \mathbb{P}(X_{E_n} \neq Y_{E_n}) = \sup_{E \in M_{\rho^{AB}}} \mathbb{P}(X_E \neq Y_E)$ for all $E \in M_{\rho^{AB}} \in \mathcal{M}^\infty$ (note that the existence of such a sequence follows from the existence of the supremum)

Now, for each E_n we define mE_n to be $\bigsqcup_{k=1}^m \frac{1}{m} E_n$

Let $\delta(x) = \frac{x-(m+1)}{m+1}$ then $(x, \delta(x))$ is the line that passes through $(0,1)$ and $(1, \frac{m}{m+1})$ (hence continuous) and the continuum of measurements $\delta(x)(mE_n) + (1-\delta(x))(E_n) \in M_{\rho^{AB}} \in \mathcal{M}^\infty$ over $x \in [0,1]$ saturate $[\mathbb{P}(X_{mE_n} \neq Y_{mE_n}), \mathbb{P}(X_{(m+1)E_n} \neq Y_{(m+1)E_n})]$ (since $\delta(0)(mE_n) + (1-\delta(0))(E_n) = mE_n$ and $\delta(1)(mE_n) + (1-\delta(0))(E_n) = (m+1)E_n$) by the linearity of the trace, now notice that

$$
\begin{aligned}
&\lim_{m\to\infty} \mathbb{P}(X_{mE_n} \neq Y_{mE_n}) \\
&= \lim_{m\to\infty} \sum_{k=1}^{m} \mathrm{tr}\left(\left(\frac{1}{m}E_1^{(k)}\right) \otimes \left(\frac{1}{m}E_2^{(k)}\right)\rho^{AB}\right) \\
&\quad + \mathrm{tr}\left(\left(\frac{1}{m}E_2^{(k)}\right) \otimes \left(\frac{1}{m}E_1^{(k)}\right)\rho^{AB}\right) + \xi && (\xi \text{ is the uncounted terms}) \\
&= \lim_{m\to\infty} \sum_{k=1}^{m} \mathrm{tr}\left(\frac{1}{m^2}E_1^{(k)} \otimes E_2^{(k)}\rho^{AB}\right) \\
&\quad + \mathrm{tr}\left(\frac{1}{m^2}E_2^{(k)} \otimes E_1^{(k)}\rho^{AB}\right) + \xi && \text{since } \otimes \text{ is bilinear}
\end{aligned}
$$

$$
\begin{aligned}
&= \lim_{m\to\infty} \sum_{k=1}^{m} \frac{1}{m^2} \operatorname{tr}\left(E_1^{(k)} \otimes E_2^{(k)} \rho^{AB}\right) \\
&\quad + \frac{1}{m^2} \operatorname{tr}\left(E_2^{(k)} \otimes E_1^{(k)} \rho^{AB}\right) + \xi && \text{since trace is a linear map} \\
&= \lim_{m\to\infty} \sum_{k=1}^{m} \frac{1}{m^2} \mathbb{P}(X_{E_n} \neq Y_{E_n}) + \xi \\
&= \lim_{m\to\infty} \frac{1}{m} \mathbb{P}(X_{E_n} \neq Y_{E_n}) + \sum_{k=1}^{m} \xi \\
&= \lim_{m\to\infty} \sum_{k=1}^{m} \xi \\
&= \lim_{m\to\infty} \sum_{k=1}^{m} \sum_{k'>k}^{m} \operatorname{tr}\left(\left(\frac{1}{m}E_1^{(k)}\right) \otimes \left(\frac{1}{m}E_1^{(k')}\right) \rho^{AB}\right) \\
&\quad + \operatorname{tr}\left(\left(\frac{1}{m}E_1^{(k)}\right) \otimes \left(\frac{1}{m}E_2^{(k')}\right) \rho^{AB}\right) \\
&\quad + \operatorname{tr}\left(\left(\frac{1}{m}E_2^{(k)}\right) \otimes \left(\frac{1}{m}E_1^{(k')}\right) \rho^{AB}\right) \\
&\quad + \operatorname{tr}\left(\left(\frac{1}{m}E_2^{(k)}\right) \otimes \left(\frac{1}{m}E_2^{(k')}\right) \rho^{AB}\right) \\
&\quad + \operatorname{tr}\left(\left(\frac{1}{m}E_1^{(k')}\right) \otimes \left(\frac{1}{m}E_1^{(k)}\right) \rho^{AB}\right) \\
&\quad + \operatorname{tr}\left(\left(\frac{1}{m}E_1^{(k')}\right) \otimes \left(\frac{1}{m}E_2^{(k)}\right) \rho^{AB}\right) \\
&\quad + \operatorname{tr}\left(\left(\frac{1}{m}E_2^{(k')}\right) \otimes \left(\frac{1}{m}E_1^{(k)}\right) \rho^{AB}\right) \\
&\quad + \operatorname{tr}\left(\left(\frac{1}{m}E_2^{(k')}\right) \otimes \left(\frac{1}{m}E_2^{(k)}\right) \rho^{AB}\right) \\
&= \lim_{m\to\infty} \sum_{k=1}^{m} \sum_{k'>k}^{m} \frac{1}{m^2} \operatorname{tr}\Big(\Big(E_1^{(k)} \otimes E_1^{(k')} \\
&\quad + E_1^{(k)} \otimes E_2^{(k')} \\
&\quad + E_2^{(k)} \otimes E_1^{(k')} + E_2^{(k)} \otimes E_2^{(k')}\Big) \rho^{AB}\Big) \\
&\quad + \frac{1}{m^2} \operatorname{tr}\Big(\Big(E_1^{(k')} \otimes E_1^{(k)} + E_1^{(k')} \otimes E_2^{(k)} && \text{since trace is a linear map} \\
&\quad + E_2^{(k')} \otimes E_1^{(k)} + E_2^{(k')} \otimes E_2^{(k)}\Big) \rho^{AB}\Big) && \text{and } \otimes \text{ is a bilinear map} \\
&= \lim_{m\to\infty} \sum_{k=1}^{m} \sum_{k'>k}^{m} \frac{2}{m^2} \operatorname{tr}(\mathrm{id}\,\rho^{AB}) && \text{by the completeness equation} \\
&= \lim_{m\to\infty} \frac{2}{m^2} \sum_{k=1}^{m} \sum_{k'>k}^{m} 1 && \text{since } \rho^{AB} \text{ is a density operator} \\
&= \lim_{m\to\infty} \frac{2}{m^2} \sum_{k=1}^{m} (m-k)
\end{aligned}
$$

$$
\begin{aligned}
&= \lim_{m\to\infty} \frac{2}{m^2} \sum_{n=1}^{m-1} n && \text{(by substitution with } n = m-k) \\
&= \lim_{m\to\infty} \frac{2}{m^2} \frac{(m-1)m}{2} && \text{sum is } m-1^{\text{th}} \text{ triangular number} \\
&= \lim_{m\to\infty} \frac{m-1}{m} \\
&= 1
\end{aligned}
$$

(note that the superscript $E^{(k)}$ are for distinguish-ability of the elements, i.e. $E^{(k)} = E^{(k')}$ when equality is understood to be equality of the linear maps but $E^{(k)} \neq E^{(k')}$ when equality is understood as being the same element in the family mE_n)

Thus we have a continuum of measurements saturating $(\inf \mathbb{P}(X_{E_n} \neq Y_{E_n}), 1)$.

Now, if $\overline{Q}(x) = p$ for some $x \in [0,1)$ then there exists a sequence of $\rho_n^{AB} \in B_x$ s.t. $\|\rho_n^A - \rho_n^B\|_{\text{TD}} \to p$ (else $\overline{Q}$ would not be initial, see proof of Lemma 13), for each of these ρ_n^{AB} we've shown that $\overline{Q}(x') \geq \lim_{n\to\infty} \|\rho_n^A - \rho_n^B\|_{\text{TD}} = \overline{Q}(x)$ for $x < x' < 1$ and thus monotone non-decreasing on $[0,1)$.

If $\rho^{AB} \in \mathcal{D}$ is such that $\|\rho^A - \rho^B\|_{\text{TD}} = 1$, then let $\rho^A - \rho^B = Q - S$ for positive semi-definite Q,S. Now: $\text{tr}(Q) = \|\rho^A - \rho^B\|_{\text{TD}} = 1 = \text{tr}(S)$, but by the linearity of the trace this is only possible if $Q = \rho^A$ and $S = \rho^B$, i.e. ρ^A and ρ^B are orthogonal and thus any binary measurement $\{E_1, E_2\} \in M_{\rho^{AB}} \in \mathcal{M}^\infty$ gives us $E_1 \perp \rho^B$ and $E_2 \perp \rho^A$ (else we fail to maximise the total variation distance with the induced distribution) which gives us $\mathbb{P}(X \neq Y) = \text{tr}(E_1 \otimes E_2 \rho^{AB}) + \text{tr}(E_2 \otimes E_1 \rho^{AB}) = 1 + 0 = 1$, thus $\overline{Q}(1) \geq 1$, but $\overline{Q} \leq 1$ and thus $\overline{Q}(1) = 1$ and since $\overline{Q} \leq 1$ and $\overline{Q}$ is monotone non-decreasing on $[0,1)$ we find $\overline{Q}$ is monotone non-decreasing on $[0,1]$. □

4.2 Optimal Coupling Function

In this section we will consider $\mathcal{D}$ to be full, thus we have monotonicity on $[0,1]$ for our initial q.cs over $\mathcal{M}^\infty$.

Take some system $\mathcal{M}^2$ and $\overline{Q}$ the initial q.c over it, then we know that $\overline{Q} \leq \text{Mon}\,\overline{Q}$ (by Prop. 19 since Prop. 20) with $\text{Mon}\,\overline{Q}$ the inital q.c for $\mathcal{M}^\infty$, then by Prop. 20, and since $\mathcal{M}^n \subseteq \mathcal{M}^\infty$ we know that for every $\overline{Q'}$ for $\mathcal{M}^n$ we have $\overline{Q} \leq \overline{Q'} \leq \text{Mon}\,\overline{Q}$, thus if we can show that $\overline{Q}$ is monotone we will discover that all of the initial q.cs over the systems $\mathcal{M}^n$ and the intial q.c over $\mathcal{M}^\infty$ are identical.

Towards this we will prove that $\overline{Q}(\mathbb{P}(X \neq Y)) = \mathbb{P}(X \neq Y)$. Let $|0\rangle, |1\rangle \in \mathcal{H}$ be orthonormal, then the pair of states $|0\rangle\langle 0|$ and $(1-p)|0\rangle\langle 0| + p|1\rangle\langle 1|$ have only one coupling, namely $\rho = |0\rangle\langle 0| \otimes ((1-p)|0\rangle\langle 0| + p|1\rangle\langle 1|)$ and thus said state is in $\mathcal{D}$, notably the eigenvalues and eigenvectors of the difference of the two states are $\pm p$ and $|0\rangle\langle 0|, |1\rangle\langle 1|$. Now consider the binary measurement $\{E_1, E_2\}$ with $E_1 \perp |0\rangle\langle 0|$ and $E_2 \perp |1\rangle\langle 1|$ then

$$
\begin{aligned}
\mathbb{P}(X \neq Y) &= \text{tr}(E_1 \otimes E_2 \rho) + \text{tr}(E_2 \otimes E_1 \rho) \\
&= 0 + \text{tr}(E_1((1-p)|0\rangle\langle 0| + p|1\rangle\langle 1|))
\end{aligned}
$$

$$
\begin{aligned}
&= p\,\mathrm{tr}(E_1 \left|1\right\rangle\left\langle 1\right|) \\
&= p \qquad\qquad \text{since } E_1 \geq \left|1\right\rangle\left\langle 1\right|
\end{aligned}
$$

Thus $\overline{Q} \geq \mathbb{P}(X \neq Y)$.

4.2.1 Residue Matrix R

We require a short detour to the concept of a residue, let ρ, σ be density operators belonging to the same Hilbert space, then we know there exist Q, S positive semi-definite such that $\rho - \sigma = Q - S$, we now show that there exists positive semi-definite R such that $\rho = Q + R$ and $\sigma = S + R$. Firstly we let $R = \rho - Q$, then $R - \sigma = -S \implies S + R = \sigma$, now consider some vector $\left|\psi\right\rangle$ in the nullspace of Q, then

$$
\begin{aligned}
0 \leq \left\langle\psi\right|\rho\left|\psi\right\rangle &= \left\langle\psi\right|(Q+R)\left|\psi\right\rangle && \text{since } \rho \text{ is positive semi-definite} \\
&= \left\langle\psi\right|R\left|\psi\right\rangle && \text{since } \left|\psi\right\rangle \text{ is in the nullspace of } Q
\end{aligned}
$$

Now for $\left|\psi'\right\rangle$ in the nullspace of S we get

$$
\begin{aligned}
\left\langle\psi'\right|(\rho - \sigma)\left|\psi'\right\rangle &= \left\langle\psi'\right|(Q - S)\left|\psi'\right\rangle \\
\left\langle\psi'\right|\rho\left|\psi'\right\rangle &\geq \left\langle\psi'\right|Q\left|\psi'\right\rangle
\end{aligned}
$$

and since $S \perp Q$ we conclude that $\rho \geq Q$, and thus

$$
\begin{aligned}
\left\langle\psi'\right|\rho\left|\psi'\right\rangle &= \left\langle\psi'\right|(Q+R)\left|\psi'\right\rangle \\
\implies \left\langle\psi'\right|(\rho - Q)\left|\psi'\right\rangle &= \left\langle\psi'\right|R\left|\psi'\right\rangle
\end{aligned}
$$

and since $\rho \geq Q$ $\rho - Q$ is positive semi-definite, and by linearity (since $Q \perp S$) we conclude R is positive semi-definite. Since $R \leq \rho$ we have $\mathrm{tr}(R) = 1 - \mathrm{tr}(Q) \leq 1$ and $\frac{R}{\mathrm{tr}(R)}$ is a density operator in the case that $R \neq 0$. We call R the residue matrix and if $R \neq 0$ then for a binary measurement $\{E_1, E_2\} \in M_{\rho\otimes\sigma} \in \mathcal{M}^2$ we call $\mathrm{tr}(E_1 \frac{R}{\mathrm{tr}(R)}) := q$ or $\mathrm{tr}(E_2 \frac{R}{\mathrm{tr}(R)}) := q$ the residue, this means that we treat $1 - q$ and q as identical (by completeness), and this is due to the symmetric nature of measurements in $\mathcal{M}^2$ (see fig. 4.1), finally we call the distribution induced by the binary measurement on R the residue distribution. Given this we may consider $\mathcal{D} = \{\rho \otimes \sigma : \rho, \sigma \in \mathcal{H} \text{ are density operators}\}$, a full set of density operators and for the M-System $\mathcal{M}^2$ over $\mathcal{D}$ we can calculate the probability of inequality explicitly: since for every measurement $\{E_1, E_2\} \in M_\rho^{AB} \in \mathcal{M}^2$ w.l.o.g we have $E_1 \perp S$ and $E_2 \perp Q$, let $q = \mathrm{tr}(E_1 \frac{R}{\mathrm{tr}(R)})$ be the residue and $p = \mathrm{tr}(Q) = \mathrm{tr}(S)$ the trace distance, then we find

$$
\begin{aligned}
&\mathbb{P}(X \neq Y) \\
&\quad= \mathrm{tr}(E_1 \otimes E_2 \rho^{AB}) + \mathrm{tr}(E_2 \otimes E_1 \rho^{AB}) \\
&\quad= \mathrm{tr}(E_1 \otimes E_2 \rho^A \otimes \rho^B) + \mathrm{tr}(E_2 \otimes E_1 \rho^A \otimes \rho^B) && \rho^{AB} = \rho^A \otimes \rho^B \text{ for our set } \mathcal{D} \\
&\quad= \mathrm{tr}(E_1 \rho^A)\,\mathrm{tr}(E_2 \rho^B) + \mathrm{tr}(E_2 \rho^A)\,\mathrm{tr}(E_1 \rho^B) \\
&\quad= \mathrm{tr}(E_1(Q+R))\,\mathrm{tr}(E_2(S+R)) && \text{by residue decomposition} \\
&\qquad+ \mathrm{tr}(E_2(Q+R))\,\mathrm{tr}(E_1(S+R))
\end{aligned}
$$

$$
\begin{aligned}
&= (\mathrm{tr}(Q)+\mathrm{tr}(E_1R))(\mathrm{tr}(S)+\mathrm{tr}(E_2R)) && \text{by linearity of trace and since}\\
&\quad + \mathrm{tr}(E_1R)\,\mathrm{tr}(E_2R) && \Pi_S \perp E_1 \geq \Pi_Q \text{ and } \Pi_Q \perp E_2 \geq \Pi_S\\
&= (p+(1-p)q)(p+(1-p)(1-q)) && \\
&\quad + (1-p)q(1-p)(1-q) && \text{by substitution of } p,q\\
&= 2(1-p)^2q(1-q)+p && \\
&\geq p = \|\rho^A-\rho^B\|_{\mathrm{TD}} && \text{since } p,q \in [0,1]
\end{aligned}
$$

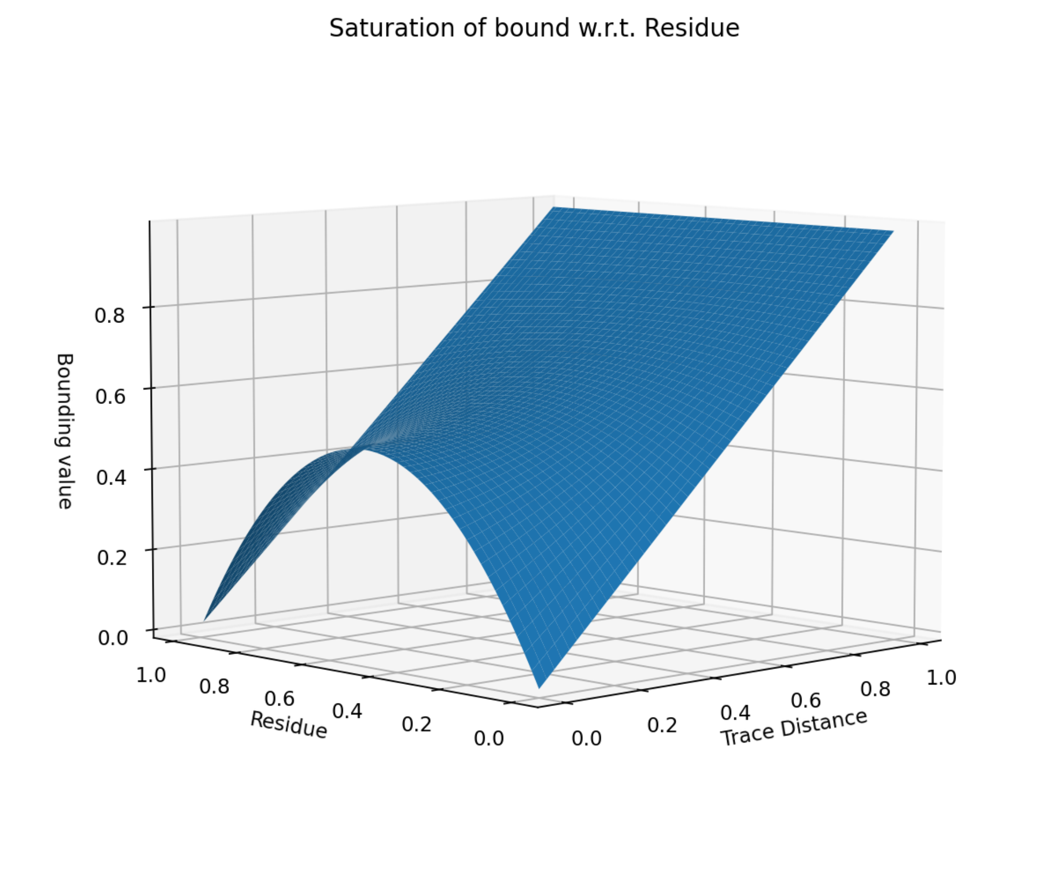


Figure 4.1: Visualisation of the impact residue has on the probability of inequality

Now for the general case (arbitrary full $\mathcal{D}$) we have

$$
\begin{aligned}
\mathbb{P}(X=Y) &= \mathrm{tr}(E_1^{\otimes 2}\rho^{AB})+\mathrm{tr}(E_2^{\otimes 2}\rho^{AB}) && \\
&\leq \mathrm{tr}(\mathrm{id}\otimes E_1\rho^{AB})+\mathrm{tr}(E_2\otimes \mathrm{id}\,\rho^{AB}) && \text{since } E_1,E_2 \leq \mathrm{id}\\
&= \mathrm{tr}(E_1\rho^B)+\mathrm{tr}(E_2\rho^A) && \text{by the universal property of partial trace}\\
&= (1-p)q+(1-p)(1-q) = 1-p &&
\end{aligned}
$$

hence $\mathbb{P}(X \neq Y) = 1-\mathbb{P}(X=Y) \geq 1-(1-p) = p$ and thus the bound holds in general meaning that our original claim is true and the initial q.c for all of our full M-Systems $\mathcal{M}^n$ for $n \geq 2$ and $\mathcal{M}^\infty$ is $\overline{Q} = \mathbb{P}(X \neq Y)$.

4.3 Results on Saturation

Back in section 4.2, optimal coupling function, we've shown that the bound $\mathbb{P}(X \neq Y)$ is optimal by looking at the spectrum of states $\rho = |0\rangle\langle 0| \otimes ((1-p)|0\rangle\langle 0| + p|1\rangle\langle 1|)$ for $p \in [0,1]$, we will now show that the worst case saturation, corresponding to a residue of $\frac{1}{2}$ (see fig. 4.1) is not only possible, but there is no measurement optimisation or coupling optimisation that can remove it, we do this by considering the spectrum given by $\rho^{AB} = (\sqrt{\frac{1+p}{2}}|0\rangle + \sqrt{\frac{1-p}{2}}|1\rangle)(\sqrt{\frac{1+p}{2}}\langle 0| + \sqrt{\frac{1-p}{2}}\langle 1|) \otimes (\sqrt{\frac{1+p}{2}}|1\rangle + \sqrt{\frac{1-p}{2}}|0\rangle)(\sqrt{\frac{1+p}{2}}\langle 1| + \sqrt{\frac{1-p}{2}}\langle 0|)$ for $p \in (0,1]$, clearly the non-zero eigenvectors of $\rho^A - \rho^B$ are $|0\rangle\langle 0|$ and $|1\rangle\langle 1|$ with eigenvalues $\pm(\frac{1+p}{2} - \frac{1-p}{2}) = \pm p$ (thus p is also the trace distance) and taking measurements $\{E_1, E_2\} \in M_{\rho^{AB}} \in \mathcal{M}^2$ with $E_1 \perp |1\rangle\langle 1|$ and $E_2 \perp |0\rangle\langle 0|$ gives us

$$\begin{aligned}
\mathbb{P}(X \neq Y) &= \mathrm{tr}(E_1\rho^A \otimes E_2\rho^B) + \mathrm{tr}(E_2\rho^A \otimes E_1\rho^B) \\
&= \left(\frac{1-p}{2}\right)^2 + \left(\frac{1+p}{2}\right)^2 \\
&= \frac{1}{2}(p^2+1)
\end{aligned}$$

and thus

$$\|\rho^A - \rho^B\|_{\mathrm{TD}} = \sqrt{2\mathbb{P}(X \neq Y) - 1}$$

We can visualise this result by the following diagram:

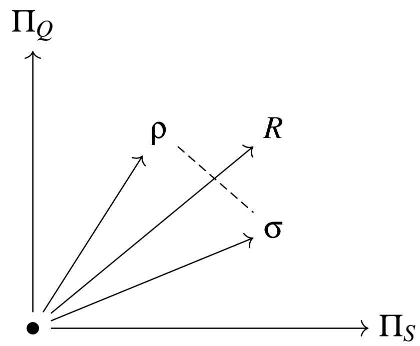


Figure 4.2: For pure states ρ, σ the residue operator lies in the span of the eigenvectors

This shows that the residue is $\frac{1}{2}$ and thus saturation is not possible irrespective of measurement or coupling (since the only coupling of a pure state is the trivial coupling).

Chapter 5

Conclusion

This chapter restates our contributions, summarises the project, and proposes potential future work.

5.1 Contributions

- General framework for understanding potential quantum couplings as a relation over collections of measurements indexed by bipartite (entangled) states.
- The infeasibility of arbitrary measurement scheme for quantum coupling.
- Coupling bound for pure states in the 1-qubit system given a Von Neumann measurement scheme with saturation under measurement optimisation.
- Monotonicity of coupling function over the maximal Total Variation measurement scheme irrespective of restriction to states.
- Equality of coupling function over the maximal Total Variation measurement scheme for full M-Systems.
- Negative result on saturation of coupling function over the maximal Variation measurement scheme for full M-Systems.

5.2 Overview

In this project we introduce a general framework for understanding and working with quantum coupling functions, justifying our choices along the way, and apply our framework to two main measurement schemes: the arbitrary measurement scheme which demonstrates the need for measurement restriction, and the maximal total variation measurement scheme, motivated by the well-known quantum analogue to the concept of total variation distance, trace distance, we demonstrate the general existence of a bound analogous to that given by coupling for full measurement systems as well as demonstrate that the quantum coupling function is essentially monotone in the most general case. The negative result on saturation motivates the study of more esoteric measurement systems for which we have laid the groundwork. We also explore the utility of our framework for pairs of pure states of the 1-qubit system with the corresponding measurement system as a part of the Von Neumann measurement scheme.

5.3 Future Work

Within the general framework, we assume the base field to be the complex numbers, $\mathbb{C}$, the key reason for this is algebraic closure for spectral decomposition so a natural extension of the framework could be to consider more general separable Hilbert spaces, which would allow results to apply to a wider domain of theoretical physics.

The work done within the Von Neumann measurement scheme is preliminary with two main roads for future development: continuing with pure states but generalising to arbitrary Hilbert spaces may be attempted through proving conjecture 1 or some alternative approach, or generalising from pure states to more general quantum states, in particular, a geometric approach seems most insightful towards this end.

We have seen that well-structured measurement dilution can lead to monotonicity, this can easily be generalised however measurement systems like those handled in section 3.4 do not admit such an argument due to their bounded cardinality yet seem to be monotone, it can easily be verified that regularity and simplicity on their own are insufficient however the result is unclear when both hold simultaneously. Such monotonicity results have implications on alternative quantum coupling analogues as there is a strong intuitive reason why the classical coupling bound must be monotone-increasing thus informing us about the structure of potential analogues.

For numerical stability, the smoothness (and consequently continuity) of the coupling bound is important and towards this end a notion of 'continuous motion' analogous to trivial motion but for states where direct isomorphisms do not exist, but a clear notion of similarity exists in the Hilbert space is a worthwhile starting point. The name 'continuous motion' comes from geometric rigidity theory.

Bibliography

Nawaf Bou-Rabee, Andreas Eberle, and Raphael Zimmer. Coupling and convergence for hamiltonian monte carlo. *The Annals of Applied Probability*, 30(3), 2020. doi: 10.1214/19-aap1528.

Bova, Francesco, Goldfarb, Avi, and Melko, Roger G. Commercial applications of quantum computing. *EPJ Quantum Technol.*, 8(1):2, 2021. doi: 10.1140/epjqt/s40507-021-00091-1. URL https://doi.org/10.1140/epjqt/s40507-021-00091-1.

Y. Cao, J. Romero, and A. Aspuru-Guzik. Potential of quantum computing for drug discovery. *IBM Journal of Research and Development*, 62(6):6:1–6:20, 2018. doi: 10.1147/JRD.2018.2888987.

David Deutsch, Artur Ekert, Richard Jozsa, Chiara Macchiavello, Sandu Popescu, and Anna Sanpera. Quantum privacy amplification and the security of quantum cryptography over noisy channels. *Phys. Rev. Lett.*, 77:2818–2821, Sep 1996. doi: 10.1103/PhysRevLett.77.2818. URL https://link.aps.org/doi/10.1103/PhysRevLett.77.2818.

Antonio García de la Barrera Amo, Manuel A. Serrano, Ignacio García Rodríguez de Guzmán, Macario Polo, and Mario Piattini. Automatic generation of test circuits for the verification of quantum deterministic algorithms. In *Proceedings of the 1st International Workshop on Quantum Programming for Software Engineering*, QP4SE 2022, page 1–6, New York, NY, USA, 2022. Association for Computing Machinery. ISBN 9781450394581. doi: 10.1145/3549036.3562055. URL https://doi.org/10.1145/3549036.3562055.

Adán Garros, Diego R. Alcoba, Pablo Capuzzi, Luis Lain, Alicia Torre, Ofelia B. Oña, and Jorge Dukelsky. Determination of electronic excitation energies within the doubly occupied configuration interaction space by means of the Hermitian operator method. *The Journal of Chemical Physics*, 159(12):124107, 09 2023. ISSN 0021-9606. doi: 10.1063/5.0168585. URL https://doi.org/10.1063/5.0168585.

Jeffrey J. Hunter. Coupling and mixing times in a markov chain. *Linear Algebra and its Applications*, 430(10):2607–2621, 2009. ISSN 0024-3795. doi: https://doi.org/10.1016/j.laa.2008.09.017. URL https://www.sciencedirect.com/science/article/pii/S0024379508004382. Special Issue devoted to selected papers presented at the 16th International Workshop on Matrices and Statistics (IWMS-2007).

Peter Janotta and Haye Hinrichsen. Generalized probability theories: what determines the structure of quantum theory? *Journal of Physics A: Mathematical and Theoretical*, 47(32):323001, jul 2014. doi: 10.1088/1751-8113/47/32/323001. URL `https://dx.doi.org/10.1088/1751-8113/47/32/323001`.

V. V Kisil. A quantum-classical bracket from p -mechanics. *Europhysics Letters (EPL)*, 72(6):873–879, December 2005. ISSN 1286-4854. doi: 10.1209/epl/i2005-10324-7. URL `http://dx.doi.org/10.1209/epl/i2005-10324-7`.

Vladimir V Kisil. p-mechanics as a physical theory: an introduction. *Journal of Physics A: Mathematical and General*, 37(1):183–204, December 2003. ISSN 1361-6447. doi: 10.1088/0305-4470/37/1/013. URL `http://dx.doi.org/10.1088/0305-4470/37/1/013`.

Vasily Kravtsov, Samuel Berweger, Joanna M. Atkin, and Markus B. Raschke. Control of plasmon emission and dynamics at the transition from classical to quantum coupling. *Nano Letters*, 14(9):5270–5275, 2014. doi: 10.1021/nl502297t. URL `https://doi.org/10.1021/nl502297t`. PMID: 25089501.

Tom Leinster. Basic category theory, 2016.

David A. Levin and Yuval Peres. *Markov Chains and Mixing Times: Second edition*. American Mathematical Soc., 2017. ISBN 978-1-4704-2962-1.

Marco Lewis, Sadegh Soudjani, and Paolo Zuliani. Formal verification of quantum programs: Theory, tools and challenges. *ACM Transactions on Quantum Computing*, oct 2023. doi: 10.1145/3624483. URL `https://doi.org/10.1145/3624483`. Just Accepted.

J. E. Moyal. Quantum mechanics as a statistical theory. *Mathematical Proceedings of the Cambridge Philosophical Society*, 45(1):99–124, 1949. doi: 10.1017/S0305004100000487.

Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, 2010. doi: 10.1017/CBO9780511976667.

S. Pirandola, U. L. Andersen, L. Banchi, M. Berta, D. Bunandar, R. Colbeck, D. Englund, T. Gehring, C. Lupo, C. Ottaviani, J. L. Pereira, M. Razavi, J. Shamsul Shaari, M. Tomamichel, V. C. Usenko, G. Vallone, P. Villoresi, and P. Wallden. Advances in quantum cryptography. *Adv. Opt. Photon.*, 12(4):1012–1236, Dec 2020. doi: 10.1364/AOP.361502. URL `https://opg.optica.org/aop/abstract.cfm?URI=aop-12-4-1012`.

Alexandre F. Ramos, José Eduardo M. Hornos, and John Reinitz. Gene regulation and noise reduction by coupling of stochastic processes. *Phys. Rev. E*, 91:020701, Feb 2015. doi: 10.1103/PhysRevE.91.020701. URL `https://link.aps.org/doi/10.1103/PhysRevE.91.020701`.

Gareth O. Roberts and Jeffrey S. Rosenthal. Coupling and ergodicity of adaptive markov chain monte carlo algorithms. *Journal of Applied Probability*, 44(2):458–475, 2007. doi: 10.1239/jap/1183667414.

Miklós Rédei and Stephen Jeffrey Summers. Quantum probability theory. *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, 38(2):390–417, 2007. ISSN 1355-2198. doi: https://doi.org/10.1016/j.shpsb.2006.05.006. URL `https://www.sciencedirect.com/science/article/pii/S1355219807000342`. Probabilities in quantum mechanics.

Yao Zhang and Qiang Ni. Recent advances in quantum machine learning. *Quantum Engineering*, 2(1):e34, 2020. doi: https://doi.org/10.1002/que2.34. URL `https://onlinelibrary.wiley.com/doi/abs/10.1002/que2.34`.

Maximillian Zinner, Florian Dahlhausen, Philip Boehme, Jan Ehlers, Linn Bieske, and Leonard Fehring. Toward the institutionalization of quantum computing in pharmaceutical research. *Drug Discovery Today*, 27(2):378–383, 2022. ISSN 1359-6446. doi: https://doi.org/10.1016/j.drudis.2021.10.006. URL `https://www.sciencedirect.com/science/article/pii/S135964462100444X`.

Appendix A

addition of measurement systems

This appendix includes addition of measurement systems, a patchwork approach to quantum coupling functions is an immediate consequence of these results but most importantly to the reader, addition gives an insight into the composition of measurement systems and allows the reader to view q.c results, not only at the level of representative sets but rather as induced by the 'influence' of every generalised element in a well-chosen representative set.

Definition 19. Let $\mathcal{M}^{(1)} = \{M^{(1)}_\rho\}_{\rho\in\mathcal{D}_1}$ and $\mathcal{M}^{(2)} = \{M^{(2)}_\rho\}_{\rho\in\mathcal{D}_2}$ be M-Systems with $\mathcal{D}_1, \mathcal{D}_2 \subset \mathcal{L}(\mathcal{H}^{\otimes 2})$ sets of density operators for some Hilbert space $\mathcal{H}$, then $\mathcal{M}^{(1)} + \mathcal{M}^{(2)}$ is the M-System over $\mathcal{D}_1 \cup \mathcal{D}_2$ with

$$\begin{aligned}
M_\rho &= \overline{M^{(1)}_\rho} \cup \overline{M^{(2)}_\rho} \text{for } \rho \in \overline{D_1}, \overline{D_2}, D_1 \cup D_2 \\
M_\rho &= M^{(1)}_\rho \text{for } \rho \notin \overline{D_2}, \rho \in \mathcal{D}_1 \\
M_\rho &= M^{(2)}_\rho \text{for } \rho \notin \overline{D_1}, \rho \in \mathcal{D}_2
\end{aligned}$$

Lemma 22. $\mathcal{M}^{(1)} + \mathcal{M}^{(2)} := \mathcal{M}$ *is an M-System.*

Proof. If $\rho \notin \overline{D_2}, \rho \in \mathcal{D}_1$ then there does not exist a unitary $U \in \mathrm{SL}(\mathcal{H})$ such that $U^{\otimes 2}\rho U^{\otimes 2\dagger} \in \mathcal{D}_2$ thus we only need to verify trivial motion for some $\rho' \in \mathcal{D}_1$ which follows from $\mathcal{M}^{(1)}$ being an M-System. And analogous to above if $\rho \notin \overline{D_1}, \rho \in \mathcal{D}_2$ thus we only need to show trivial motion for $\rho \in \overline{D_1}, \overline{D_2}, D_1 \cup D_2$, observe that if $U^{\otimes 2}\rho' U^{\otimes 2\dagger} = \rho$ then by unital closure $\rho' \in \overline{D_1}, \overline{D_2}$ and so $M_{\rho'} = \overline{M^{(1)}_{\rho'}} \cup \overline{M^{(2)}_{\rho'}}$ and since both $\overline{\mathcal{M}^{(1)}}$ and $\overline{\mathcal{M}^{2}}$ are M-Systems we have

$$\begin{aligned}
M_\rho &= \overline{M^{(1)}_\rho} \cup \overline{M^{(2)}_\rho} \\
&= \{\{UM_iU^\dagger\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in \overline{M^{(1)}_{\rho'}}\} \cup \{\{UM_iU^\dagger\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in \overline{M^{(2)}_{\rho'}}\} \\
&= \{\{UM_iU^\dagger\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in \overline{M^{(1)}_{\rho'}} \cup \overline{M^{(2)}_{\rho'}}\}
\end{aligned}$$

$$= \{\{UM_iU^\dagger\}_{i\in\mathcal{I}} : \{M_i\}_{i\in\mathcal{I}} \in M_{\rho'}\}$$

thus we have trivial motion and so $\mathcal{M} = \mathcal{M}^{(1)} + \mathcal{M}^{(2)}$ is an M-System. □

Lemma 23. *Let $\mathcal{M}^{(1)}$ and $\mathcal{M}^{(2)}$ be M-Systems with (initial) q.cs Q_1 and Q_2 respectively, then a (initial) q.c over $\mathcal{M}^{(1)} + \mathcal{M}^{(2)}$ is $Q_1 \vee Q_2$.*

Proof. If $M \in M_{\rho^{AB}}$ then either $M \in \overline{M^{(1)}_{\rho^{AB}}}$ and $\|\rho^A - \rho^B\|_{\text{TD}} \leq Q_1(\mathbb{P}(X \neq Y)) \leq (Q_1 \vee Q_2)(\mathbb{P}(X \neq Y))$ and analogously for $M \in \overline{M^{(2)}_{\rho^{AB}}}$ thus $Q_1 \vee Q_2$ is a q.c for the M-System $\mathcal{M}^{(1)} + \mathcal{M}^{(2)}$. And if Q_1 and Q_2 are initial then for every $x \in [0,1]$ there exists a sequence of operators ρ_n^{AB} and σ_n^{AB} such that $\|\rho_n^A - \rho_n^B\|_{\text{TD}} \to Q_1(\mathbb{P}(X \neq Y))$ and $\|\sigma_n^A - \sigma_n^B\|_{\text{TD}} \to Q_2(\mathbb{P}(X \neq Y))$ as $n \to \infty$ from which we immediately conclude that $Q_1 \vee Q_2$ is initial. □