

Mixed States and POVMs

9.1 Introduction

As the decades of the twentieth century rolled on, quantum mechanics (QM) became more and more sophisticated and mathematical. Understanding what this theory means intuitively was confounded not only by nonclassical concepts such as wave–particle duality and quantum interference, but also by issues to do with observation. The Newtonian classical mechanics (CM) paradigm of reality, wherein reductionist laws of physics describe observer-independent dynamics of systems under observation (SUOs) with observer-independent properties, was found to be inadequate. Quantum theorists were confronted with the *measurement problem*, which attempts to understand, explain, and rationalize the laws of QM that underpin the processes of observation that go on in the laboratory. They are not the same as those of CM in several puzzling respects.

Historically, the first sign of the measurement problem was Planck's quantization of energy (Planck, 1900b) and the second was Bohr's veto on radiation damping in hydrogen (Bohr, 1913). These occurred in the first quarter of the twentieth century, a period in physics often referred to as *Old Quantum Mechanics*. Another indicator that intuition was inadequate was Born's interpretation of the squared modulus of the Schrödinger wave function as a probability density (Born, 1926).¹ That interpretation has everything to do with observers and observation, because probability without an observer is a vacuous concept.

Eventually, the *projection-valued measure* (PVM) formalism emerged, championed by von Neumann in an influential book on the mathematical formulation of QM (von Neumann, 1955). Subsequently, pioneers such as Ludwig (Ludwig, 1983a,b) and Kraus (Kraus, 1974, 1983) refined the theory into the general *positive operator-valued measure* (POVM) formalism that we shall discuss and use.

¹ Born appears to have at first taken the *magnitude* of the wave function as the probability density, but corrected himself in time.

The quantized detector network (QDN) approach to quantum experiments is most naturally expressed in the PVM formalism, as QDN focuses on the individual detectors in the laboratory. However, the POVM formalism is more general than the PVM formalism, giving a description of multiple detector processes similar to QDN. This raises the question of how the two approaches, QDN and POVM, are related. The aim of this chapter is to explore this relationship.

Before we review the PVM and POVM formalisms, we review some essential mathematical concepts.

9.2 Sets and Measures

Most of the mathematics used in this book involves spaces, which are sets with additional structure such as inner products (Howson, 1972).

Definition 9.1 A sigma-algebra on set A is a collection Σ^A of subsets of A such that

1. Σ^A includes the empty subset \emptyset .
2. Σ^A is closed under complement: if E is an element of Σ^A , then so is its complement in A , denoted E^c . Since by property 1, the empty set \emptyset belongs to Σ^A and its complement is A , then property 2 means that A itself is a member of Σ^A .
3. Σ^A is closed under countable unions, which means that if we pick any countable number E^1, E^2, \dots, E^n of elements in Σ^A , then their union $\cup_{i=1}^n E^i$ is also in Σ^A .
4. Σ^A is closed under countable intersections, which means that if we pick any finite number E^1, E^2, \dots, E^n of elements of Σ^A , then their intersection $\cap_{i=1}^n E^i$ is also in Σ^A . Note that this intersection could be empty, but that possibility is covered by property 1.

Definition 9.2 The *extended reals* \mathbb{R}^* is the set of real numbers \mathbb{R} and two extra elements, $+\infty$ and $-\infty$. These latter two elements are referred to as *plus infinity* and *minus infinity*, respectively, and are interpreted accordingly.

Definition 9.3 Given a sigma-algebra Σ^A over set A , a *measure* on A assigns an extended real number $\mu(E)$ to each element E of Σ^A such that

1. *Nonnegativity*: for any element E in Σ^A , $\mu(E) \geq 0$.
2. *Measure of empty set*: $\mu(\emptyset) = 0$.
3. *Countable additivity*: for any countable collection $\{E^1, E^2, \dots\}$ of pairwise disjoint elements of Σ^A , meaning that $E^i \cap E^j = \emptyset$ for $i \neq j$, then

$$\mu\left(\bigcup_{i=1}^{\infty} E^i\right) = \sum_{i=1}^{\infty} \mu(E^i). \quad (9.1)$$

In applications to quantum physics, the set A referred to in the above definitions will consist of all possible outcomes of an experiment; the sigma-algebra will consist of all possible ways of grouping those outcomes; and the measure μ will be the assignment of probabilities to the elements of Σ^A .

9.3 Hilbert Spaces

Hilbert spaces are complex vector spaces with a suitable inner product concept. In this chapter, we shall use the well-known Dirac bracket notation, following Paris (2012). In most of this book we deal with finite-dimensional Hilbert spaces, as the guiding philosophy of QDN is to model what goes on in the laboratory. No infinities are ever actually encountered in the laboratory; at worst, a readout on a counter goes off-scale.

Definition 9.4 An orthonormal basis (ONB) for a d -dimensional Hilbert space \mathcal{H} is a set of elements $\{|\psi^n\rangle : n = 1, 2, \dots, d\}$ of \mathcal{H} with the following properties:

1. **Orthonormality:** $\langle\psi^n|\psi^m\rangle = \delta^{nm}$, $1 \leq n, m \leq d$, where δ^{nm} is the Kronecker delta.
2. **Completeness/resolution of the identity:**

$$\sum_{n=1}^d |\psi^n\rangle\langle\psi^n| = I^{\mathcal{H}}, \quad (9.2)$$

where $I^{\mathcal{H}}$ is the identity operator on \mathcal{H} .

9.4 Operators and Observables

An *operator* is any rule that assigns an element of one Hilbert space to some element either in the same Hilbert space or in another Hilbert space. There are various kinds of operators that are important to us here. A *linear operator* O from Hilbert space \mathcal{H}^1 to Hilbert space \mathcal{H}^2 is one such that if $|\Psi\rangle$ and $|\Phi\rangle$ are arbitrary elements of \mathcal{H}^1 and α and β are arbitrary complex numbers, then

$$O(\alpha|\Psi\rangle + \beta|\Phi\rangle) = \alpha O|\Psi\rangle + \beta O|\Phi\rangle, \quad (9.3)$$

where we note that addition on the left-hand side of (9.3) is in \mathcal{H}^1 , while addition on the right-hand side is in \mathcal{H}^2 .

The linear space of linear operators from \mathcal{H} to \mathcal{H} is denoted $L(\mathcal{H})$ and is itself a Hilbert space (Paris, 2012).

A *positive operator* O over Hilbert space \mathcal{H} is one such that for any element $|\Psi\rangle$ of \mathcal{H} , we have

$$\langle\Psi|O|\Psi\rangle \geq 0. \quad (9.4)$$

A positive operator is self-adjoint.

An observable X is a self-adjoint operator that admits a discrete *spectral decomposition*; i.e., we can write

$$X = \sum_{n=1}^d x^n P^n, \tag{9.5}$$

where the x^n are real and the eigenvalues of X , and the *projectors* P^n are given by $P^n \equiv |x^n\rangle\langle x^n|$. Here the normalized eigenvectors $|x^n\rangle$ satisfy the eigenvalue equation

$$X|x^n\rangle = x^n|x^n\rangle \tag{9.6}$$

and form an ONB for \mathcal{H} .² Orthonormality then leads to the product rule

$$P^n P^m = \delta^{nm} P^n \tag{9.7}$$

and the completeness sum

$$\sum_{n=1}^d P^n = I^{\mathcal{H}}. \tag{9.8}$$

9.5 Trace

If $\{|\psi^n\rangle : n = 1, 2, \dots, d\}$ is an ONB for \mathcal{H} , then the *trace* $\text{Tr}\{O\}$ of an operator O is defined by

$$\text{Tr}\{O\} \equiv \sum_{n=1}^d \langle \psi^n | O | \psi^n \rangle. \tag{9.9}$$

The trace of an operator is independent of choice of ONB for \mathcal{H} .

Given an arbitrary state $|\Psi\rangle$ in \mathcal{H} , then we can use any ONB to show that

$$\langle \Psi | O | \Psi \rangle = \text{Tr}\{O|\Psi\rangle\langle \Psi|\}. \tag{9.10}$$

This result is crucial to the density operator and POVM formalisms widely applied in QM.

9.6 Projection-Valued Measure

We are now in a position to discuss PVMs in standard QM.

Given an observable X , the probability $\text{Pr}(x^n|\Psi)$ of final outcome x^n given initial normalized state $|\Psi\rangle$ is according to the Born rule (Born, 1926) given by

$$\begin{aligned} \text{Pr}(x^n|\Psi) &= |\langle x^n | U | \Psi \rangle|^2 = \langle \Psi | U^\dagger | x^n \rangle \langle x^n | U | \Psi \rangle \\ &= \langle \Psi | U^\dagger P^n U | \Psi \rangle = \text{Tr}\{P^n U \rho U^\dagger\}, \end{aligned} \tag{9.11}$$

² This can always be arranged, even if some of the eigenvalues are degenerate.

where U is the unitary evolution operator taking the initial state $|\Psi\rangle$ to its final state $U|\Psi\rangle$ at the time of measurement and ρ is the initial *density operator*, defined by

$$\rho \equiv |\Psi\rangle\langle\Psi| \tag{9.12}$$

in this instance.

The *expectation value* $\langle X \rangle_\Psi$ of the observable X conditional on Ψ is given by

$$\begin{aligned} \langle X \rangle_\Psi &\equiv \sum_{n=1}^d x \Pr(x^n|\Psi) = \sum_{n=1}^d x^n \text{Tr}\{P^n U \rho U^\dagger\} \\ &= \text{Tr} \left\{ \left[\sum_{n=1}^d x^n P^n \right] U \rho U^\dagger \right\} = \text{Tr}\{XU \rho U^\dagger\}. \end{aligned} \tag{9.13}$$

9.7 Mixed States

Suppose an observer carries out an experiment consisting of a large number of runs but is unsure, at the start of each run, of the initial state. Suppose further that the observer’s ignorance can be quantified into the statement that for each run, the initial state is taken from a discrete probability space Ω , that is, a finite distribution of possible states, each labeled by superscript κ , running from 1 to some finite integer K , such that the probability of preparing state $|\Psi^\kappa\rangle$ is ω^κ :

$$\Omega \equiv \left\{ \omega^\kappa, |\Psi^\kappa\rangle : \sum_{\kappa=1}^K \omega^\kappa = 1, \quad \langle \Psi^\kappa | \Psi^\kappa \rangle = 1 \right\}. \tag{9.14}$$

Here the possible initial states are normalized but not necessarily mutually orthogonal. The number K of possibilities is arbitrary and can exceed the dimension d of \mathcal{H}^S . The probabilities ω^κ are *epistemic* in character, that is, classical probabilities. Such a random initial state is referred to as a *mixed state* when $K > 1$. When $K = 1$, the observer’s ignorance about the initial state is zero and the corresponding unique element of the Hilbert space is referred to as a *pure state*.

The expectation value $\langle X \rangle_\rho$ of the observable X conditional on a mixed state ρ is now

$$\begin{aligned} \langle X \rangle_\rho &= \sum_{\kappa=1}^K \omega^\kappa \langle \psi^\kappa | U^\dagger X U | \psi^\kappa \rangle \\ &= \text{Tr}\{XU \underbrace{\sum_{\kappa=1}^K \omega^\kappa |\psi^\kappa\rangle\langle\psi^\kappa|}_{\rho} U^\dagger\} = \text{Tr}\{XU \rho U^\dagger\}, \end{aligned} \tag{9.15}$$

where

$$\rho \equiv \sum_{\kappa=1}^K \omega^\kappa |\psi^\kappa\rangle\langle\psi^\kappa| \tag{9.16}$$

is the appropriate generalization of the density matrix operator (9.12) to the mixed state situation.

It is easy to show that a density operator is a positive operator and has unit trace. This means that the eigenvalues of a density operator are nonnegative and sum to unity.

9.8 Partial Trace

The above formalism is standard quantum theory as applied to a single Hilbert space, typically the space of SUO states. We now extend the discussion to the tensor product of two Hilbert spaces, \mathcal{H}^S and \mathcal{H}^A , where in anticipation of our later needs, S will stand for SUO and A will stand for *apparatus* or, more technically, *ancilla*.³ \mathcal{H}^S will have dimension d and \mathcal{H}^A will have dimension D .

Given two finite-dimensional Hilbert spaces $\mathcal{H}^S, \mathcal{H}^A$, not necessarily of the same dimension, consider a state $|\Psi^{SA}\rangle$ in the tensor product $\mathcal{H}^S \otimes \mathcal{H}^A$. Note that we shall henceforth use *round* brackets to denote states in such an SUO-apparatus tensor product space, rather than angular brackets, and call them *total states*. Then the associated density operator is defined by

$$\rho^{SA} \equiv |\Psi^{SA}\rangle\langle\Psi^{SA}|. \tag{9.17}$$

Now suppose $X \in L(\mathcal{H}^S)$ is an observable over \mathcal{H}^S . Then we can write

$$X = \sum_{n=1}^d x^n P^n. \tag{9.18}$$

Now construct the operator $\hat{P}^n \equiv P^n \otimes I^A$ in $L(\mathcal{H}^S \otimes \mathcal{H}^A)$, where I^A is the identity operator over \mathcal{H}^A . Then

$$\Pr(x^n|\Psi^{SA}) = \langle\Psi^{SA}|U^\dagger \hat{P}^n U|\Psi^{SA}\rangle = \text{Tr}_{AB}\{\hat{P}^n U \rho^{SA} U^\dagger\}. \tag{9.19}$$

Here the subscript AB reminds us we are taking the full trace, that is, in the tensor product space $\mathcal{H}^S \otimes \mathcal{H}^A$.

The concept of *partial trace* is related to the concept of partial question that we discussed in the previous chapter. Partial traces are defined by constructing ONBs for the component Hilbert spaces and summing only over some of them. Suppose $\{|s^m\rangle : m = 1, 2, \dots, d\}$ is an ONB for \mathcal{H}^S and $\{|a^n\rangle : n = 1, 2, \dots, D\}$ is an ONB basis for \mathcal{H}^A . Then $\{|s^m, a^n\rangle \equiv |s^m\rangle \otimes |a^n\rangle : m = 1, 2, \dots, d, n = 1, 2, \dots, D\}$ is an ONB basis for $\mathcal{H}^S \otimes \mathcal{H}^A$.

Suppose V is an operator over \mathcal{H}^S and W is an operator over \mathcal{H}^A . Then the *full trace* $\text{Tr}_{SA}\{V \otimes W\}$ of the tensor product operator $V \otimes W$ is given by

$$\begin{aligned} \text{Tr}_{SA}\{V \otimes W\} &\equiv \sum_{m=1}^d \sum_{n=1}^D \langle s^m, a^n | V \otimes W | s^m, a^n \rangle \\ &= \left\{ \sum_{m=1}^d \langle s^m | V | s^m \rangle \right\} \left\{ \sum_{n=1}^D \langle a^n | W | a^n \rangle \right\}. \end{aligned} \tag{9.20}$$

³ In standard QM, ancillas are often treated as auxiliary, almost incidental aspects. In QDN, they are essential and as important as SUOs.

There are two partial traces available. $\text{Tr}_S\{V \otimes W\}$ is a partial trace over the SUO degrees of freedom, giving

$$\text{Tr}_S\{V \otimes W\} = \sum_{m=1}^d \langle s^m | V \otimes W | s^m \rangle = \left\{ \sum_{m=1}^d \langle s^m | V | s^m \rangle \right\} W, \quad (9.21)$$

and is an operator over \mathcal{H}^A . Similarly, $\text{Tr}_A\{V \otimes W\}$ is a partial trace over the apparatus degrees of freedom, giving

$$\text{Tr}_A\{V \otimes W\} = \sum_{n=1}^D \langle a^n | V \otimes W | a^n \rangle = V \left\{ \sum_{n=1}^D \langle a^n | W | a^n \rangle \right\}, \quad (9.22)$$

and is an operator over \mathcal{H}^S .

Given a density operator ρ^{SA} over $\mathcal{H}^S \otimes \mathcal{H}^A$, then we define the partial traces

$$\rho^S \equiv \text{Tr}_A\{\rho^{SA}\}, \quad \rho^A \equiv \text{Tr}_S\{\rho^{SA}\}. \quad (9.23)$$

Then ρ^S is a density operator over \mathcal{H}^S and ρ^A is a density operator over \mathcal{H}^A , with

$$\text{Tr}_S\{\rho^S\} = \text{Tr}_A\{\rho^A\} = 1. \quad (9.24)$$

Circularity

For a single Hilbert space \mathcal{H} , the trace of operators A, B, \dots, Z satisfies the circularity property

$$\text{Tr}_H\{ABC \dots Z\} = \text{Tr}_H\{BC \dots ZA\}. \quad (9.25)$$

This property holds also for tensor products of Hilbert spaces. If R^1, R^2, \dots, R^N are operators over $\mathcal{H}^S \otimes \mathcal{H}^A$, then

$$\text{Tr}_{SA}\{R^1 R^2 \dots R^N\} = \text{Tr}_{SA}\{R^2 R^3 \dots R^N R^1\}. \quad (9.26)$$

Circularity does not hold for partial traces.

9.9 Purification

Suppose \mathcal{H}^S is a Hilbert space of dimension d , representing states of some SUO. Consider a density operator ρ^S over \mathcal{H}^S . From previous sections, we can find a set $\{|\psi^m\rangle : m = 1 \dots d\}$ of normalized eigenvectors of ρ^S with nonnegative eigenvalues, that is,

$$\rho^S |\psi^m\rangle = \lambda^m |\psi^m\rangle, \quad m = 1, 2, \dots, d, \quad \lambda^m \geq 0. \quad (9.27)$$

Then we can write

$$\rho^S = \sum_{m=1}^d \lambda^m |\psi^m\rangle \langle \psi^m|. \quad (9.28)$$

We can assume orthonormality, that is, $\langle \psi^m | \psi^n \rangle = \delta^{mn}$.

Now construct another Hilbert space \mathcal{H}^A with $\dim \mathcal{H}^A = D \geq d$, with an ONB $\{|\theta^n : n = 1, 2, \dots, D\}$. Next, define a pure state $|\psi^{SA}\rangle$ in $\mathcal{H}^S \otimes \mathcal{H}^A$ of the form

$$|\psi^{SA}\rangle \equiv \sum_{n=1}^d \sqrt{\lambda^n} |\psi^n\rangle \otimes |\theta^n\rangle. \tag{9.29}$$

The density operator ρ^{SA} associated with this pure state is then given by

$$\rho^{SA} \equiv |\psi^{SA}\rangle \langle \psi^{SA}| = \sum_{m,n=1}^d \sqrt{\lambda^m \lambda^n} |\psi^m\rangle \langle \psi^n| \otimes |\theta^m\rangle \langle \theta^n|. \tag{9.30}$$

Now partially trace ρ^{SA} over \mathcal{H}^A :

$$\begin{aligned} \text{Tr}_A\{\rho^{SA}\} &\equiv \sum_{c=1}^D \langle \theta^c | \rho^{SA} | \theta^c \rangle = \sum_{c=1}^D \langle \theta^c | \sum_{m,n=1}^d \sqrt{\lambda^m \lambda^n} |\psi^m\rangle \langle \psi^n| \otimes |\theta^m\rangle \langle \theta^n| \theta^c \rangle \\ &= \sum_{c=1}^D \sum_{m,n=1}^d \sqrt{\lambda^m \lambda^n} |\psi^m\rangle \langle \psi^n| \underbrace{\langle \theta^c | \theta^m \rangle}_{\delta^{cm}} \underbrace{\langle \theta^n | \theta^c \rangle}_{\delta^{nc}} \\ &= \sum_{m=1}^d \lambda^m |\psi^m\rangle \langle \psi^m|, \end{aligned} \tag{9.31}$$

that is,

$$\text{Tr}_A\{\rho^{SA}\} = \rho^S. \tag{9.32}$$

In words, we can represent the density operator for a mixed state in one Hilbert space by the density operator for a pure state in a larger Hilbert space. This fundamental result opens the door to Naimark’s theorem (below). The state $|\psi^{SA}\rangle$ is called a *purification* of ρ^S . There are infinitely many possible purifications of a given density operator.

9.10 Purity and Entropy

Definition 9.5 Given a density operator ρ with spectrum of eigenvalues $\{\lambda^k : k = 1, 2, \dots, d\}$, define the *purity* $\mu[\rho]$ by

$$\mu[\rho] \equiv \sum_{k=1}^d (\lambda^k)^2. \tag{9.33}$$

It is straightforward to prove that for any density operator, $d^{-1} \leq \mu[\rho] \leq 1$.

Mixed states ignore correlation information encoded between an SUO and its environment. Given a density operator ρ , another measure of information loss associated with ρ is the *von Neumann entropy*, defined by

$$S[\rho] \equiv -\text{Tr}\{\rho \ln \rho\} = -\sum_k \lambda^k \ln \lambda^k. \tag{9.34}$$

Then it is straightforward to show that $0 \leq S[\rho] \leq \ln d$. Von Neumann entropy is a monotonically decreasing function of purity and vice-versa (Paris, 2012). A pure state has purity 1 and von Neumann entropy zero, while a maximally mixed state has entropy $\ln d$ and purity $1/d$.

9.11 POVMs

The Born rule for mixed states can be rewritten in a form that can be generalized, leading to the POVM formalism, a more general approach to quantum measurement than the PVM formalism.

In standard QM, given a density operator ρ^S on a d -dimensional SUO Hilbert space \mathcal{H}^S and observable $X \equiv \sum_{m=1}^d x^m P^m$, then the probability $\Pr(x^m | \rho^S)$ of outcome x^m is given by

$$\Pr(x^m | \rho^S) \equiv \text{Tr}\{P^m U \rho^S U^\dagger P^m\}, \quad (9.35)$$

where we use $P^n P^n = P^n$.

Now suppose we can find a set $\{M^n : n = 1, 2, \dots, N\}$ of operators called *Kraus* (or *detection*) operators such that

$$\sum_{n=1}^N M^{n\dagger} M^n = I^S. \quad (9.36)$$

Then the generalization of (9.35) is to assert that

$$\Pr(y^n | \rho^S) \equiv \text{Tr}\{M^n \rho^S M^{n\dagger}\} \quad (9.37)$$

is the probability associated with detection outcome associated with M^n , where now the number N of possible outcomes is not necessarily equal to $d \equiv \dim \mathcal{H}^S$.

We define the *POVM elements* $\{E^n : n = 1, 2, \dots, N\}$ of the probability (or positive) operator-valued measure (POVM) by

$$E^n \equiv M^{n\dagger} M^n. \quad (9.38)$$

Then (9.36) gives

$$\sum_{n=1}^N E^n = I^{\mathcal{H}^S}. \quad (9.39)$$

The POVM operators E^n are positive.

The detection operators M^n are defined up to unitary transformations; that is, given a detection operator M^n , then for unitary operator V , $M'^n \equiv V^n M^n$ is a valid detection operator giving the same POVM element $E'^n \equiv M'^{n\dagger} M'^n$ as M^n , i.e.,

$$E'^n = E^n. \quad (9.40)$$

This scheme is called a *generalized measurement*.

9.12 Naimark's Theorem

This theorem is critical in the formal justification and rationalization of QDN. The theorem goes under the name of Naimark, but Naimark was not concerned with application to quantum theory per se.

The theorem has two parts (Paris, 2012). We write it out here in its QDN form, where S refers to the SUO and A refers to *apparatus* or **ancilla**.

Theorem 9.6 Part 1

Suppose we are given a POVM set $\{E^n : n = 1, 2, \dots, N\}$ on SUO Hilbert space \mathcal{H}^S with finite dimension d . Then we know that the E^n are positive operators and

$$\sum_{n=1}^N E^n = I^S. \tag{9.41}$$

Then there exists a Hilbert space \mathcal{H}^A of dimension at least N , and a pure state $|\omega^A\rangle$ in \mathcal{H}^A such that

1. The density operator $\rho^A \equiv |\omega^A\rangle\langle\omega^A| \in L(\mathcal{H}^A)$, the Hilbert space of linear operator over \mathcal{H}^A .
2. There is some unitary evolution operator (in QDN a semi-unitary operator) $U \in L(\mathcal{H}^S \otimes \mathcal{H}^A)$ such that

$$U^\dagger U = U U^\dagger = I^{SA}. \tag{9.42}$$

3. There is a set $\{P^n\}$ of projectors over \mathcal{H}^A ,
such that

$$E^n = \text{Tr}_A\{I^S \otimes P^n U I^S \otimes \rho^A U^\dagger\}. \tag{9.43}$$

Note that the U operator can encode any dynamical evolution in the combined system.

Part 2

In this part, we derive an expression for the detection operators $\{M^n\}$.

Suppose an initial mixed state is prepared, such that in $\mathcal{H}^S \otimes \mathcal{H}^A$ it is described by density operator

$$\rho_0^{SA} \equiv \rho_0^S \otimes |\omega_0^A\rangle\langle\omega_0^A| \tag{9.44}$$

and then allowed to evolve under unitary evolution U , giving the final density operator

$$\rho^{SA} = U \rho_0^{SA} U^\dagger. \tag{9.45}$$

Then a projective measurement to test for outcome $|x^n\rangle$ of observable X is made via the apparatus. The probability $\text{Pr}(x^n | \rho_0^{SA})$ is given by the equivalent of the Born rule, in this case

$$\Pr(x^n | \rho_0^{SA}) = \text{Tr}_{SA} \{ \rho^{SA} I^S \otimes P^n \}, \tag{9.46}$$

where $P^n \equiv |x^n\rangle\langle x^n|$. Then

$$\begin{aligned} \Pr(x^n | \rho_0^{SA}) &= \text{Tr}_{SA} \{ U \rho_0^{SA} U^\dagger I^S \otimes P^n \} \\ &= \text{Tr}_{SA} \{ U \rho_0^S \otimes |\omega_0^A\rangle\langle \omega_0^A| U^\dagger I^S \otimes |x^n\rangle\langle x^n| \} \\ &= \text{Tr}_{SA} \{ \rho_0^S \otimes |\omega_0^A\rangle\langle \omega_0^A| U^\dagger I^S \otimes |x^n\rangle\langle x^n| U \} \\ &= \text{Tr}_S \{ \rho_0^S \langle \omega_0^A| U^\dagger I^S \otimes |x^n\rangle\langle x^n| U |\omega_0^A\rangle \} \\ &= \text{Tr}_S \{ \rho_0^S \langle \omega_0^A| U^\dagger |x^n\rangle\langle x^n| U |\omega_0^A\rangle \} \\ &= \text{Tr}_S \{ \underbrace{|x^n\rangle\langle x^n| U |\omega_0^A\rangle}_{M^n} \rho_0^S \underbrace{\langle \omega_0^A| U^\dagger |x^n\rangle}_{M^{n\dagger}} \} \end{aligned} \tag{9.47}$$

i.e.

$$\Pr(x^n | \rho_0^{SA}) = \text{Tr}_S \{ M^n \rho_0^S M^{n\dagger} \} = \text{Tr}_S \{ E^n \rho_0^S \}, \tag{9.48}$$

where $E^n \equiv M^{n\dagger} M^n$.

9.13 QDN and POVM Theory

We turn our attention now to the relationship between QDN and POVMs. This is important because a generalized QDN-POVM formalism is used extensively in our computer algebra (CA) implementation of QDN, program MAIN, discussed in Chapter 12 and used in all our specific calculations.

The first step is to recognize that the quantum registers we are concerned with model only the labstates, that is, the apparatus states, and say nothing per se about the imagined SUO states. As we stressed previously, QDN was not designed to give specific information about what happens in the information void. Therefore, the quantum physics of SUOs has to be appended “by hand”. This is achieved by introducing a stage-dependent Hilbert space \mathcal{H}_n^S at each stage Σ_n to contain the SUO “internal” states, and a separate quantum register \mathcal{Q}_n to contain the signal state of the apparatus. Elements of \mathcal{H}_n^S will be called *system states*, elements of \mathcal{Q}_n are called *labstates*, and elements of $\mathcal{H}_n \equiv \mathcal{H}_n^S \otimes \mathcal{Q}_n$ will be called *total states*.

Notation

In the following, Dirac’s bracket notation $|\psi_n\rangle$ is used for system states; our bold notation \mathbf{i}_n denotes computational basis representation (CBR) of labstates; and modified Dirac brackets $|\Psi_n\rangle = |\psi_n, \mathbf{i}_n\rangle \equiv |\psi_n\rangle \otimes \mathbf{i}_n$ describe total states. We make an exception to our rule suppressing tensor product symbols in the case of total states, in order to separate out system states and labstates.

By definition, system states are unobservable directly and there is no natural preferred basis for \mathcal{H}_n^S .⁴ Therefore, we are free to choose any convenient

⁴ The principle of “general covariance,” or independence of frame of reference, is meaningful as far as system states are involved, but vacuous as far as labstates are concerned.

orthonormal basis for \mathcal{H}^S . We shall denote elements of our choice by $|\alpha_n\rangle$, that is, with lowercase Greek labels, with the inner product rule $\langle\alpha_n|\beta_n\rangle \equiv \delta^{\alpha\beta}$, and assume that \mathcal{H}_n^S has finite dimension d_n . For instance, $d_n = 2$ if \mathcal{H}_n describes vertical and horizontal electromagnetic polarization eigenstates (ignoring momenta and other attributes).

Summations occur frequently in the following, so we make the following simplification:

$$\sum_{\alpha=1}^{d_n} \sum_{i=1}^{2^{r_n}-1} \rightarrow \sum_{\alpha i}^{[n]}, \tag{9.49}$$

where r_n is the rank of \mathcal{Q}_n .

Initial Total State

A pure initial total state $|\Psi_0\rangle$ and its dual $\langle\Psi_0|$ will take the general form

$$|\Psi_0\rangle \equiv \sum_i^{[0]} \psi_0^{\alpha i} |\alpha_0\rangle \otimes \mathbf{i}_0, \quad \langle\Psi_0| = \sum_{\alpha i}^{[0]} \psi_0^{\alpha i*} \langle\alpha_0| \otimes \overline{\mathbf{i}}_0, \tag{9.50}$$

where $\psi_0^{\alpha i*}$ is the complex conjugate of $\psi_0^{\alpha i}$. If the initial total state is normalized to unity, then we have

$$\langle\Psi_0|\Psi_0\rangle = \sum_{\alpha i}^{[0]} |\psi_0^{\alpha i}|^2 = 1. \tag{9.51}$$

Final Total State

Assuming semi-unitary evolution, the final total state $|\Psi_N\rangle$ is given by

$$|\Psi_N\rangle \equiv U_{N,0}|\Psi_0\rangle, \quad N \geq 0, \tag{9.52}$$

where Σ_N is the final stage and the contextual evolution operator $U_{N,0}$ is given by

$$U_{N,0} \equiv \sum_{\alpha i}^{[N]} \sum_{\beta j}^{[0]} U_{N,0}^{\alpha i, \beta j} |\alpha_N\rangle \langle\beta_0| \otimes \mathbf{i}_N \overline{\mathbf{j}}_0. \tag{9.53}$$

The retraction operator $\overline{U}_{N,0}$ is given by

$$\overline{U}_{N,0} = \sum_{\alpha i}^{[N]} \sum_{\beta j}^{[0]} U_{N,0}^{\alpha i, \beta j*} |\beta_0\rangle \langle\alpha_N| \otimes \mathbf{j}_0 \overline{\mathbf{i}}_N. \tag{9.54}$$

The semi-unitary condition $\overline{U}_{N,0}U_{N,0} = I_0$, where I_0 is the identity operator for the initial total space \mathcal{H}_0 , requires the conditions

$$\sum_{\alpha i}^{[N]} U_{N,0}^{\alpha i, \beta j*} U_{N,0}^{\alpha i, \gamma k} = \delta^{\beta\gamma} \delta^{jk}. \tag{9.55}$$

QDN POVM Operators

The QDN Kraus operators are defined as

$$\begin{aligned} M_{N,0}^i &\equiv \overline{\mathbf{i}}_N U_{N,0} = \sum_{\alpha}^{[N]} \sum_{\beta_j}^{[0]} U_{N,0}^{\alpha i, \beta_j} |\alpha_N\rangle \langle \beta_0| \otimes \overline{\mathbf{j}}_0, \\ \overline{M}_{N,0}^i &\equiv \overline{U}_{N,0} \mathbf{i}_N = \sum_{\alpha}^{[N]} \sum_{\beta_j}^{[0]} U_{N,0}^{\alpha i, \beta_j^*} |\beta_0\rangle \langle \alpha_N| \otimes \mathbf{j}_0, \end{aligned} \quad (9.56)$$

giving the POVM operators

$$\begin{aligned} E_{N,0}^i &\equiv \overline{M}_{N,0}^i M_{N,0}^i \\ &= \sum_{\beta_j}^{[0]} \sum_{\delta_k}^{[0]} \left\{ \sum_{\alpha}^{[N]} U_{N,0}^{\alpha i, \beta_j^*} U_{N,0}^{\alpha i, \delta_k} \right\} |\beta_0\rangle \langle \delta_0| \otimes \mathbf{j}_0 \overline{\mathbf{k}}_0, \quad i = 0, 1, 2, \dots, 2^{r_N} - 1. \end{aligned} \quad (9.57)$$

Using the semi-unitary conditions (9.36), we readily find

$$\sum_i^{[0]} E_{N,0}^i = I_0, \quad (9.58)$$

which is the QDN analogue of the standard POVM condition (9.39).

Interpretation

We may readily understand the QDN POVM formalism if we consider the possible questions that the observer could ask. Those questions can be only asked about the signal status of the apparatus. If the final stage normalized total state is $|\Psi_N\rangle$ and the final stage apparatus has rank r_N , then there is a grand total of 2^{r_N} maximal questions, each of them equivalent to a projector of the form $I_N^S \otimes \mathbf{i}_N \overline{\mathbf{i}}_N$, for $i = 0, 1, 2, \dots, 2^{r_N} - 1$. The probability $P(\mathbf{i}_N | \Psi_0)$ that the final labstate is \mathbf{i}_N is given by

$$\begin{aligned} P(\mathbf{i}_N | \Psi_0) &\equiv (\Psi_N | \mathbf{i}_N \overline{\mathbf{i}}_N | \Psi_N) = (\Psi_0 | \overline{U}_{N,0} \mathbf{i}_N \overline{\mathbf{i}}_N U_{N,0} | \Psi_0) \\ &= (\Psi_0 | \underbrace{\overline{U}_{N,0} \mathbf{i}_N \overline{\mathbf{i}}_N U_{N,0}}_{\overline{M}_{N,0}^i M_{N,0}^i} | \Psi_0) = (\Psi_0 | \underbrace{\overline{M}_{N,0}^i M_{N,0}^i}_{E_{N,0}^i} | \Psi_0) \end{aligned} \quad (9.59)$$

$$= \text{Tr} \{ E_{N,0}^i \varrho_0 \}, \quad (9.60)$$

where $\varrho_0 \equiv |\Psi_0\rangle \langle \Psi_0|$ is the initial stage density operator.

We saw in Chapter 8 that we can also ask partial questions, involving only a subset of all the final state detectors. We can answer these questions as well, because any partial question is equivalent to some combination of maximal questions.

Example 9.7 Consider a rank-three quantum register. There are $2^3 = 8$ maximal questions, corresponding to the eight projection operators associated with the CBR. Specifically, we have $Q^0 \equiv P^1 P^2 P^3 = \overline{\mathbf{00}}$, $Q^1 \equiv \widehat{P}^1 P^2 P^3 = \overline{\mathbf{11}}$, \dots , $Q^7 \equiv \widehat{P}^1 \widehat{P}^2 \widehat{P}^3 = \overline{\mathbf{77}}$.

Suppose we wanted to ask the partial question $\widehat{\mathbb{P}}^2$, that is, look only at detector 2 and ask whether it is in its signal state. Then we use the rule that for $i = 1, 2, \dots, d$, $\mathbb{P}^i + \widehat{\mathbb{P}}^i = \mathbb{I}$, the register identity, to write

$$\begin{aligned}\widehat{\mathbb{P}}^2 &= \mathbb{I}\widehat{\mathbb{P}}^2\mathbb{I} = (\mathbb{P}^1 + \widehat{\mathbb{P}}^1)\widehat{\mathbb{P}}^2(\mathbb{P}^3 + \widehat{\mathbb{P}}^3) \\ &= \mathbb{P}^1\widehat{\mathbb{P}}^2\mathbb{P}^3 + \widehat{\mathbb{P}}^1\widehat{\mathbb{P}}^2\mathbb{P}^3 + \mathbb{P}^1\widehat{\mathbb{P}}^2\widehat{\mathbb{P}}^3 + \widehat{\mathbb{P}}^1\widehat{\mathbb{P}}^2\widehat{\mathbb{P}}^3 \\ &= \mathbb{Q}^2 + \mathbb{Q}^3 + \mathbb{Q}^6 + \mathbb{Q}^7.\end{aligned}\tag{9.61}$$

We conclude from this that knowledge of all the maximal questions and their answers allows us to answer all partial questions.

Mixed Initial States

The above has assumed that the initial total state is a pure one. We can readily extend the formalism to the case of mixed initial states. All we need do is replace the pure density operator $\varrho_0 \equiv |\Psi_0\rangle\langle\Psi_0|$ with the appropriate mixed density operator. This will have the generic form

$$\varrho_0 \equiv \sum_{\kappa} \omega^{\kappa} |\Psi_0^{\kappa}\rangle\langle\Psi_0^{\kappa}|,\tag{9.62}$$

where the ω^{κ} are probabilities summing to unity and $|\Psi_0^{\kappa}\rangle$ is the normalized total state occurring with probability ω^{κ} in the mixture.

There is an interesting possibility here: not only could the randomness be associated with the system states, but there could be uncertainty about the apparatus. In other words, we should be prepared for the possibility that the apparatus at any given stage is not determined beforehand but is created by random processes. This raises deeper questions to do with the general theory of observation that will certainly need to be addressed in the future. We discuss some aspects of this topic in Chapter 21, on self-intervening networks.

There are three important aspects to our modeling. First, in common with standard quantum modeling of pointer states, our initial apparatus register (at stage Σ_0) will be a rank-one quantum register \mathcal{Q}_1 referred to as a *preparation switch*. This models the logic of state preparation: if the observer knows that an SUO state $|\Psi\rangle$ has been prepared, then that state is tensored with element $\mathbf{1}_0$ of \mathcal{Q}_0 , whereas if such a state has *not* been prepared, then that state is tensored with element $\mathbf{0}_0$ of \mathcal{Q}_0 . We see from this that QDN attaches significance to what has *not* been done as much as to what has been done. This is reminiscent of Renniger's thought experiment, where an absence of observation has measurable consequences (Renniger, 1953).

The second aspect concerns the interpretation of what is going on. In QDN, only signal states of the apparatus are physically meaningful. The SUO and therefore the mathematical representation of its states is a convenient fiction encoding contextuality. Therefore, we do not need to treat \mathcal{H}^S on the same footing as \mathcal{Q}_n . It may be convenient to employ the Schrödinger picture for evolution of

SUO states and treat \mathcal{H}^S as stage independent.⁵ That is certainly not the case for the quantum registers \mathcal{Q}_n .

The third aspect concerns the notion of *purification* that we discussed above for standard QM. There it was pointed out that the dimension of the ancilla Hilbert space \mathcal{H}^A had to be at least as great as the number of independent states in the prepared mixture that was being purified, and that there was always an infinite number of ancillas that could be employed. In the case of QDN, neither of these comments applies. The analogue of the ancilla concept is the quantum register modeling the apparatus, and the rank of that register is determined by the number of detectors that the observer has constructed. That number is independent of the dimensionality of \mathcal{H}^S . Moreover, the concept of preferred basis does not apply to the standard ancilla concept, whereas it is relevant in QDN. The moral here is that standard QM treats states of SUO as the primary objects of interest, whereas QDN relegates them to auxiliary devices and elevates the apparatus to be the only thing that matters. This is exactly in line with Wheeler’s participatory principle, mentioned previously.

We start our analysis therefore with a statement as to what is known at initial stage Σ_0 . We will assume that a mixed SUO state has been prepared at stage Σ_0 ,⁶ such that the initial density matrix ρ_0^{SA} is an element of $L(\mathcal{H}^S \otimes \mathcal{Q}_0)$ given by

$$\rho_0^{SA} \equiv \rho^S \otimes \mathbf{1}_0 \bar{\mathbf{I}}_0 = \rho^S \otimes \widehat{\mathbb{P}}_0^1, \tag{9.63}$$

where ρ^S is a density operator, an element of $L(\mathcal{H}^S)$.

We now imagine that the combined SUO-apparatus state evolves from stage Σ_0 to some final stage, Σ_N , where $N > 0$. Consider quantum evolution from Hilbert space $\mathcal{H}^S \otimes \mathcal{Q}_n$ at stage Σ_n to Hilbert space $\mathcal{H}^S \otimes \mathcal{Q}_{n+1}$ at stage Σ_{n+1} , where \mathcal{H}^S is the SUO Hilbert space of dimension d and $\mathcal{Q}_n, \mathcal{Q}_{n+1}$ are the quantum registers representing labstates of the apparatus. An ONB at Σ_n is given by $\{|A, \mathbf{i}_n\rangle \equiv |A\rangle \otimes \mathbf{i}_n : i = 0, 1, \dots, d_n\}$ with the orthonormalization $(A, \mathbf{i}_n | B, \mathbf{j}_n) = \delta^{AB} \delta^{ij}$, while at Σ_{n+1} we have ONB $\{|A, \mathbf{i}_{n+1}\rangle \equiv |A\rangle \otimes \mathbf{i}_{n+1} : i = 0, 1, \dots, d_{n+1}\}$ with the orthonormalization $(A, \mathbf{i}_{n+1} | B, \mathbf{j}_{n+1}) = \delta^{AB} \delta^{ij}$. Here $d_n \equiv 2^{r_n} - 1$.

Pure quantum evolution is given by

$$U_{n+1,n} |A, \mathbf{i}_n\rangle = \sum_{B=1}^d \sum_{j=0}^{d_{n+1}} U_{n+1,n}^{BA,ji} |B, \mathbf{j}_{n+1}\rangle : \quad i = 0, 2, \dots, d_n. \tag{9.64}$$

⁵ In our computer algebra program MAIN, discussed in Chapter 12, we take the system space to change from stage to stage.

⁶ States of SUOs are treated in QDN as convenient repositories of context. By their actions in the state preparation process, an observer will in general be entitled to model some of that context in terms of a density operator representing a mixed state of an SUO.

Using completeness, this gives the dyadic representation of $U_{n+1,n}$

$$U_{n+1,n} = \sum_{A,B=1}^d \sum_{j=0}^{d_{n+1}} \sum_{i=0}^{d_n} |B, \mathbf{j}_{n+1}\rangle U_{n+1,n}^{BA,ji} \langle A, \mathbf{i}_n|. \tag{9.65}$$

The retraction operator $\bar{U}_{n+1,n}$ is defined to be

$$\bar{U}_{n+1,n} = \sum_{A,B=1}^d \sum_{j=0}^{d_{n+1}} \sum_{i=0}^{d_n} |A, \mathbf{i}_n\rangle U_{n+1,n}^{BA,ji*} \langle B, \mathbf{j}_{n+1}|. \tag{9.66}$$

By definition, we have

$$\bar{U}_{n+1,n} U_{n+1,n} = I^S \otimes I_1^A, \tag{9.67}$$

where I^S is the identity over \mathcal{H}^S and I_1^A is the identity over \mathcal{Q}_1 . From this, we arrive at the semi-unitary conditions

$$\sum_{C=1}^d \sum_{j=0}^{d_{n+1}} U_{n+1,n}^{CA,ja*} U_{n+1,n}^{CB,jb} = \delta^{AB} \delta^{ab}. \tag{9.68}$$

Now consider a pure total state

$$|\Psi_0\rangle \equiv \sum_{A=1}^d \Psi_0^A |A\rangle \otimes \mathbf{1}_0, \quad \sum_{A=1}^d |\Psi_0^A|^2 = 1, \tag{9.69}$$

evolving from state Σ_0 to stage Σ_1 , giving total state $|\Psi_1\rangle \equiv U_{1,0}|\Psi_0\rangle$.

Continuing this process, we find the state at stage Σ_N is given by $|\Psi_N\rangle = U_{N,0}|\Psi_0\rangle$, where $U_{N,0} \equiv U_{N,N-1}U_{N-1,N-2} \dots U_{1,0}$.

Suppose now the observer asks a partial question \mathbb{Q}_N^θ of the state of the apparatus at stage Σ_N . The expectation value $E[\mathbb{Q}_N^\theta|\Psi_0]$ of the answer is given by

$$E[\mathbb{Q}_N^\theta|\Psi_0] \equiv (\Psi_N|I^S \otimes \mathbb{Q}_N^\theta|\Psi_N) = \sum_{A,B=1}^d \Psi_0^{A*} \Psi_0^B \langle A|E_N^\theta|B\rangle, \tag{9.70}$$

where

$$E_N^\theta \equiv \bar{\mathbf{1}}_0 \bar{U}_{N,0} I^S \otimes \mathbb{Q}_N^\theta U_{N,0} \mathbf{1}_0. \tag{9.71}$$

If now the initial state is a mixed state, such that the initial SUO state $|\Psi_0^\alpha\rangle$ is given with probability ω^α , then the expectation value is given by

$$E[\mathbb{Q}_N^\theta|\boldsymbol{\rho}_0] = \text{Tr}_S\{\boldsymbol{\rho}_0^A E_N^\theta\}, \tag{9.72}$$

where

$$\boldsymbol{\rho}_0^A \equiv \sum_{\alpha} \omega^\alpha |\Psi_0^\alpha\rangle \langle \Psi_0^\alpha|. \tag{9.73}$$

This is the QDN generalization of the standard POVM formalism.

We note that, provided we sum θ over all elements of an identity class Θ only,⁷ then

$$\sum_{\theta \text{ in } \Theta} E_N^\theta = \overline{\mathbf{1}_0} \overline{U}_{N,0} I^S \otimes \sum_{\theta \text{ in } \Theta} Q_N^\theta U_{N,0} \mathbf{1}_0 = \overline{\mathbf{1}_0} \overline{U}_{N,0} I^S \otimes \mathbb{I}_N U_{N,0} \mathbf{1}_0 = I^S. \quad (9.74)$$

Hence

$$\sum_{\theta \text{ in } \Theta} E[Q_N^\theta | \boldsymbol{\rho}_0] = \text{Tr}_S \left\{ \boldsymbol{\rho}_0^A \sum_{\theta \text{ in } \Theta} E_N^\theta \right\} = \text{Tr}_S \{ \boldsymbol{\rho}_0^A I^S \} = 1. \quad (9.75)$$

The interpretation of the expectation values $E[Q_N^\theta | \boldsymbol{\rho}_0]$ therefore is consistent with probability, provided we restrict θ to a single identity class.

⁷ Identity classes are discussed in the previous chapter.