

PHYS450 THEORY OF OPEN QUANTUM SYSTEMS

Note Title

JENS KOCH, NORTHWESTERN UNIVERSITY 1/2/2013

Textbook

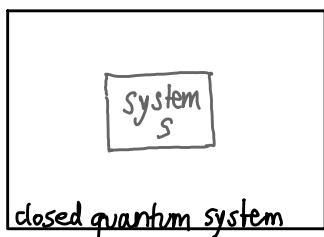
H.-P. Breuer, F. Petruccione: *The Theory of Open Quantum Systems* (Oxford University Press)

Other literature

- A. M. Zagoskin: *Quantum Engineering* (Cambridge University Press)
- R. Alicki, K. Lendi: *Quantum Dynamical Semigroups and Applications* (Springer)
- H. W. Wiseman, G. J. Milburn: *Quantum Measurement and Control* (Cambridge University Press)
- S. Haroche, J.-M. Raimond: *Exploring the Quantum* (Cambridge University Press)
- P. E. Kloeden, E. Platen: *Numerical solution of stochastic differential equations* (Springer)

Preface: Motivation and Overview

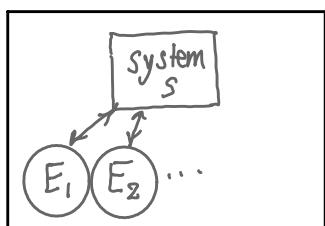
The traditional way of learning quantum mechanics consists of studying closed quantum systems (think of a harmonic oscillator, a hydrogen atom, a particle in a potential).



A closed quantum system, even though embedded into the "universe"*, is assumed to be

- decoupled from the rest of the "universe"
- fully described by its Hamiltonian H .

The truth is: except perhaps for the universe itself, no system is truly closed. (An atom couples to the electromagnetic field, leading to relaxation by photo-emission. A conduction electron (or quasi-particle) interacts with impurities and imperfections in the crystal lattice. Etc.)



The "degree of openness" depends on the coupling strength between the system of interest (S) and other systems in its environment (E_1, E_2, \dots), as well as on the time scale during which the system is to be observed / modeled.

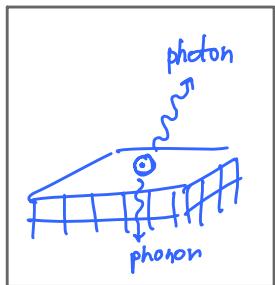
* "Universe" here means, loosely speaking, the rest of the physical world. In many cases, it is useful to picture the direct environment of the system or the experimenter's lab, rather than vast space and galaxies.

Closed-system approach

include all participating systems in your Hamiltonian and solve Schrödinger equation (or calculate Green's functions etc.)

Drawbacks:

- The combined system $S \otimes E_1 \otimes E_2 \dots$ is often too large and the Schrödinger equation hence intractable.
- The goal may be to extract properties of S only, i.e. quantities that are accessible by applying measurements to S alone. In this case, calculating the detailed behavior of E_1, E_2, \dots is overkill.
- Oftentimes, the precise nature of E_1, E_2, \dots and their exact form of coupling to S are not well known. Yet, for the effects on S , these details may not matter much. Think, e.g., of a surface atom in an excited state. The effect of relaxation on the atom is the same, independent of whether the relaxation occurs due to photon or phonon emission!



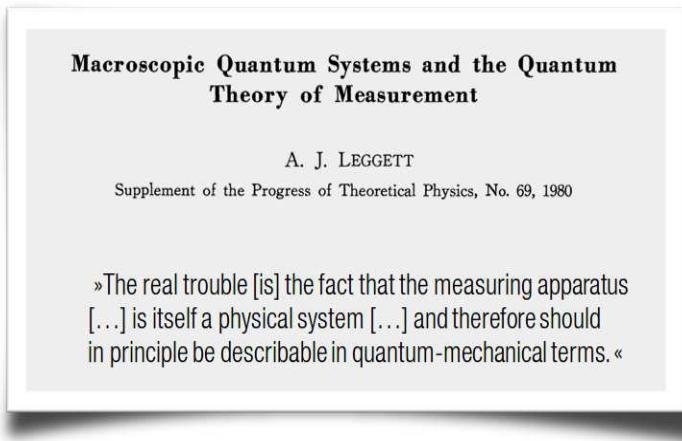
Much of your quantum mechanics knowledge may be based on closed systems. There are, however, at least two places where openness of a system peaks through in any introductory QM class:

■ time-dependent Hamiltonians $H(t)$

If you believe in energy conservation, you will have to admit that the system must be exchanging energy with some other system and hence be coupled.

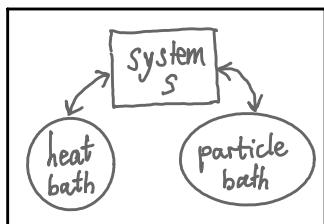
measurement

Even though QM completely fails to say what constitutes a measurement, it is clear that coupling to another system — the measurement apparatus — is a necessary requirement.



Note: If you are here because of a hope that this class or the theory of open quantum systems in general could cure this horrific state of affairs, then you will be utterly disappointed.

Quite likely, you also got a flavor of openness of quantum systems in the context of statistical mechanics. There, the coupling of a quantum system with heat and particle baths is essential for the description of equilibrium properties within the canonical and grand-canonical ensembles.

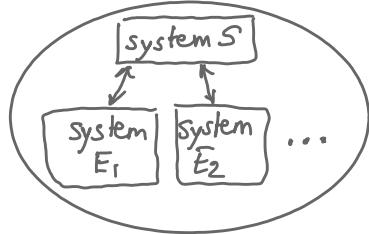


A central object for calculating equilibrium expectation values is the equilibrium density matrix of the system:

$$\text{canonical : } \rho = \frac{1}{Z} e^{-\beta H} \quad Z = \text{tr } e^{-\beta H}$$

$$\text{grand-canonical : } \rho = \frac{1}{Z} e^{-\beta(H - \mu N)} \quad Z^* = \text{tr } e^{-\beta(H - \mu N)}$$

The notion of open quantum systems goes beyond this. Think of a system S , coupled to other systems of distinct types, sizes, ...



What can we learn about the dynamics inside system S , while other systems E_1, E_2, \dots interact with it?

TOPICS OF INTEREST INCLUDE

- time dependence of observables
 - e.g., - gate fidelities for quantum operations in an implementation of a quantum algorithm
 - quantum feedback
- expectation values in nonequilibrium steady states
 - e.g. - photon state inside a driven and lossy cavity
- nature and quantitative description of decoherence
 - e.g. - loss of phase information in a qubit superposition state
- ensemble description: Markovian master equations
Single-shot description: Quantum trajectories / stochastic Schrödinger equation

Open-system approach

The theory of open quantum systems is firmly based on the standard quantum mechanics you know. In fact, as you will see, much of it is explicitly derived from closed-system quantum mechanics in a strategy that could be described as intentional selective amnesia: We want to know everything going on in our system of interest S but forget the rest. All effects of E_1, E_2, \dots are to be included in a much more efficient evolution equation for S alone.

1. Quantum Mechanics for Quantum Engineers

[Chapter Title by Zagorskin]

1.1 Whirlwind Review: The 5 Axioms of Quantum Mechanics

We are all familiar with quantum mechanics, maybe even experts. Since Feynman, however, forever tells us that "nobody understands quantum mechanics," it seems useful to recapitulate the bare bones skeleton of quantum mechanics in the form of its five* basic axioms:

I MATH FRAMEWORK

The instantaneous state of a quantum system at time t is given by a normalized vector $|\psi(t)\rangle \in \mathcal{H}$ from an appropriate Hilbert space \mathcal{H} .

II UNITARY TIME EVOLUTION

The time evolution is governed by the Schrödinger equation $i\hbar\partial_t |\psi(t)\rangle = H|\psi(t)\rangle$ where the Hamiltonian H is a hermitean operator associated with the system energy.

(► Time evolution is unitary: $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ w/ $U = e^{-iHt/\hbar}$)
↑ unitary propagator

III OBSERVABLES

Observables are measurable quantities (e.g. energy, momentum of a particle,...) and are represented by hermitean operators $A = A^\dagger$. The measured value** is always one of the eigenvalues of A .

IV COLLAPSE OF THE WAVE FUNCTION [given for spec A non-degenerate]

Measurement generally perturbs the system by changing its state. Immediately after measuring the value a_n (where $A|a_n\rangle = a_n|a_n\rangle$), the system is in state $|a_n\rangle$.** (► Non-unitary and t -irreversible evolution.)

* Some other authors including Zagorskin speak of four axioms. The question of 4 vs. 5 is not terribly important for us.

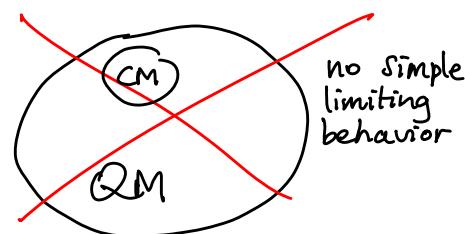
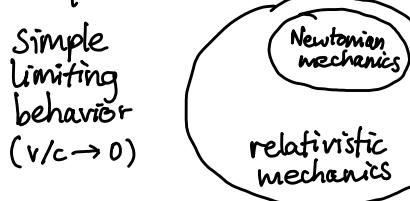
** In an ideal, projective measurement — we will discuss more general measurement types later.

V BORN'S RULE

For a given state $|\psi\rangle$, the probability to obtain the result a_n when measuring A is given by $p_n = |\langle a_n | \psi \rangle|^2$.

REMARKS

- (1) For a complete set of axioms, you may additionally want to include rules for quantization, how to construct joint Hilbert spaces from multiple subsystems, rules for systems of identical particles etc.)
- (2) If we accept the above axioms, then we acknowledge that there are two fundamentally different types of evolution
 - unitary evolution under Schrödinger eq.
 - irreversible state changes under measurement.
- (3) If we accept I - V as axioms (independent statements that cannot be derived from each other!), then quantum mechanics is not complete and classical physics is not a limiting behavior of quantum mechanics.



Why? The axioms introduce the notion of a "measurement" without giving any explanation as to what constitutes a measurement!

- (4) Axioms IV & V assume observables with non-degenerate spectra. For the general case, note:

$$\text{post-state } |a_n\rangle = \frac{|a_n\rangle\langle a_n| \psi \rangle}{\langle a_n | \psi \rangle} = \frac{P_n |\psi\rangle}{\sqrt{\langle \psi | P_n | \psi \rangle}}$$

w/ $P_n = |a_n\rangle\langle a_n|$ projector
on subspace for eigenvalue a_n

$$\text{probability: } p_n = |\langle a_n | \psi \rangle|^2 = \langle \psi | P_n | \psi \rangle$$

These are the appropriate expressions to use when spec A has degeneracies.
(In that case, degenerate subspaces are multi-dimensional.)

Example: Axioms in action — derive: $\langle A \rangle_\psi = \langle \psi | A | \psi \rangle$

Let A be an observable for \mathcal{H} and $|\psi\rangle \in \mathcal{H}$ a state. The expectation value $\langle A \rangle_\psi$ is defined to be the average measurement result when measuring A on a large ensemble of $N \gg 1$ states prepared to be $|\psi\rangle$.

Thus,

$$\begin{aligned}\langle A \rangle_\psi &\stackrel{\text{III}}{=} \sum_n \frac{N_n}{N} a_n \stackrel{N \gg 1}{=} \sum_n p_n a_n \stackrel{\text{IV}}{=} \sum_n |\langle a_n | \psi \rangle|^2 a_n \\ &= \sum_n \langle \psi | a_n \rangle a_n \langle a_n | \psi \rangle = \langle \psi | \underbrace{\left(\sum_n a_n |\langle a_n | \psi \rangle\right)}_A | \psi \rangle = \langle \psi | A | \psi \rangle\end{aligned}$$

$a_n (n=1,2,\dots)$: eigenvalues of A

N_n : number of experiments where a_n is measurement result.

1.2 Composite Systems, Entangled States (pure)

Consider two quantum systems ($\alpha=1,2$) with separate Hilbert spaces \mathcal{H}_α and Hamiltonians H_α . In many situations, we would like to describe the two systems jointly (perhaps because you have brought them into close contact and they interact with each other).

The joint Hilbert space of the two systems is the direct product $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Given bases $\{|\psi_n\rangle_\alpha\}_{n=1,2,\dots} \subset \mathcal{H}_\alpha$, a basis for \mathcal{H} is $\{|\psi_n\rangle_1 \otimes |\psi_m\rangle_2\}_{\substack{n=1,2,\dots \\ m=1,2,\dots}}$.

Accordingly,

$$\dim \mathcal{H} = (\dim \mathcal{H}_1) \cdot (\dim \mathcal{H}_2).$$

Example: Consider two spin- $\frac{1}{2}$ systems. Bases: $\{|\uparrow\rangle_\alpha, |\downarrow\rangle_\alpha\} \subset \mathcal{H}_\alpha$.

Basis for the joint Hilbert space: $\{|\uparrow_1\uparrow_2\rangle, |\uparrow_1\downarrow_2\rangle, |\downarrow_1\uparrow_2\rangle, |\downarrow_1\downarrow_2\rangle\}$.

Since $\{|\psi_n, \psi_m\rangle \equiv |\psi_n\rangle_1 \otimes |\psi_m\rangle_2\}$ is a basis, every state $|\Psi\rangle \in \mathcal{H}$ has a unique decomposition

$$|\Psi\rangle = \sum_n \sum_m c_{nm} |\psi_n, \psi_m\rangle \quad \text{with } c_{nm} \in \mathbb{C}.$$

The direct product of two operators $A: \mathcal{H}_1 \rightarrow \mathcal{H}_1$ and $B: \mathcal{H}_2 \rightarrow \mathcal{H}_2$ is defined accordingly:

$$\begin{aligned} \Omega: \mathcal{H}_1 \otimes \mathcal{H}_2 &\rightarrow \mathcal{H}_1 \otimes \mathcal{H}_2 \\ |\psi_n, \psi_m\rangle &\mapsto \Omega|\psi_n, \psi_m\rangle \equiv (A|\psi_n\rangle) \otimes (B|\psi_m\rangle) \end{aligned}$$

The matrix elements of $\Omega = A \otimes B$ are

$$\langle n', m' | A \otimes B | n, m \rangle = \langle n' | A | n \rangle \langle m' | B | m \rangle = A_{nn'} B_{mm'}$$

To obtain $A \otimes B$ in matrix form for given matrices $A_{n \times n}$ and $B_{m \times m}$, we must choose a convention for the order of double indices (n, m) .

Convention: "last goes fast", i.e.

$$\begin{aligned} 1: & |n=1, m=1\rangle \\ 2: & |1, 2\rangle \\ \vdots & \vdots \\ M: & |1, M\rangle \\ M+1: & |2, 1\rangle \\ \vdots & \vdots \\ M+N: & |N, M\rangle \end{aligned}$$

Thus,

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1N}B \\ a_{21}B & a_{22}B & \cdots & a_{2N}B \\ \vdots & & & \\ a_{N1}B & a_{N2}B & \cdots & a_{NN}B \end{pmatrix},$$

where each entry $a_{ij}B$ is still a matrix.

This is sometimes also referred to as 'Kronecker product.'

Whenever a system is composed of multiple components (or subsystems), it makes sense to ask whether the system is in an **entangled state**.

In the case of a **bi-partite** system (two subsystems) a state $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is called entangled iff the state cannot be written as a product state $|\Psi\rangle = |\psi\rangle_1 \otimes |\phi\rangle_2$ for any $|\psi\rangle_1 \in \mathcal{H}_1$ and $|\phi\rangle_2 \in \mathcal{H}_2$.

Note: ■ Example:

$|S=1, M=1\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2$ is a product state (not entangled),
 $|S=1, M=0\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ is an entangled state.

■ In a (bi-partite) entangled state, each subsystem "loses its quantum identity" (Haroche & Raimond). For the example of the two spins: the picture that each spin carries with it its own wavefunction that encodes all properties is not correct. In an entangled state, a

joint wavefunction of the two spins must be used which describes the shared properties of the two atoms (even if they are spatially separated).

This poses an important question for the description of open quantum systems: if system and environment get entangled, a single ket $| \psi \rangle \in \mathcal{H}_{\text{sys}}$ will not adequately describe the system — what will?

We will address this question in the next section.

- Entangled states play a crucial role in quantum computing and quantum cryptography (without entanglement no exp. speedup relative to a classical computer).

R. Josza, N. Linden, Proc. R. Soc. Lond. A (2003), 459 2011–2032

- Much of this can easily be generalized to more than two subsystems and multi-partite entanglement.

Math Interlude: The trace (tr)

The trace of an operator $A: \mathcal{H} \rightarrow \mathcal{H}$ is given by the sum of its diagonal matrix elements w.r.t. an orthonormal basis $\{|m\rangle\}_{m=1,2,\dots,M}$ of the Hilbert space \mathcal{H} :

$$\text{tr } A = \sum_{m=1}^M \langle m | A | m \rangle.$$

Remarks

- The trace is independent of the orthonormal basis chosen to calculate it.

PROOF: Let $\{|v\rangle\}$ be a second ONB. Then,

$$\begin{aligned} \sum_m \langle m | A | m \rangle &= \sum_m \sum_{v,v'} \langle m | v \rangle \langle v | A | v' \rangle \langle v' | m \rangle \quad (\sum_v |v\rangle \langle v| = \mathbb{1}: \text{completeness}) \\ &= \sum_{v,v'} \sum_m \langle v' | m \rangle \langle m | v \rangle \langle v | A | v' \rangle = \sum_v \langle v | A | v \rangle \end{aligned}$$

- The trace of any hermitian operator is real-valued and identical to the sum of its eigenvalues.
- The trace is cyclically invariant, i.e. $\text{tr}(ABC) = \text{tr}(BCA) = \text{tr}(CAB)$
PROOF: same strategy as above, i.e., use definition, completeness, rearrange terms

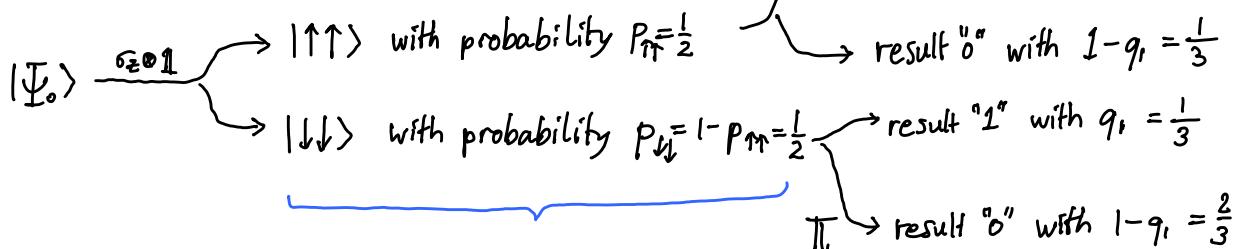
1.3 The Density Matrix

Motivation

Consider a system of two spin- $\frac{1}{2}$'s, initially in the state $|\Psi_0\rangle = (|\uparrow\uparrow\rangle + i|\downarrow\downarrow\rangle)/\sqrt{2}$.

We first measure $\sigma_z \otimes \mathbb{1}$ and subsequently $\Pi = \mathbb{1} \otimes |\phi\rangle\langle\phi|$ with $|\phi\rangle = \sqrt{\frac{2}{3}}|\uparrow\rangle + i\sqrt{\frac{1}{3}}|\downarrow\rangle$. What is the expectation value $\langle\Pi\rangle$?

Pedestrian solution



Problem: this statistical mixture
cannot be compactly described
by a ket (pure state)

$$\text{Result: } \langle\Pi\rangle = p_{\uparrow\uparrow}q_{\Pi} \cdot 1 + p_{\downarrow\downarrow}q_{\Pi} \cdot 1 = \frac{1}{2} \cdot \frac{2}{3} + \frac{1}{2} \cdot \frac{1}{3} = \frac{1}{2}$$

More sophisticated solution

$$\begin{aligned}\langle\Pi\rangle &= p_{\uparrow\uparrow} \cdot \langle\Pi\rangle_{\uparrow\uparrow} + p_{\downarrow\downarrow} \langle\Pi\rangle_{\downarrow\downarrow} = p_{\uparrow\uparrow} \langle\uparrow\uparrow|\Pi|\uparrow\uparrow\rangle + p_{\downarrow\downarrow} \langle\downarrow\downarrow|\Pi|\downarrow\downarrow\rangle \\ &= p_{\uparrow\uparrow} \text{tr}(|\uparrow\uparrow\rangle\langle\uparrow\uparrow|\Pi) + p_{\downarrow\downarrow} \text{tr}(|\downarrow\downarrow\rangle\langle\downarrow\downarrow|\Pi) \\ &= \text{tr} \left[\underbrace{(p_{\uparrow\uparrow}|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + p_{\downarrow\downarrow}|\downarrow\downarrow\rangle\langle\downarrow\downarrow|)}_{\equiv \rho} \Pi \right] = \text{tr}(\rho\Pi) = \langle\Pi\rangle_{\rho}\end{aligned}$$

$\equiv \rho$: density matrix or statistical operator

describes the ensemble state after the first measurement

Check: $\rho = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$

$$\Pi = \mathbb{1} \otimes |\phi\rangle\langle\phi| = \mathbb{1} \otimes \left(\sqrt{\frac{2}{3}}|\uparrow\rangle + \frac{i}{\sqrt{3}}|\downarrow\rangle \right) \left(\sqrt{\frac{2}{3}}\langle\uparrow| - \frac{i}{\sqrt{3}}\langle\downarrow| \right)$$

$$= \mathbb{1} \otimes \left(\frac{2}{3}|\uparrow\rangle\langle\uparrow| - \frac{i\sqrt{2}}{3}|\uparrow\rangle\langle\downarrow| + \frac{i\sqrt{2}}{3}|\downarrow\rangle\langle\uparrow| + \frac{1}{3}|\downarrow\rangle\langle\downarrow| \right)$$

$$\Pi = \begin{pmatrix} \frac{2}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix}$$

$$\therefore \rho\Pi = \begin{pmatrix} \frac{1}{2}\frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}\frac{1}{3} \end{pmatrix}$$

do not need to calculate
these to obtain $\text{tr}(\rho\Pi)$

$$\therefore \text{tr}(\rho\Pi) = \frac{1}{2} \quad \checkmark$$

DEFINITION

Let $\{|\psi_n\rangle\}_{n=1,\dots,N} \subset \mathcal{H}$ be a set of normalized (not necessarily orthogonal) states. The operator

$$\rho = \sum_{n=1}^N p_n |\psi_n\rangle\langle\psi_n|$$

with $0 \leq p_n \leq 1$: probability to be in state $|\psi_n\rangle$ and $\sum_{n=1}^N p_n = 1$ (normalization), describes the ensemble state of a quantum system.

The operator ρ is called the **density matrix**.

Vice versa, any operator R that can be brought into this form of a **probability-weighted sum of projectors** represents a valid density matrix.

REMARKS :

(1) Ensemble expectation values of an observable A with respect to the "state" ρ are given by $\langle A \rangle_\rho = \text{tr}(A\rho) = \text{tr}(\rho A)$

(2) The normalization condition $\sum_{n=1}^N p_n = 1$ for the state $\rho = \sum_{n=1}^N p_n |\psi_n\rangle\langle\psi_n|$, is equivalent to the condition $\text{tr } \rho = 1$.

(3) All density matrices are **hermitean**.

(4) All eigenvalues of a density matrix are real, non-negative and sum up to 1. The property of having real, non-negative eigenvalues is sometimes expressed as: ρ is a positive (semi-definite) matrix. (Vice versa, by employing the spectral representation, every positive hermitean operator with unity trace is a valid density matrix.)

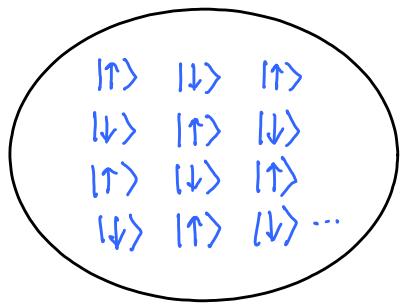
(5) The representation of ρ as a probability weighted sum of projectors is not unique.

EXAMPLE : Consider a spin- $\frac{1}{2}$. Let $|\uparrow\rangle, |\downarrow\rangle$ be the σ_z eigenstates and $|\pm\rangle = (|\uparrow\rangle \pm |\downarrow\rangle)/\sqrt{2}$ the σ_x eigenstates. Then

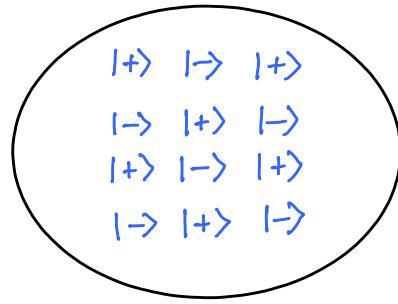
$$\rho = \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow| = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \text{ and}$$

$$\begin{aligned} \rho' &= \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow| = \frac{1}{2} \cdot \frac{1}{2} (|\uparrow\rangle + |\downarrow\rangle)(\langle\uparrow| + \langle\downarrow|) + \frac{1}{2} \cdot \frac{1}{2} (|\uparrow\rangle - |\downarrow\rangle)(\langle\uparrow| - \langle\downarrow|) \\ &= \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow| = \rho \end{aligned}$$

Consequence: the ensembles



and



look different but are IDENTICAL (same ρ). No measurement scheme, no matter how ingenious, could distinguish between these two.

(6) If ρ_1 and ρ_2 are density matrices, then $\rho = p\rho_1 + (1-p)\rho_2$ ^(*) is also a density matrix for all $0 \leq p \leq 1$. (Think of p as a probability.)

PROOF: Since ρ_1, ρ_2 are density matrices, we have

$$\rho_1 = \sum_{n=1}^N \alpha_n |\psi_n\rangle\langle\psi_n| \text{ and } \rho_2 = \sum_{m=1}^M \beta_m |\phi_m\rangle\langle\phi_m|, \text{ where } 0 \leq \alpha_n, \beta_m \leq 1 \text{ and } \sum_{n=1}^N \alpha_n = \sum_{m=1}^M \beta_m = 1. \text{ Thus,}$$

(*) Mathematically, the set of density matrices \mathcal{R}_{re} is thus convex.



$$\rho = \sum_{n=1}^N p\alpha_n |\psi_n\rangle\langle\psi_n| + \sum_{m=1}^M (1-p)\beta_m |\phi_m\rangle\langle\phi_m| = \sum_{e=1}^{N+M} \gamma_e |\chi_e\rangle\langle\chi_e|$$

with $0 \leq \gamma_e \leq 1$ and $\sum_e \gamma_e = \sum_n p\alpha_n + \sum_m (1-p)\beta_m = p + (1-p) = 1$.

(7) Our good old kets translate easily into the language of density matrices: the state $|\psi\rangle$ is associated with the density matrix $\rho = |\psi\rangle\langle\psi|$. Whenever ρ takes this simple form, we say the system is in a **pure state**.

$$\begin{aligned} \text{We have: } \rho \text{ is pure} &\Leftrightarrow \rho = \rho^2 \\ &\Leftrightarrow \text{spec } \rho = \{1, 0, 0, \dots, 0\} \\ &\Leftrightarrow \text{tr}(\rho^2) = 1 \end{aligned}$$

(8) Expressing pure states by means of the density matrix $\rho = |\psi\rangle\langle\psi|$ immediately gets rid of non-observable phase information: $|\psi\rangle$ and $e^{i\varphi}|\psi\rangle$ lead to the same density matrix $\rho = |\psi\rangle\langle\psi|$. In other words, $\rho = |\psi\rangle\langle\psi|$ represents a **ray** in Hilbert space.

(9) The description of quantum mechanics in terms of kets (i.e., pure states) is completely contained in the description via density matrices.

► Let us rephrase axioms I through IV in the language of density matrices!

1.4 Deja vu: QM Axioms in Density Matrix Language

I MATH FRAMEWORK

The instantaneous state of a quantum system at time t is given by a density matrix $\rho(t) \in \mathbb{R}_{\geq 0}$ (set of density matrices for Hilbert space \mathcal{H} ; see also Problem Set #1).

II UNITARY TIME EVOLUTION

The time evolution is governed by the von-Neumann equation
 $i\hbar \partial_t \rho(t) = [H, \rho(t)]$ where H is the system's Hamiltonian.

► Using the unitary propagator $U(t)$, we can easily write the solution as
 $\rho(t) = U(t) \rho(0) U^\dagger(t)$.

PROOF:

1. [von-Neumann equation]

$$\begin{aligned} i\hbar \partial_t \rho &= i\hbar \partial_t \left(\sum_n p_n |\psi_n\rangle \langle \psi_n| \right) = \sum_n p_n (i\hbar \partial_t |\psi_n\rangle) \langle \psi_n| + \sum_n p_n |\psi_n\rangle (i\hbar \langle \psi_n| \partial_t) \\ &= \sum_n p_n H |\psi_n\rangle \langle \psi_n| + \sum_n p_n |\psi_n\rangle \langle \psi_n| (-H) = [H, \rho] \end{aligned}$$

2. Consider $\rho(0) = \sum_n p_n |\psi_n\rangle \langle \psi_n|$, i.e., with probability p_n we start in the pure state $|\psi_n\rangle$. Time evolution of this state is given by $|\psi_n\rangle \mapsto U(t)|\psi_n\rangle$ (hence, $\langle \psi_n| \mapsto \langle \psi_n| U^\dagger(t)$). Thus, $\rho(0) \mapsto U(t)\rho(0)U^\dagger(t)$; use $U(t) = e^{-iHt/\hbar}$ to confirm directly.

III OBSERVABLES — unchanged! —

IV COLLAPSE OF THE DENSITY MATRIX

Let $A = \sum_{m=1}^M a_m P_m$ be an observable with eigenvalues a_m (pairwise different) and P_m the projectors onto the (pairwise orthogonal) eigenspaces.

For a given ensemble state $\rho = \sum_{n=1}^N p_n |n\rangle \langle n|$, A is measured. The resulting new ensemble is $\rho' = \sum_{m=1}^M P_m \rho P_m$ (unconditional post-measurement state)

The resulting sub-ensemble ρ_e of all instances in which the measurement result a_e was obtained, is

$$\rho_e = \frac{P_e \rho P_e}{\text{tr}(\rho P_e)}$$

(post-measurement state conditioned on measurement result a_e)

PROOF: For each member state $|n\rangle$ in the ρ ensemble, the possible states after measuring A are $P_m|n\rangle/\sqrt{\langle n|P_m|n\rangle}$ with probability $p_m = \langle n|P_m|n\rangle$. Thus, the post-measurement ensemble is

$$\rho' = \sum_{n=1}^N p_n \sum_{m=1}^M p_m \frac{1}{\langle n|P_m|n\rangle} P_m|n\rangle\langle n|P_m = \sum_m p_m \left(\sum_{n=1}^N p_n |n\rangle\langle n| \right) P_m$$

For sub-ensemble, only include $m=l$.

V BORN'S RULE

For any member state of the ensemble described by the density matrix ρ , the probability to observe the measurement result a_ℓ is $p_e = \text{tr}(\rho P_\ell)$ w/ P_ℓ being the projector onto the eigenspace for a_ℓ .

PROOF: Let $\rho = \sum_n p_n |n\rangle\langle n|$. Then, the probability of measuring a_ℓ for member state $|n\rangle$ is $\langle n|P_\ell|n\rangle$.
 $\therefore p_e = \sum_n p_n \langle n|P_\ell|n\rangle = \text{tr}(\rho P_\ell)$

Audience Question: In the motivational example discussed in the beginning of section 1.3, it turns out that the same result, $\langle \Pi \rangle = \frac{1}{2}$, is obtained when the intermediate measurement of $A_1 = \sigma_z \otimes \mathbb{1}$ is dropped. Why?

Answer: Indeed, one also obtains

$$\langle \Pi \rangle_\rho = \text{tr}(\Pi \rho) = \text{tr} \left[\begin{pmatrix} \frac{2}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 1/2 & 0 & 0 & -i/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i/2 & 0 & 0 & 1/2 \end{pmatrix} \right] = \text{tr} \left[\begin{pmatrix} \frac{2}{3} \cdot \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{3} \cdot \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{2}{3} \cdot \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \cdot \frac{1}{2} \end{pmatrix} \right] = \frac{1}{2}$$

This is an accident of the selected example rather than a general result.

To see this, let us denote the first and second observable ($\alpha=1,2$)

by $\Omega_\alpha = \sum_n \lambda_n^{(\alpha)} P_n^{(\alpha)}$, where for each α , the $P_n^{(\alpha)}$ operators are projectors onto the mutually orthogonal eigenspaces of the observables.

Then the two expectation values in question are

$$(1) \langle \Omega_2 \rangle_{\rho_0} = \text{tr}(\Pi \rho_0)$$

$$(2) \langle \Omega_2 \rangle_{\rho_1} = \text{tr}(\Omega_2 \rho_1) = \text{tr}\left(\Omega_2 \sum_n P_n^{(1)} \rho_1 P_n^{(1)}\right)$$

A sufficient (but not necessary!) condition for $\langle \Omega_2 \rangle_{\rho_0} = \langle \Omega_2 \rangle_{\rho_1}$ is

$$[\Omega_2, P_n^{(1)}] = 0 \quad \forall n \quad \text{or} \quad [\rho_0, P_n^{(1)}] = 0 \quad \forall n.$$

It is the former condition that happens to hold in the example.

For an example where the two expectation values differ, consider

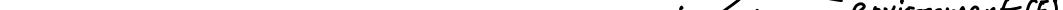
$$\rho_0 = |\psi_0\rangle\langle\psi_0| \quad \text{with} \quad |\psi_0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle), \quad \Omega_1 = \sigma_z \otimes \mathbb{1}, \quad \Omega_2 = \sigma_x \otimes \sigma_x.$$

(see Problem Set #1).

1.5 The State of an Open Quantum System

Consider, once again, a quantum system S in contact with its environment E . We may imagine the combination of S and E to be a closed system, described by either a pure state $|\Psi\rangle \in \mathcal{H}_S \otimes \mathcal{H}_E \equiv \mathcal{H}$ or by a statistical mixture $\rho \in \mathcal{R}_{\mathcal{H}}$. As we saw in Section 1.3, in the presence of entanglement, $|\Psi\rangle$ cannot be reduced to a product state; hence, no single ket $|\psi\rangle_S \in \mathcal{H}_S$ can reflect the peculiar state of the open system S . However, all properties that can be extracted from $|\Psi\rangle$ by measurements on S alone can be expressed by a **reduced density matrix ρ_S** .

To see this and define the appropriate ρ_S , start from $\rho \in \mathcal{R}_{\mathcal{H}}$ where $\rho = |\Psi\rangle\langle\Psi|$ for the special case of a pure state. (The following considerations work just as well when ρ is a mixed state.) Measurements of S

alone are represented by observables of the form $\Omega = A \otimes \mathbb{1} \equiv A_S \mathbb{1}_E$ (where $A_S^+ = A_S$).


Then, $\langle \Omega \rangle_p = \text{tr} [\rho \Omega] = \text{tr} [\rho A_S \mathbb{1}_E] = \sum_{m=1}^M \langle m | \rho A_S \mathbb{1}_E | m \rangle$, where

$\{|m\rangle\}_{m=1,\dots,M} = \{|n,l\rangle = |n\rangle_S |l\rangle_E\}_{\substack{n=1,\dots,N \\ l=1,\dots,L}}$ is an ONB of $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$.

Rewrite:

$$\begin{aligned}
 \langle \Omega \rangle_p &= \sum_{n=1}^N \sum_{\ell=1}^L \langle n, \ell | \rho A_S \mathbb{1}_E | n, \ell \rangle = \sum_{n, \ell} \underbrace{\langle n |}_{S_E} \underbrace{\langle \ell |}_{S_E} \rho A_S \mathbb{1}_E \underbrace{\langle n \rangle_S}_{\langle \ell \rangle_E} \\
 &= \sum_{n, \ell} \langle n | \underbrace{\langle \ell | \rho | \ell \rangle_E}_{A_S} \underbrace{A_S | n \rangle_S}_{\langle n |} = \sum_n \underbrace{\langle n |}_{S_E} \left(\sum_{\ell} \underbrace{\langle \ell | \rho | \ell \rangle_E}_{A_S} \right) \underbrace{A_S | n \rangle_S}_{\langle n |} \\
 &= \text{tr}_S (\rho_S A_S) \quad \rho_S \equiv \text{tr}_E \rho
 \end{aligned}$$

This looks promising — same form as before!
Need to confirm that ρ_s is a system density matrix.

Here, tr_E (tr_S) is a partial trace using only the environment (the system) orthonormal basis in the summation.

Note:

- The partial trace $\text{tr}_E A$ of any operator $A: \mathcal{H}_S \otimes \mathcal{H}_E \rightarrow \mathcal{H}_S \otimes \mathcal{H}_E$ is still an operator, namely on \mathcal{H}_S .

$$\begin{aligned}
 \text{PROOF: } A &= \sum_{n_1, n_2} \sum_{\ell_1, \ell_2} a_{n_2 \ell_2, n_1 \ell_1} |n_2, \ell_2\rangle \langle n_1, \ell_1| \\
 \Rightarrow \text{tr}_E A &= \sum_{\ell} \langle \ell | A | \ell \rangle_E = \sum_{\ell_1, \ell_2} \sum_{n_1, n_2} a_{n_2 \ell_2, n_1 \ell_1} |n_2\rangle_S \langle \ell | \ell_2 \rangle_E \langle n_1 |_E \langle \ell_1 | \ell \rangle \\
 &= \sum_{n_1 n_2} \left(\sum_{\ell} a_{n_2 \ell, n_1 \ell} \right) |n_2\rangle_S \langle n_1 | \quad \text{which is an operator on } \mathcal{H}_S.
 \end{aligned}$$

- A common mistake of unfortunate popularity is to employ the cyclic invariance to a partial trace. This procedure is wrong since the objects to be permuted are still operators:

$\text{tr}_S(\Omega_1\Omega_2\Omega_3) \neq \text{tr}_S(\Omega_2\Omega_3\Omega_1)$ in general.

- The partial trace of a density matrix is a density matrix for the remaining subsystem.

PROOF: Let ρ be hermitean, positive and have unit trace, i.e.

$$\rho = \sum_K p_K |K\rangle\langle K| \text{ with } |K\rangle \in \mathcal{D}_S \otimes \mathcal{D}_E \text{ and}$$

$$\rho_S = \text{tr}_E \rho = \sum_K p_K \sum_{\ell} \langle \ell | K \rangle \langle K | \ell \rangle_E. \text{ Hermiticity follows from}$$

$$\begin{aligned} (\rho_S)_{nn'} &= \langle n | \rho_S | n' \rangle_S = \sum_K p_K \sum_{\ell} \langle n | \ell \rangle \langle K | n' \rangle \\ &= \sum_K p_K \sum_{\ell} (\langle n' | \ell \rangle \langle K | n \rangle)^* = (\langle n' | \rho_S | n \rangle)^* = (\rho_S)_{n'n}^* \end{aligned}$$

$$\begin{aligned} \text{Positivity follows from: } \langle \psi | \rho_S | \psi \rangle_S &= \langle \psi | \sum_K p_K \sum_{\ell} \langle \ell | K \rangle \langle K | \ell \rangle_E | \psi \rangle_S \\ &= \sum_{\ell} \langle \psi | \ell \rangle \rho_S | \psi \rangle \geq 0 \text{ (since } \rho \text{ is positive).} \end{aligned}$$

Unit trace of ρ_S follows directly from $\text{tr} \rho = 1$.

As a result, $\rho_S = \text{tr}_E \rho$ is a valid density matrix of the system S and deserves the name "reduced density matrix".

CAVEAT: Some caution is required in interpreting statements such as "the system is in the state $\rho_S = \text{tr}_E \rho$."

What we have proven is merely: we can calculate all ensemble averages of system observables by using the system ensemble state ρ_S . Properties going beyond this such as system-environment correlations are not captured by ρ_S . In particular, this is the case when system and environment are entangled. (In that case, ρ_S is sometimes referred to as an "improper mixed state," see [BP] p. 73.)

If $S+E$ is in a pure product state, no such problem occurs:

$$|\Psi\rangle = |\psi\rangle_S |\phi\rangle_E \Rightarrow \rho = |\psi\rangle_S |\psi\rangle_E \langle \psi | \langle \phi |$$

$$\Rightarrow \rho_S = \text{tr}_E \rho = |\psi\rangle_S \langle \psi | \text{ (pure state)}$$

For a pure entangled state (example: two spin- $\frac{1}{2}$'s), however, we find

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \Rightarrow \rho = \frac{1}{2}(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\uparrow\uparrow\rangle\langle\downarrow\downarrow| + |\downarrow\downarrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|)$$

$$\Rightarrow \rho_1 = \text{tr}_2 \rho = \langle \uparrow_2 | \rho | \uparrow_2 \rangle + \langle \downarrow_2 | \rho | \downarrow_2 \rangle = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)$$

which is a mixed state.

This yields a convenient way of testing a pure state of a bi-partite system for entanglement:

TEST FOR BIPARTITE ENTANGLEMENT

The pure state $\rho = |\Psi\rangle\langle\Psi|$, $|\Psi\rangle \in \mathcal{H}_S \otimes \mathcal{H}_E$ is entangled
 $\Leftrightarrow \rho_S = \text{tr}_E \rho$ is not pure.

Example: Consider two spin- $\frac{1}{2}$'s in the joint state $\rho = \frac{1}{3} \begin{pmatrix} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow \\ 1 & 1 & 0 & -1 \\ 1 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & 1 \end{pmatrix}$.
 Is this state pure? Is it entangled?

Answer: Calculate ρ^2 and find $\rho^2 = \rho \therefore \rho$ is pure.

Next, calculate

$$\rho_1 = \text{tr}_2 \rho = \begin{pmatrix} \langle \uparrow | \rho | \uparrow \rangle & \langle \uparrow | \rho | \downarrow \rangle \\ \langle \downarrow | \rho | \uparrow \rangle & \langle \downarrow | \rho | \downarrow \rangle \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

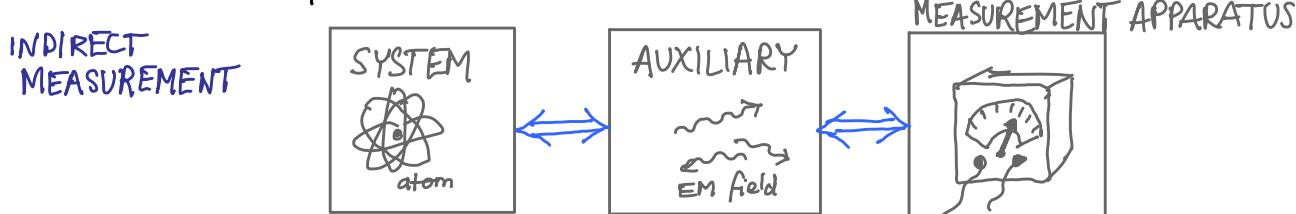
$$\rho_1^2 = \frac{1}{9} \begin{pmatrix} 5 & -2 \\ -2 & 2 \end{pmatrix} \neq \rho_1 \quad \therefore \rho \text{ is entangled.}$$

1.6 Generalized Measurement Theory

Measurements are a crucial part of developing and testing any physical theory. Those of our QM axioms that are related to measurements (state collapse and Born's rule) are based on the picture of ideal, projective measurements. Evidently, this appealingly simple perspective has several shortcomings:

Theoretically, any Hermitian operator is a perfectly fine choice for an observable. However, experimentalists do not possess buckets of Hermitian operators for measurement. Rather, careful thinking is required to devise ways of extracting information from a system. Usually, for any given system, only a limited number of observables are easily accessible in an experiment. Figuring out how to measure is a crucial task for a quantum engineer.

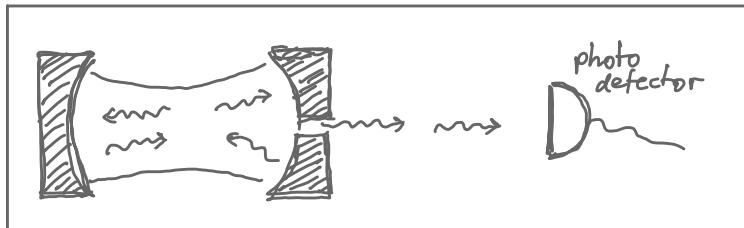
In many cases of interest, the measurement of a quantum system follows an indirect measurement approach. The quantum system to be measured (think about an atom, for example) may not be wired to the measurement apparatus. It couples, however, to the electro-magnetic field which, in turn, is more easily accessible (think photo detector, for instance).



In certain types of measurements, the conditional post-measurement state does not correspond to the projected state. In some cases, this is referred to as a destructive measurement. Example: measure the photon content of a system by directing all photons to a photo

detector. Once all "clicks" have been counted, we know the photon number — but all registered photons are gone!

DESTRUCTIVE
MEASUREMENT



Moreover, measurements commonly involve **uncertainties and errors**.

For instance, photo detectors have a "dark count rate" at which clicks are triggered in the absence of a photon. As another example, take any position measurement x of a particle in 1D. The measurement result will never be a single eigenvalue of \hat{x} (which would be a point!). Instead the measurement will give an interval $[x - \Delta x, x + \Delta x]$.

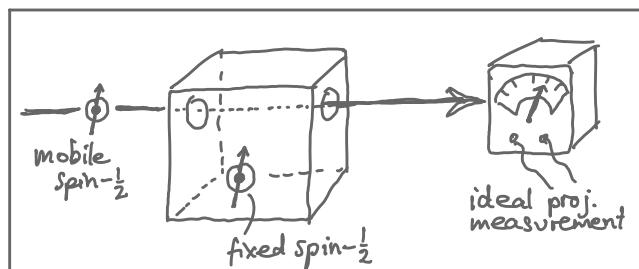
(This measurement uncertainty would not necessarily be due to Heisenberg's uncertainty principle.)

Question: Given the axioms for ideal projective measurements, can we derive a more flexible, realistic and general description of quantum measurements?

Case study

To further motivate a generalized measurement theory and outline its form, let us consider a system consisting of

- a spatially fixed spin- $\frac{1}{2}$ (e.g., nuclear spin of a trapped atom)
- an auxiliary and mobile spin- $\frac{1}{2}$ of the same sort
- a measurement apparatus that can perform a σ_z measurement of the mobile spin- $\frac{1}{2}$.



The idea of a simple indirect measurement is to allow the mobile spin to interact with the fixed one in a "fly-by." Subsequently, we imagine applying an ideal projective measurement of σ_z to the mobile spin.

Let us assume that during the fly-by the two spins are coupled for a time Δt with constant coupling given by

$$H = hg(\sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+). \quad \begin{matrix} 1: \text{fixed} \\ 2: \text{mobile} \end{matrix}$$

For given initial state $|\Psi_0\rangle = |\phi\rangle |1\rangle_2$, what is the post-measurement state of the fixed spin? Since no projective measurement is applied to the fixed spin, we cannot directly apply the axioms to obtain this state. However, the axioms allow us to infer that state as follows.

To describe the time evolution during the interaction period, we first calculate the propagator $e^{-iHt/\hbar}$.

$$H = hg \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \therefore e^{-iHt/\hbar} = \exp \left[-2\pi i g t \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \right]$$

Shortcut: remember that $e^{i\varphi \vec{n} \cdot \vec{S}} = e^{i\frac{\varphi}{2} \vec{n} \cdot \vec{\sigma}} = \cos \frac{\varphi}{2} \cdot \mathbb{1} + i \sin \frac{\varphi}{2} (\vec{n} \cdot \vec{\sigma})$. (Here: $\vec{n} = \hat{e}_x$.)

$$\Rightarrow e^{-iHt/\hbar} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\pi g t) & -i \sin(2\pi g t) & 0 \\ 0 & -i \sin(2\pi g t) & \cos(2\pi g t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Lengthier pedestrian way:

$$U H U^\dagger = hg \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad w/ \quad U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$e^{-iHt/\hbar} = e^{-iU^\dagger H U^\dagger U t/\hbar} = U^\dagger e^{-iH \text{diag}(U) t/\hbar} U = U^\dagger \text{diag}(1, e^{-2\pi i g t}, e^{2\pi i g t}, 1) U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \boxed{U} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

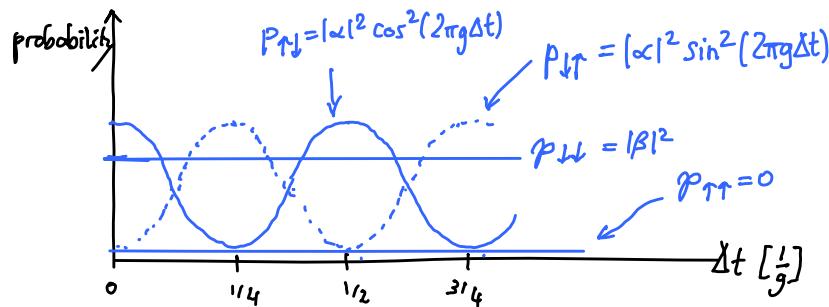
$$w/ \quad u = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} e^{-i\varphi} & 0 \\ 0 & e^{i\varphi} \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} e^{-i\varphi} & e^{-i\varphi} \\ e^{i\varphi} & -e^{i\varphi} \end{pmatrix} = \begin{pmatrix} \cos \varphi & -i \sin \varphi \\ -i \sin \varphi & \cos \varphi \end{pmatrix} = \begin{pmatrix} \cos(2\pi g t) & -i \sin(2\pi g t) \\ -i \sin(2\pi g t) & \cos(2\pi g t) \end{pmatrix}$$

Next, employ the propagator to extract the state after the fly-by:

$$\text{initial state: } |\Psi_0\rangle = (\alpha |1\rangle_1 + \beta |0\rangle_1) \otimes |1\rangle_2 = \begin{pmatrix} 0 \\ \alpha \\ 0 \\ \beta \end{pmatrix} \begin{matrix} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{matrix}$$

$$\text{post fly-by: } \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\pi g \Delta t) & -i \sin(2\pi g \Delta t) & 0 \\ 0 & -i \sin(2\pi g \Delta t) & \cos(2\pi g \Delta t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \alpha \\ 0 \\ \beta \end{pmatrix} \begin{matrix} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{matrix} = \begin{pmatrix} 0 \\ \alpha \cos(2\pi g \Delta t) \\ -i \alpha \sin(2\pi g \Delta t) \\ \beta \end{pmatrix}$$

Thus, the amplitude to be in the state $|11\rangle$ remains unchanged (β) while the probability amplitude for $|1\downarrow\rangle$ periodically swaps with $|1\uparrow\rangle$:



Finally, apply a σ_z measurement to the mobile spin:

pre-measurement state:

abbreviate: $c \equiv \cos(2\pi g \Delta t)$, $s \equiv \sin(2\pi g \Delta t)$

$$\rho = |\Psi_1\rangle \langle \Psi_1| = \begin{pmatrix} 0 \\ -i\alpha s \\ \beta \end{pmatrix} \otimes (0 \ \alpha^* c \ i\alpha^* s \ \beta^*) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |\alpha|^2 c^2 & i|\alpha|^2 c s & \alpha \beta^* c \\ 0 & -i|\alpha|^2 c s & |\alpha|^2 s^2 & -i\alpha \beta^* s \\ 0 & \alpha^* \beta c & i\alpha^* \beta s & |\beta|^2 \end{pmatrix}$$

observable:

$$1 \otimes \sigma_z^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = 1 \cdot P_i - 1 \cdot P_{-i}, \quad w/ \quad P_i = \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{\text{projectors}}, \quad P_{-i} = \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\text{projectors}}$$

Measurement results and conditional post-measurement states:

Result $\sigma_2^z = 1$

Probability for this measurement outcome:

$$p_1 = \text{tr}(P_1 \rho) = \text{tr} \begin{pmatrix} 0 & * & * & * \\ * & 0 & * & * \\ * & * & |\alpha|^2 s^2 & * \\ * & * & * & 0 \end{pmatrix} = |\alpha|^2 \sin^2(2\pi g \Delta t)$$

Conditional post-measurement state:

$$\rho_1 = \frac{P_1 \rho P_1}{p_1} = p_1^{-1} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |\alpha|^2 c^2 & i|\alpha| c s & \alpha \beta^* c \\ 0 & -i|\alpha|^2 c s & |\alpha|^2 s^2 & -i\alpha \beta^* s \\ 0 & \alpha^* \beta c & i\alpha^* \beta s & |\beta|^2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = |\downarrow\uparrow\rangle\langle\downarrow\uparrow|$$

selected by the projector

Reduced density matrix for the fixed spin: $\rho_{\text{fix}} = \text{tr}_2 \rho_1 = |\downarrow\rangle\langle\downarrow\downarrow|$

Result $\sigma_2^z = -1$

Probability for this measurement outcome: $p_{-1} = 1 - p_1 = 1 - |\alpha|^2 \sin^2(2\pi g \Delta t)$

Conditional post-measurement state:

$$\begin{aligned} \rho_{-1} &= p_{-1}^{-1} P_{-1} \rho P_{-1} = p_{-1}^{-1} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |\alpha|^2 c^2 & i|\alpha| c s & \alpha \beta^* c \\ 0 & -i|\alpha|^2 c s & |\alpha|^2 s^2 & -i\alpha \beta^* s \\ 0 & \alpha^* \beta c & i\alpha^* \beta s & |\beta|^2 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ &= \frac{1}{1 - |\alpha|^2 s^2} \begin{pmatrix} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow \\ 0 & 0 & 0 & 0 \\ 0 & |\alpha|^2 (1-s^2) & 0 & \alpha \beta^* c \\ 0 & 0 & 0 & 1 - |\alpha|^2 \end{pmatrix} \begin{matrix} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{matrix} \end{aligned}$$

Reduced density matrix for the fixed spin:

$$\rho_{\text{fix}} = \text{tr}_2 \rho_{-1} = \frac{1}{1 - |\alpha|^2 s^2} \left(|\alpha|^2 (1-s^2) |\uparrow\rangle\langle\uparrow| + (1 - |\alpha|^2) |\downarrow\rangle\langle\downarrow| + \alpha^* \beta c |\uparrow\rangle\langle\downarrow| + \alpha \beta^* c |\downarrow\rangle\langle\uparrow| \right)$$

Let us focus on two specific interaction times: $\Delta t = \frac{1}{4} \frac{1}{g}$ and $\Delta t \ll \frac{1}{g}$.

$$\Delta t = \frac{1}{4} \frac{1}{g}$$

In this case, $\cos(2\pi g \Delta t) = 0$ and $\sin(2\pi g \Delta t) = 1$, so the interaction time is adjusted to perform a perfect swap $|\uparrow\downarrow\rangle \rightarrow |\downarrow\uparrow\rangle$.

The indirect measurement boils down to:

$\sigma_z^z = -1$: probability for this outcome is $|\beta|^2 = 1 - |\alpha|^2$.

Conditional post-measurement state for fixed spin: $\rho_{fix} = |\downarrow\rangle\langle\downarrow\downarrow|$

$\sigma_z^z = +1$: probability for outcome: $|\alpha|^2$

Conditional post-measurement state for fixed spin: $\rho_{fix} = |\downarrow\rangle\langle\downarrow\downarrow|$

This is an ideal but destructive measurement.

$$\Delta t \ll 1$$

Now, $\cos(2\pi g \Delta t) = 1 - \frac{1}{2}(2\pi g \Delta t)^2 + \mathcal{O}(\Delta t^3)$, $\sin(2\pi g \Delta t) \approx 2\pi g \Delta t + \mathcal{O}(\Delta t^3)$ and almost no swapping occurs. Abbreviating $\epsilon = 2\pi g \Delta t$, we then obtain:

$\sigma_z^z = -1$: probability for this outcome is $\rho_{-1} \approx 1 - |\alpha|^2 \epsilon^2 \ (\approx 1)$

Conditional post-measurement state for fixed spin:

$$\rho_{fix} = \frac{|\alpha|^2(1-\epsilon^2)}{1-|\alpha|^2\epsilon^2} |\uparrow\rangle\langle\uparrow\uparrow| + \frac{1-|\alpha|^2}{1-|\alpha|^2\epsilon^2} |\downarrow\rangle\langle\downarrow\downarrow| + \left[\frac{\alpha^* \beta (1-\frac{1}{2}\epsilon^2)}{1-|\alpha|^2\epsilon^2} |\uparrow\rangle\langle\downarrow\downarrow| + h.c. \right]$$

$\sigma_z^z = +1$: probability for outcome: $\rho_{+1} \approx |\alpha|^2 \epsilon^2 \ll 1$

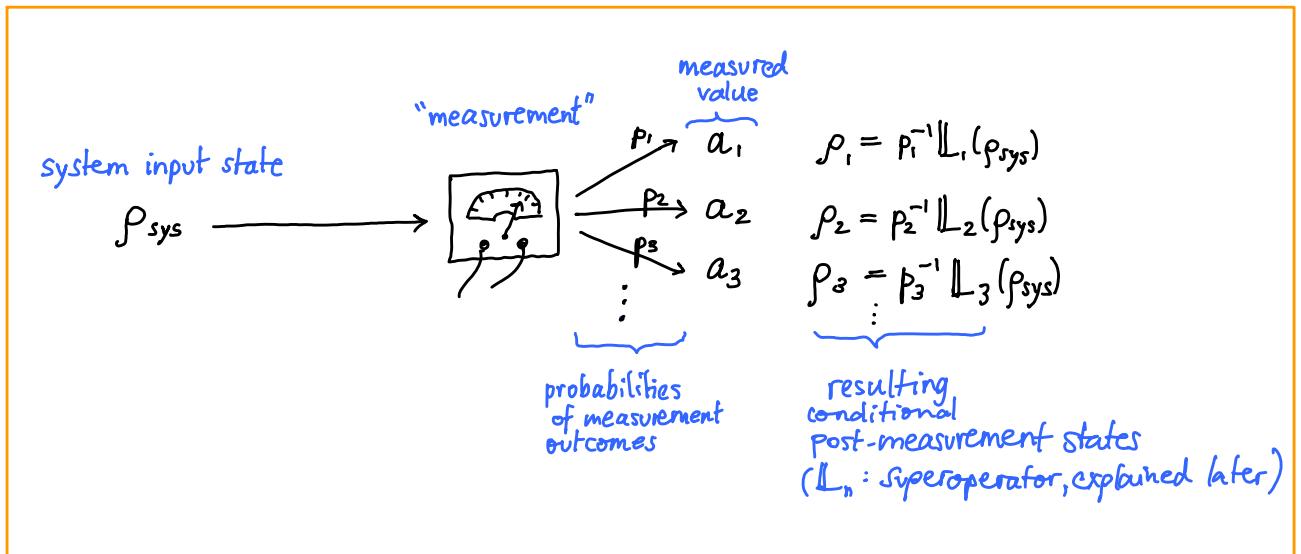
Conditional post-measurement state for fixed spin:

$$\rho_{fix} = |\downarrow\downarrow\rangle\langle\downarrow\downarrow|$$

→ This corresponds to a weak but destructive measurement of σ_z^z .

When using the alternative interaction Hamiltonian $H_I = \hbar g \sigma_1^+ \sigma_1^- \sigma_2^x$, we can turn this into a QND measurement of σ_z^z .

Fundamental building blocks of generalized measurements



From our discussion above it is clear that indirect measurements represent one class of generalized measurements which differ from pure projective ones. We will find out below that the viewpoint of indirect measurements is actually a lot more powerful: any generalized measurement with the basic building blocks sketched above can be interpreted as originating from an appropriate indirect measurement. It is thus very useful to rephrase our case study in general terms.

For the indirect measurement, the system (input state: ρ_{sys}) is brought into contact with an auxiliary system ("E") prepared in a fixed initial state ρ_E (independent of ρ_{sys}). Together, the combined system evolves and, possibly, becomes entangled:

$$\rho_0 = \rho_{sys} \otimes \rho_E \rightarrow \rho_i = U \rho_{sys} \otimes \rho_E U^\dagger$$

ρ_i then acts as the pre-measurement state for an ideal projective measurement of an observable in "E": $\mathbb{1}_{sys} \otimes A_E$ ($A_E = A_E^\dagger$).

Using the spectral decomposition $A_E = \sum_{\mu} a_{\mu} P_{\mu}$ (w/ $P_{\mu} P_{\nu} = \delta_{\mu\nu} P_{\mu}$), the possible measurement outcomes are given by $\{a_n\}$.

The conditional post-measurement state of the combined system is given by $P_{\mu} \rho_i P_{\mu} / p_{\mu}$. Once traced over the "E" degrees of freedom, we obtain the resulting reduced density matrix for the system:

$$\rho'_{sys, \mu} = \frac{1}{p_{\mu}} \text{tr}_E (P_{\mu} \rho_i P_{\mu}) = \frac{1}{p_{\mu}} \text{tr}_E (U \rho_{sys} \otimes \rho_E U^{\dagger} P_{\mu})$$

Note how the projector P_{μ} in the "E" subspace will select either a single contribution in the tr_E or multiple ones $\{|n_E^{(\mu)}\rangle\}$ forming an ONB in the degenerate eigenspace of a_{μ} . Both possibilities are summarized by

$$\begin{aligned} \text{tr}_E (P_{\mu} \rho_i P_{\mu}) &= \text{tr}_E (U \rho_{sys} \otimes \rho_E U^{\dagger} P_{\mu}) = \sum_n^{(\mu)} \langle n_E^{(\mu)} | U \rho_{sys} \otimes \rho_E U^{\dagger} | n_E^{(\mu)} \rangle \\ &= \sum_n^{(\mu)} \sum_{\substack{i_1, m_1 \\ i_2, m_2}} \langle n_E^{(\mu)} | U | i_1, m_1 \rangle \langle i_1, m_1 | \rho_{sys} \otimes \rho_E | i_2, m_2 \rangle \langle i_2, m_2 | U^{\dagger} | n_E^{(\mu)} \rangle \end{aligned}$$

Choose the "E" ONB such that $\rho_E = \sum_m p_m |m\rangle \langle m|$ is diagonal. Then,

$$\begin{aligned} \text{tr}_E (P_{\mu} \rho_i P_{\mu}) &= \sum_n^{(\mu)} \sum_m \langle n_E^{(\mu)} | U | m \rangle p_m \rho_{sys} \langle m | U^{\dagger} | n_E^{(\mu)} \rangle \\ &= \sum_n^{(\mu)} \sum_m M_{nm}^{\mu} \rho_{sys} (M_{nm}^{\mu})^{\dagger} \quad w/ \quad M_{nm}^{\mu} \equiv \sqrt{p_m} \langle n_E^{(\mu)} | U | m \rangle \end{aligned}$$

The probability for outcome a_{μ} to occur is

$$\begin{aligned} p_{\mu} &= \text{tr}(P_{\mu} \rho_i P_{\mu}) = \text{tr}_{sys} \text{tr}_E (P_{\mu} \rho_i P_{\mu}) = \sum_n^{(\mu)} \sum_m \text{tr}_{sys} (M_{nm}^{\mu} \rho_{sys} (M_{nm}^{\mu})^{\dagger}) \\ &= \text{tr}_{sys} \left(\rho_{sys} \sum_n^{(\mu)} \sum_m (M_{nm}^{\mu})^{\dagger} M_{nm}^{\mu} \right) \end{aligned}$$

Summary and Remarks: Generalized Measurements

- In a general (indirect) measurement scheme, every measurement outcome a_μ is associated with a set of measurement operators

$$\{ M_{nm}^\mu \mid M_{nm}^\mu = \langle n^{(\mu)} | U | m \rangle \sqrt{p_m} \}$$

ONB for the "E"
 eigenspace of a_μ ↗ ONB for "E" that
 diagonalizes ρ_E

Each M_{nm}^μ is an operator in \mathcal{H}_{sys} and not generally hermitean.

- The probability for measurement outcome a_μ is given in terms of $\{M_{nm}^\mu\}$ by

$$p_\mu = \text{tr}_{\text{sys}} \left[\rho_{\text{sys}} \sum_n \sum_m^{(\mu)} (M_{nm}^\mu)^\dagger M_{nm}^\mu \right] = \text{tr}_{\text{sys}} (\rho_{\text{sys}} F_\mu)$$

The operator $F_\mu \equiv \sum_n \sum_m^{(\mu)} (M_{nm}^\mu)^\dagger M_{nm}^\mu$ is called an "effect". It is hermitean, positive, and satisfies $\sum_\mu F_\mu = 1$.

PROOF : Hermiticity of F_μ is obvious. Positivity follows from

$$\langle \psi | F_\mu | \psi \rangle = \sum_n \sum_m^{(\mu)} \langle \psi | (M_{nm}^\mu)^\dagger M_{nm}^\mu | \psi \rangle = \sum_n \sum_m^{(\mu)} \| M_{nm}^\mu | \psi \rangle \|^2 \geq 0$$

The completeness relation is obtained via

$$\begin{aligned} \sum_\mu F_\mu &= \sum_\mu \sum_n \sum_m^{(\mu)} (M_{nm}^\mu)^\dagger M_{nm}^\mu = \sum_\mu \sum_n \sum_m^{(\mu)} \underbrace{\left(\langle n^{(\mu)} | U | m \rangle \right)^\dagger}_{\text{still operator!}} \langle n^{(\mu)} | U | m \rangle \cdot \mathbb{1}_{\text{sys}} \\ &= \sum_m \langle m | U^\dagger | \underbrace{\sum_\mu \sum_n^{(\mu)} | n^{(\mu)} \rangle \langle n^{(\mu)} | U | m \rangle}_{= \mathbb{1}_E} \rangle = \sum_m \langle m | m \rangle \cdot \mathbb{1}_{\text{sys}} = \mathbb{1}_{\text{sys}} \end{aligned}$$

- The conditional post-measurement state is

$$\rho_{\text{sys}} \xrightarrow{a_\mu} \rho'_{\text{sys}, \mu} = \frac{1}{p_\mu} \mathbb{L}_\mu(\rho_{\text{sys}}) = \frac{1}{p_\mu} \sum_n^{(\mu)} \sum_m M_{nm}^\mu \rho_{\text{sys}} (M_{nm}^\mu)^\dagger.$$

Here, $\mathbb{L}_\mu(\rho_{\text{sys}})$ is called an "operation." \mathbb{L}_μ is linear in ρ_{sys} and must map a density matrix to another density matrix (up to normalization). Such maps are generally called super-operators.

- Generalized measurements as described above are also referred to as **POVM based measurements** where the acronym stands for Positive Operator Valued Measure. This is to be contrasted with **PVM based measurements** (projection valued measure). These form a subset of POVMs, as is easily checked by considering $M^\mu = P_M$.

Kraus's Representation Theorem for Operations

If you are carefully following the logic behind our introduction of generalized measurements as stemming from indirect measurements, you are pondering about an important question right now: why are we so sure that indirect measurements really give us the most general description possible? Could it be that there is something even more general that lies beyond our new description of measurements?

This question is an important and, by no means, trivial one. The representation theorem for operations by Kraus* gives the definitive answer that, indeed, all physical possibilities are captured by considering indirect measurements. Kraus' theorem states that an operation

$$\rho' = \frac{\mathbb{L}(\rho)}{\text{tr } \mathbb{L}(\rho)}$$

satisfies the following conditions if and only if there is a set of measurement operators $\{M_k\}_{k=1,2,\dots}$ such that

" $\sum_k M_k^+ M_k \leq \mathbb{I}$ " : read as statement about eigenvalues!

Automatically, $\sum_k M_k^+ M_k$ is hermitean and positive. Demand $0 \leq m_j \leq 1$ for its eigenvalues.

and $\mathbb{L}(\rho) = \sum_k M_k \rho M_k^+$.

* K. Kraus, "States, Effects and Operations," vol. 190 of Lecture Notes in Physics (Springer, 1983)

Conditions:

- (1) $\text{tr } \mathbb{L}(\rho)$ satisfies $0 \leq \text{tr } \mathbb{L}(\rho) \leq 1$ and hence can be interpreted as a probability.
- (2) The map \mathbb{L} is convex linear, i.e. $\mathbb{L}(\sum_i p_i \rho_i) = \sum_i p_i \mathbb{L}(\rho_i)$ ($0 \leq p_i \leq 1, \sum_i p_i = 1$)
- (3) The map \mathbb{L} is "completely positive."

Before proceeding with the proof, we need to understand the meaning of **complete positivity** demanded in (3). **Positivity** of \mathbb{L} means that for any positive ρ , $\mathbb{L}(\rho)$ is positive as well. Complete positivity goes one step further: not only should $\mathbb{L}(\rho)$ be positive but its tensor product $\text{id}_E \otimes \mathbb{L}(\rho_E \otimes \rho)$ should also be positive for any environment system "E". The physical motivation for this condition is simple: imagine extending the system to include an additional subsystem 'E.' If 'E' and the original system remain separate, then the operation should simply extend to a new superoperator $\text{id}_E \otimes \mathbb{L}_\mu$, which must also be positive.

You might wonder whether there are any positive maps that are not completely positive. The answer is: yes, there are!

Example:

Consider the map $\mathbb{L}(\rho) = \rho^t$ (only transpose, no complex conjugation). Clearly \mathbb{L} is positive since

$$\begin{aligned} \rho \text{ positive} &\Leftrightarrow \langle \psi | \rho | \psi \rangle \geq 0 \quad \forall |\psi\rangle = \sum_n \alpha_n |n\rangle \in \mathcal{H} \\ &\Leftrightarrow \langle \psi | \rho | \psi \rangle = \sum_n \sum_m \alpha_n^* \alpha_m \underbrace{\langle n | \rho | m \rangle}_{\rho_{nm}} = \sum_{n,m} \alpha_n^* \alpha_m \rho_{mn}^* = \left(\sum_{n,m} \alpha_n \alpha_m^* \rho_{mn} \right)^* \\ &= (\langle \psi | \rho^t | \psi \rangle)^* \geq 0 \Leftrightarrow \rho^t \text{ is positive.} \end{aligned}$$

Now, consider two spins. Let $\mathbb{L}_1(\rho_1) = \rho_1^t$ act on spin 1 but not spin 2. The joint operation on both spins hence takes the form $\text{id}_2 \otimes \mathbb{L}_1$. When mapping the state $\rho = |\phi\rangle\langle\phi|$ with $|\phi\rangle = (|1\rangle\langle 1| + |2\rangle\langle 2|)/\sqrt{2}$ we obtain:

$$\begin{aligned} \text{id}_{\mathbb{L}_2} \otimes \mathbb{L}_1 (|\phi\rangle\langle\phi|) &= \text{id}_{\mathbb{L}_2} \otimes \mathbb{L}_1 (|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) \cdot \frac{1}{2} \\ &= \frac{1}{2} \left[|\uparrow_2\rangle\langle\uparrow_2| \otimes \mathbb{L}_1 (|\uparrow_1\rangle\langle\uparrow_1|) + |\uparrow_2\rangle\langle\downarrow_2| \otimes \mathbb{L}_1 (|\uparrow_1\rangle\langle\downarrow_1|) \right. \\ &\quad \left. + |\downarrow_2\rangle\langle\uparrow_2| \otimes \mathbb{L}_1 (|\downarrow_1\rangle\langle\uparrow_1|) + |\downarrow_2\rangle\langle\downarrow_2| \otimes \mathbb{L}_1 (|\downarrow_1\rangle\langle\downarrow_1|) \right] \end{aligned}$$

Now, represent the operators for spin 1 in matrix form and take the transpose:

$$\begin{aligned} \mathbb{L}_1 (|\uparrow_1\rangle\langle\uparrow_1|) &= \mathbb{L}_1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}^T = |\uparrow_1\rangle\langle\uparrow_1|, \quad \mathbb{L}_1 (|\downarrow_1\rangle\langle\downarrow_1|) = |\downarrow_1\rangle\langle\downarrow_1| \\ \mathbb{L}_1 (|\uparrow_1\rangle\langle\downarrow_1|) &= |\downarrow_1\rangle\langle\uparrow_1|, \quad \mathbb{L}_1 (|\downarrow_1\rangle\langle\uparrow_1|) = |\uparrow_1\rangle\langle\downarrow_1| \end{aligned}$$

$$\begin{aligned} \Rightarrow \text{id}_{\mathbb{L}_2} \otimes \mathbb{L}_1 (|\phi\rangle\langle\phi|) &= \frac{1}{2} (|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow| + |\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|) \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad \text{This is } \underline{\text{not}} \text{ positive. (One of the eigenvalues is } -1.) \end{aligned}$$

SKETCH OF PROOF (Kraus's Representation Theorem):

(a) Show that the form $\mathbb{L}(\rho) = \sum_k M_k \rho M_k^\dagger$ implies conditions (1), (2) & (3).

$$(1) \quad \text{tr } \mathbb{L}(\rho) = \text{tr} (\sum_k M_k \rho M_k^\dagger) = \text{tr} (\rho \sum_k M_k^\dagger M_k) = \text{tr} \left[\underbrace{\rho}_{\tilde{\rho}} \underbrace{\sum_k M_k^\dagger M_k}_{\text{diag}} \right]$$

with $0 \leq m_j \leq 1$. $\Rightarrow 0 \leq \text{tr } \mathbb{L}(\rho) \leq 1$.

$$(2) \quad \text{Let } \rho = \sum_i p_i \rho_i.$$

$$\Rightarrow \mathbb{L}(\rho) = \sum_i \sum_k M_k (p_i \rho_i) M_k^\dagger = \sum_i p_i \sum_k M_k \rho_i M_k^\dagger = \sum_i p_i \mathbb{L}(\rho_i)$$

Note: due to linearity, we may skip the parentheses: $\mathbb{L}(\rho) = \mathbb{L}\rho$

(3) Consider $\mathcal{H} = \mathcal{H}_{\text{sys}} \otimes \mathcal{H}_E$ and $\rho \in \mathbb{R}_{\geq 0}$ (thus, ρ is positive).

Then, $\rho' = \text{id}_{\mathcal{H}_E} \otimes \mathbb{L}_{\text{sys}} (\rho) = \sum_k \mathbb{I}_E M_k \rho M_k^\dagger$ and hence for $|\psi\rangle \in \mathcal{H}$ we find

$$\langle \psi | \rho' | \psi \rangle = \sum_k \langle \psi | M_k \rho M_k^\dagger | \psi \rangle = \sum_k \langle \phi_k | \rho | \phi_k \rangle \geq 0$$

$|\phi_k\rangle \equiv M_k^\dagger |\psi\rangle$ ρ positive.

(b) Need to show: if $\mathbb{L}(\rho)$ satisfies conditions (1)–(3) it has the form $\mathbb{L}(\rho) = \sum_k M_k \rho M_k^\dagger$. To prove this we explicitly construct the measurement operators $\{M_k\}$. To make use of complete positivity, we will need to enlarge our Hilbert space to $\mathcal{H} = \mathcal{H}_{\text{sys}} \otimes \mathcal{H}_E$. Choose \mathcal{H}_E to be a copy of \mathcal{H}_{sys} , so that an ONB $\{|n_{\text{sys}}\rangle\}$ of \mathcal{H}_{sys} is mirrored by an equivalent ONB $\{|n_E\rangle\}$ in \mathcal{H}_E .

Start by considering the entangled state $|f\rangle = \sum_n |n_{\text{sys}}, n_E\rangle / \sqrt{N}$, and use the extension of \mathbb{L} to obtain

$$\sigma = \text{id}_{\mathcal{H}_E} \otimes \mathbb{L} (|f\rangle \langle f|) \cdot N$$

Since $|f\rangle \langle f|$ is positive and \mathbb{L} is completely positive, σ is positive and, hence, has a spectral representation

$$\sigma = \sum_k |\sigma_k\rangle \langle \sigma_k| \quad (\text{note: } |\sigma_k\rangle \text{ not normalized!})$$

where $\{|\sigma_k\rangle\}$ is an OB in $\mathcal{H} = \mathcal{H}_{\text{sys}} \otimes \mathcal{H}_E$. Finally, for every $|\psi_{\text{sys}}\rangle = \sum_n \psi_n |n_{\text{sys}}\rangle \in \mathcal{H}_{\text{sys}}$ we define a mirror state in \mathcal{H}_E by

$$|\psi_E\rangle = \sum_n \psi_n^* |n_E\rangle.$$

Now, the measurement operators are introduced by

$$M_k |\psi_{\text{sys}}\rangle \equiv \langle \psi_E | \sigma_k \rangle = \sum_n \psi_n \underbrace{\langle n_E |}_{\in \mathcal{H}_E} \underbrace{\sigma_k}_{\in \mathcal{H}} \langle n_E | \psi_E \rangle \in \mathcal{H}_{\text{sys}},$$

so that

$$\begin{aligned} \sum_k M_k |\psi_{\text{sys}}\rangle \langle \psi_{\text{sys}} | M_k^\dagger &= \sum_k \sum_{n,n'} \psi_n \langle n_E | \sigma_k \rangle \langle \sigma_k | n'_E \rangle \psi_{n'}^* \\ &= \sum_{n,n'} \psi_n \langle n_E | \text{id}_{\mathcal{H}_E} \otimes \mathbb{L} (|f\rangle \langle f|) |n'_E \rangle \psi_{n'}^* \\ &= \sum_{n,n'} \psi_n \langle n_E | \sum_m |m_E\rangle \langle m_E| \otimes \mathbb{L} (|f\rangle \langle f|) |n'_E \rangle \psi_{n'}^* \\ &= \sum_{n,n'} \psi_n \langle n_E | \sum_m |m_E\rangle \langle m_E| \otimes \mathbb{L} (|f\rangle \langle f|) |n'_E \rangle \psi_{n'}^* \\ &= \sum_n \psi_n^* \psi_n \mathbb{L} (|f\rangle \langle f|) = \mathbb{L} (|\psi_{\text{sys}}\rangle \langle \psi_{\text{sys}}|) \end{aligned}$$

By virtue of convex linearity (condition (2)) this generalizes to all mixed states in \mathcal{H}_{sys} .

Finally note that the condition $1 \geq \text{tr } \mathbb{L}(\rho) \geq 0$ leads to

$$1 \geq \text{tr } \mathbb{L}(\rho) = \text{tr} \left(\sum_k M_k \rho M_k^\dagger \right) = \text{tr} \left(\rho \sum_k M_k^\dagger M_k \right) \geq 0$$

For any eigenstate $|m_j\rangle$ of $\sum_k M_k^\dagger M_k$ with eigenvalue λ_j , we obtain

$$1 \geq \text{tr} \left(|m_j\rangle \langle m_j| \sum_k M_k^\dagger M_k \right) = \langle m_j | \sum_k M_k^\dagger M_k | m_j \rangle = \lambda_j \geq 0. \quad \square$$

Examples of Generalized Measurements

Ideal projective measurements as a special case of generalized measurements:

In this case, measurement outcomes $\{a_\mu\}$ are the eigenvalues of an observable $A = \sum_\mu a_\mu P_\mu$. The projectors P_μ ($P_\nu P_\mu = \delta_{\nu\mu} P_\mu$) play the role of the measurement operators $M^{\mu} = P_\mu$. (Recall: projectors are always hermitean and satisfy $\sum_\mu P_\mu = \mathbb{1}$ due to hermiticity of A .)

\therefore conditional post-measurement state:

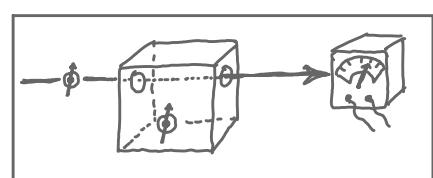
$$\rho' = \frac{1}{P_\mu} \mathbb{L}_\mu \rho = \frac{1}{P_\mu} M^\mu \rho (M^\mu)^\dagger = \frac{1}{P_\mu} P_\mu \rho P_\mu$$

probability: $p_\mu = \text{tr } \mathbb{L}_\mu \rho = \text{tr} (P_\mu \rho P_\mu) = \text{tr} (\rho P_\mu)$

Two spin- $\frac{1}{2}$'s — example from above

Measurement outcomes: $\{a_\mu\} = \{-1, +1\}$

Recall the definition of the measurement operators:



$$\{ M_{nm}^\mu \mid M_{nm}^\mu = \langle n^{(\mu)} | U | m \rangle \sqrt{p_m} \}$$

↙ use $\mu = \pm 1$ for the measurement outcomes
 ↗ ONB for the "E" eigenspace of a_μ
 ↗ ONB for "E" that diagonalizes ρ_E

PS#2

$$\rho_E = |\downarrow_2\rangle\langle\downarrow_2| \text{ (initial state of mobile spin)} \Rightarrow |\uparrow_2\rangle\sqrt{p_{\uparrow}} = 0, \quad |\downarrow_2\rangle\sqrt{p_{\downarrow}} = |\downarrow_2\rangle$$

The eigenspaces of spin 2 for the outcomes $\mu = \pm 1$ are both one-dimensional:

$$\mu = +1: \quad |n_2^{(+)}\rangle = |\uparrow_2\rangle$$

$$\mu = -1: \quad |n_2^{(-)}\rangle = |\downarrow_2\rangle$$

We calculated the propagator above:

$$U = \begin{pmatrix} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow \\ 1 & 0 & 0 & 0 \\ 0 & \cos(2\pi g t) & -i \sin(2\pi g t) & 0 \\ 0 & -i \sin(2\pi g t) & \cos(2\pi g t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \sum_{\substack{\alpha, \beta \\ \alpha', \beta' \in \{\uparrow, \downarrow\}}} U_{\alpha\beta, \alpha'\beta'} |\alpha\beta\rangle \langle \alpha'\beta'|$$

$$\langle \uparrow\downarrow | U | \downarrow\downarrow \rangle = U_{\uparrow\downarrow, \downarrow\downarrow}$$

row $\alpha\beta$ column $\alpha'\beta'$

$$M_{(\uparrow\downarrow)}^{+1} = \langle n_2^{(+)} | U | \downarrow_2 \rangle = \langle \uparrow_2 | U | \downarrow_2 \rangle$$

$$= \begin{pmatrix} 0 & 0 \\ -is & 0 \end{pmatrix}$$

$$U = \begin{pmatrix} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow \\ 1 & 0 & 0 & 0 \\ 0 & \cos(2\pi g t) & -i \sin(2\pi g t) & 0 \\ 0 & -i \sin(2\pi g t) & \cos(2\pi g t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{matrix} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{matrix}$$

$$M_{(\downarrow\downarrow)}^{-1} = \langle n_2^{(-)} | U | \downarrow_2 \rangle = \langle \downarrow_2 | U | \downarrow_2 \rangle$$

$$= \begin{pmatrix} c & 0 \\ 0 & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow \\ 1 & 0 & 0 & 0 \\ 0 & \cos(2\pi g t) & -i \sin(2\pi g t) & 0 \\ 0 & -i \sin(2\pi g t) & \cos(2\pi g t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{matrix} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{matrix}$$

$$\text{Check: } (M^{+1})^T (M^{+1}) + (M^{-1})^T (M^{-1}) = \begin{pmatrix} 0 & is \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ -is & 0 \end{pmatrix} + \begin{pmatrix} c & 0 \\ 0 & 1 \end{pmatrix}^2 = \begin{pmatrix} s^2 + c^2 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}$$

Photo detection with finite efficiency [compare also PS#2]

Consider the detection of photons with a photo multiplier, and input states

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad \text{with zero photons } (|0\rangle) \text{ or one photon } (|1\rangle) \text{ present.}$$

Assume that detection of the one-photon component occurs with efficiency $0 < \eta < 1$ and is fully destructive.

In this scenario, the measurement operators can be constructed without explicit reference to the nature of the indirect measurement scheme. To start, we note that the two basic measurement outcomes are

$\mu=1$ — photon detected, and

$\mu=0$ — no photon detected.

Our task is to construct the two measurement operators $M_{\mu=1,0}$.

$\mu=1$: For the input state $\rho_0 = |1\rangle\langle 1|$, a photon is detected with probability $p=\eta$, i.e.,

$$\rho_0 = |1\rangle\langle 1| \xrightarrow{p=\eta} \mu=1, \text{ conditional post-measurement state: } \frac{M_1|1\rangle\langle 1|M_1^\dagger}{\text{tr}(|1\rangle\langle 1|M_1^\dagger M_1)} \stackrel{!}{=} |0\rangle\langle 0| \quad (\text{destructive})$$

$$\Rightarrow M_1|1\rangle = \mu|0\rangle \quad (\because \langle 1|M_1^\dagger = \mu^* \langle 0|)$$

$$\mu \text{ is fixed by: } p_{\mu=1, |1\rangle\langle 1|} \stackrel{!}{=} \eta = \text{tr}(|1\rangle\langle 1|M_1^\dagger M_1) = |\mu|^2$$

$$\therefore \mu = \sqrt{\eta} e^{i\varphi} \quad (\text{can choose } \varphi=0; \text{ phase is irrelevant!})$$

To determine M_1 fully, we also need: $M_1|0\rangle = \alpha|0\rangle + \beta|1\rangle$

Since

$$0 \stackrel{!}{=} p_{\mu=1, |0\rangle\langle 0|} = \text{tr}(M_1^\dagger M_1 |0\rangle\langle 0|) = \langle 0|M_1^\dagger M_1|0\rangle \\ = |\alpha|^2 + |\beta|^2 \Rightarrow \alpha = \beta = 0.$$

$$\text{Thus, } M_1 = \sqrt{\eta} |0\rangle\langle 1|.$$

$\mu=0$: The result $\mu=0$ is always obtained for input state $|0\rangle$, and with probability $p=1-\eta$ if the input state is $|1\rangle$, i.e.,

$$\rho_0 = |0\rangle\langle 0| \xrightarrow{p=1} |0\rangle\langle 0| \stackrel{!}{=} \frac{M_0|0\rangle\langle 0|M_0^\dagger}{\text{tr}(|0\rangle\langle 0|M_0^\dagger M_0)} \Rightarrow M_0|0\rangle = \mu|0\rangle$$

$$\text{and } p_{\mu=0, |0\rangle\langle 0|} = 1 = \text{tr}(|0\rangle\langle 0|M_0^\dagger M_0) = \langle 0|M_0^\dagger M_0|0\rangle = |\mu|^2$$

$$\Rightarrow \mu=1 \quad (\text{up to irrelevant phase})$$

$$\rho_0 = |1\rangle\langle 1| \xrightarrow{P=1-\eta} |1\rangle\langle 1| \stackrel{!}{=} \frac{M_1|1\rangle\langle 1|M_1^+}{\text{tr}(|1\rangle\langle 1|M_1^+M_1)} \Rightarrow M_1|1\rangle = \lambda|1\rangle$$

and $\rho_{\mu=0,|1\rangle\langle 1|} \stackrel{!}{=} 1-\eta = \text{tr}(|1\rangle\langle 1|M_1^+M_1) = |\lambda|^2$
 $\therefore \lambda = \sqrt{1-\eta}$ (up to an irrelevant phase).

Thus, $M_0 = |0\rangle\langle 0| + \sqrt{1-\eta}|1\rangle\langle 1|$

Check: $M_0^+M_0 + M_0^+M_1 = |0\rangle\langle 0| + (1-\eta)|1\rangle\langle 1| + \eta|1\rangle\langle 0| |0\rangle\langle 1|$
 $= |0\rangle\langle 0| + |1\rangle\langle 1| = \mathbb{1} \quad - \text{as it must be.}$

Measurement of continuous variable with finite resolution

Consider the measurement of an observable with continuous spectrum, such as the position \hat{x} of a particle (here, for simplicity, in 1d). Given the ideal measurement outcome x_0 , there is a conditional probability distribution $p(x|x_0)$ for the measurement apparatus to report the result x , e.g. a gaussian

$$p(x|x_0) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]$$

The probability to measure " x " given " x_0 " is hence

$$\rho_{x,|x_0\rangle\langle x_0|} = p(x|x_0) \stackrel{!}{=} \text{tr}(M_x^+M_x|x_0\rangle\langle x_0|) = \langle x_0|M_x^+M_x|x_0\rangle$$

Case 1: If the collapse is perfect despite the imprecise measurement, then
 $|x_0\rangle\langle x_0| \rightarrow |x_0\rangle\langle x_0| = \frac{M_x|x_0\rangle\langle x_0|M_x^+}{\text{tr}(|x_0\rangle\langle x_0|M_x^+M_x)} \quad \therefore M_x|x_0\rangle = \mu|x_0\rangle$

and $\rho_{x,|x_0\rangle\langle x_0|} = p(x|x_0) = |\mu|^2 \quad \therefore M_x = \int dx_0 \sqrt{p(x|x_0)} |x_0\rangle\langle x_0|$

check: $\int dx M_x^+M_x = \int dx \int dx_0 \int dx'_0 \sqrt{p(x|x_0)} \sqrt{p(x|x'_0)} |x_0\rangle\langle x_0| \underbrace{|x'_0\rangle\langle x'_0|}_{S(x_0-x'_0)}$
 $= \int dx \int dx_0 p(x|x_0) |x_0\rangle\langle x_0| = \int dx_0 |x_0\rangle\langle x_0| = \mathbb{1}$

Case 2: The collapsed state after measurement may differ from $|x_0\rangle\langle x_0|$, corresponding to additional measurement back-action specific to the measurement apparatus. In this case, additional information is necessary to fully determine $\{M_x\}$. [→ measurement tomography]

Non-uniqueness and minimal Kraus sum representation

Consider an operation Φ , represented by a certain Kraus sum

$\Phi(\rho) = \sum_k M_k \rho M_k^\dagger$ with $\sum_k M_k^\dagger M_k = \mathbb{I}$. Is this representation unique or can we find an alternative set of operators $\{\tilde{M}_\mu\}$, $\sum_\mu \tilde{M}_\mu^\dagger \tilde{M}_\mu$ representing the same operation Φ ?

The Kraus sum representation is not unique, as the following example shows:

Consider $\Phi(\rho) = M_1 \rho M_1^\dagger + M_2 \rho M_2^\dagger$, and define alternative measurement operators

$$\tilde{M}_1 = \frac{1}{\sqrt{2}}(M_1 + M_2) \quad \text{and} \quad \tilde{M}_2 = \frac{1}{\sqrt{2}}(M_1 - M_2).$$

$$\begin{aligned} \text{Then } \tilde{M}_1 \rho \tilde{M}_1^\dagger + \tilde{M}_2 \rho \tilde{M}_2^\dagger &= \frac{1}{2}(M_1 + M_2)\rho(M_1^\dagger + M_2^\dagger) + \frac{1}{2}(M_1 - M_2)\rho(M_1^\dagger - M_2^\dagger) \\ &= M_1 \rho M_1^\dagger + M_2 \rho M_2^\dagger = \Phi(\rho) \end{aligned}$$

You may have recognized that the transformation $\tilde{M}_j = \sum_k u_{jk} M_k$ above corresponds to a rotation by 90° , i.e., (u_{jk}) is orthogonal. It is easy to check that any unitary transformation will do:

Let $\tilde{M}_j = \sum_k u_{jk} M_k$ with unitary (u_{jk}) . Then,

$$\begin{aligned} \sum_j \tilde{M}_j \rho \tilde{M}_j^\dagger &= \sum_j \sum_{k,\ell} u_{jk} M_k \rho u_{j\ell}^* M_\ell^\dagger = \sum_{k,\ell} \underbrace{\sum_j (u_{jk} u_{j\ell}^*)}_{\delta_{k\ell}} M_k \rho M_\ell^\dagger \\ &= \sum_k M_k \rho M_k^\dagger. \end{aligned}$$

Vice versa, one can show* that $\Phi(\rho) = \sum_k M_k \rho M_k^\dagger = \tilde{\Phi}(\rho) = \sum_\ell \tilde{M}_\ell \rho \tilde{M}_\ell^\dagger$ implies that M_k and \tilde{M}_ℓ are related by a unitary transformation. (If the Kraus sums involve different numbers of terms, simply enlarge the set with the smaller number, say, $\{M_k\}$ by additional zero matrices.)

Note: ■ since $\text{cp}(\mathcal{H}) = N^2$ for $\dim \mathcal{H} = N$, one can always transform to a basis in which the Kraus sum consists of N^2 (or fewer) terms.

■ This criterion for two measurements being the same does not apply to the conditional post-measurement state.

* See Breuer & Petruccione for proof.

1.7 Time evolution of the Reduced Density Matrix

In Section 1.5, we identified the reduced density matrix $\rho_s = \text{tr}_E \rho_{\text{total}}$ as the appropriate vehicle for describing an open quantum system coupled to an environment E . In particular, we convinced ourselves that all interesting system properties (extracted from measurement of system observables) can be obtained from $\rho_s = \text{tr}_E \rho_{\text{total}}$. This result is encouraging but not fully satisfactory: to obtain ρ_s we need, it seems, the total density matrix of system + environment E . However, the whole point of the open quantum system concept is to avoid the detailed modeling of the processes taking place in the environment!

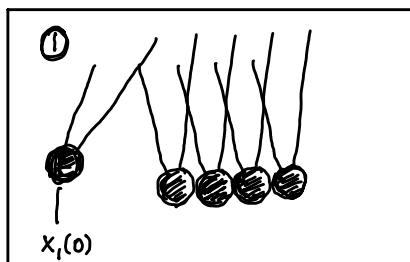
A central question, thus, is: given an initial state $\rho_{\text{total}}(t=0)$, is there an equation of motion describing the reduced density matrix alone, i.e.

$$(*) \quad \frac{d}{dt} \rho_s = \mathbb{G} \rho_s \quad \text{with initial condition } \rho(0) = \text{tr}_E \rho_{\text{total}}(0) \\ \text{and appropriate Superoperator } \mathbb{G}?$$

Note: this form already implements linearity. Moreover, it has an important property associated with the name of Markov: to evaluate the change of the reduced density matrix at time t , $d\rho_s(t) = \mathbb{G}\rho_s(t) dt$, we only invoke the instantaneous state of the reduced density matrix at that specific time — no record of the history of $\rho_s(t')$ at earlier times $t' < t$ is needed. We say that $(*)$ is Markovian — usually called a Markovian master equation.

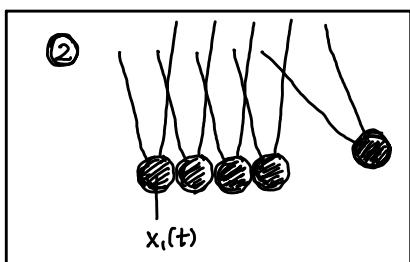
It is tempting to take the Markov property for granted — after all, any equation of motion that has the form of an ordinary or partial differential equation of finite order in time is Markovian (Newton's equation, Schrödinger equation, wave equation etc.). In a way, this merely reflects our preference for describing closed systems. It is very simple to find examples of non-Markovian behavior for open systems.

- Example of non-Markovian behavior in a classical system
Consider Newton's cradle:



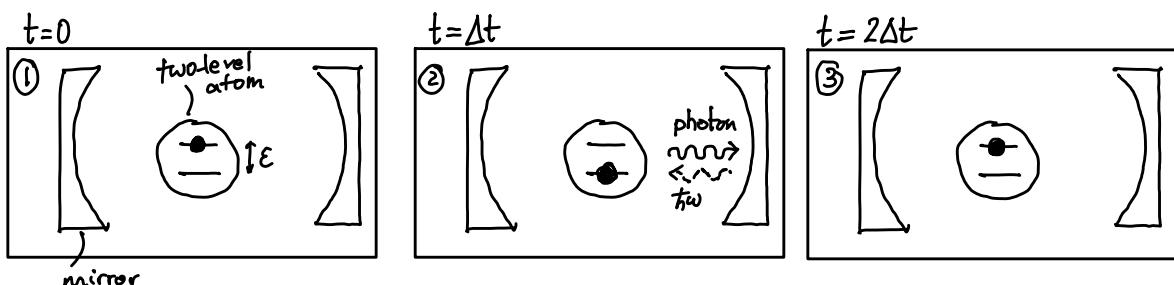
We might attempt deriving an equation of motion for the position $x_i(t)$ of the first ball alone,

$$m \frac{d^2}{dt^2} x_i(t) \stackrel{?}{=} f(x_i(t), \dot{x}_i(t))$$



It is clear that no such Markovian equation can be correct: in ② $x_i(t) = \dot{x}_i(t) = 0$. However the earlier displacement $x_i(0)$ at $t=0$ will influence the future dynamics of x_i .

- Example of non-Markovian behavior in a quantum system



Two-level atom and cavity mode described by the Jaynes-Cummings model :

$$H = \hbar \omega a^\dagger a + \frac{\epsilon}{2} \sigma_z + g(a^\dagger \sigma^- + a \sigma^+)$$

An initial state with atom excitation, $|\sigma_z = \frac{1}{2}, n=0\rangle$, may appear to decay to $|\sigma_z = \frac{1}{2}, n=1\rangle$ but actually coherently oscillates back to the initial state. This cannot be represented by a Markovian EOM for the atom alone, i.e. $\frac{d}{dt} \rho_{\text{atom}} = G \rho_{\text{atom}}$ will not work.

Heuristic discussion:

Under what circumstances may the Markovian description of an open quantum system be appropriate?

I. "Big" environment

To avoid memory effects, the presence of the system should not significantly alter the state of the environment. In a somewhat vague sense, the environment must be "big" and involve a "large" number of degrees of freedom.

Think of a single particle with kinetic energy $E_{\text{kin}} \ll k_B T$, which is brought into contact with a bath containing a large number of particles in a thermal state. Due to collisions, the particle will thermalize, hardly changing the state of the particle bath.

Note: For the last statement to hold, indeed a large number $N \gg 1$ of particles is needed. If we want Poincaré recurrence times to be infinite, we need an infinite number $N \rightarrow \infty$.

However, even an infinite number of degrees of freedom may not always be big enough.

Think of a two-level system coupled to a resonator, e.g., a transmission line resonator of length L . The resonator has an infinite number of modes with eigenfrequencies $\omega_n = \frac{c\pi}{L} \cdot n$ ($n=1,2,3,\dots$), so it could seem that the resonator would act like a good, "large" environment. This is not so: once the atom relaxes radiatively, a photonic wavepacket forms and travels to the far end of the resonator. There it gets reflected and may indeed act back on the two-level system. When viewing the two-level system as an open quantum system, this situation would certainly involve non-Markovian memory effects. The only way out is to take the limit $L \rightarrow \infty$, in which case the wavepacket will never be reflected and the resonator modes form a continuum.



2. The Environment "measures"

Closely connected to the assumption of a "large" bath in a state ρ_E that is not altered by the system is the expectation that no entanglement builds up between the system and the bath. Many derivations of the master equation will hence claim that

$$\rho_{\text{total}}(t) \approx \rho_s(t) \otimes \rho_E,$$

i.e. the change of ρ_E due to the system is neglected and the overall density matrix is, approximately, a product state.

Note: this assumption does not hold at all for the above example of radiative decay into a long (or even semi-infinite) transmission line: the bath states before and after the decay are clearly orthogonal.

Moreover, we expect there to be entanglement unless the bath itself is an open system, or "effectively performs a measurement on the system." (The last phrase, of course, contains the entire measurement problem and continues to fail explaining what makes a physical process a measurement.)

3. Separation of Time Scales

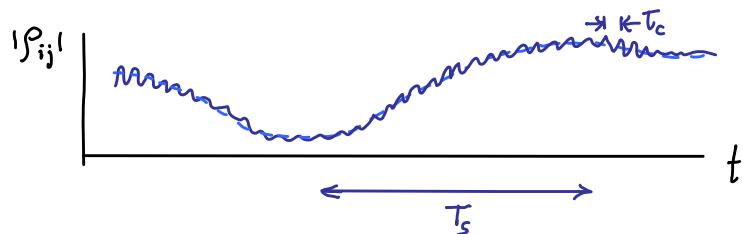
Even when working under the assumption that $\rho_{\text{total}} \approx \rho_s(t) \otimes \rho_E$, we must always admit system-bath correlations on a short time scale τ_c , the correlation time. τ_c is often described loosely as the time period over which the bath "forgets" that it ever interacted with the system. More rigorously, this can be quantified with the decay of bath correlation functions such as $\langle B(t')B^+(t) \rangle \sim e^{-(t'-t)/\tau_c}$. In the example of a semi-infinite TLS and resonator, τ_c can be viewed as the time period necessary for the wavepacket to exit the interaction region close to the TLS.

The formulation of the master equation is then based upon the separation of time scales $\tau_c \ll T_s$, where T_s is the typical

time scale for the evolution of the system. This inequality allows for coarse graining in time,

$$\tau_c \ll \Delta t \ll T_s,$$

and the master equation will give an appropriate model at the time scale Δt but will not capture the much more rapid dynamics at the time scale τ_c .



Note: a detailed verification of the validity of the three described conditions must necessarily be based on a full microscopic model of the environment and its coupling to the system of interest. Such microscopic derivations of the master equation are oftentimes difficult, very specific to a particular system — and, unfortunately not always fully convincing. Moreover, in many cases of interest both the precise nature of the environment and its coupling to the system are not known. In such cases, the Markovian description serves as an invaluable starting point for modeling — the validity of which is ultimately established by successful comparison of theoretical predictions with experimental data.*

Lindblad Master Equation

Keeping in mind the above conditions, we now derive the general form for the Markovian evolution of the reduced density matrix ρ_s . Excluding possible memory effects and using coarse graining of times as described above, we start from the ansatz

$$\frac{d}{dt} \rho_s \simeq \frac{\rho_s(t + \Delta t) - \rho_s(t)}{\Delta t} = \frac{\mathcal{L}_{\Delta t}(\rho_s(t)) - \rho_s(t)}{\Delta t}$$

where the superoperator $\mathcal{L}_{\Delta t}$ maps $\rho_s(t)$ to the reduced density matrix at the

* Such logic has, of course, to be taken with a grain of salt, if we want to keep an open mind about the possibility that experiments could one day signal deviations from standard QM.

later time $(t + \Delta t)$. (Within the terminology of generalized measurements, $\mathbb{L}_{\Delta t}$ is an "operation.") Now, Kraus's representation theorem states that there are operators $\{M_\mu\}_{\mu=1,2,\dots}$ with $\sum_r M_r^\dagger M_r = \mathbb{1}$ such that

$$\mathbb{L}_{\Delta t} \rho_s = \sum_\mu M_\mu \rho_s M_\mu^\dagger = \rho_s + \Delta t \cdot \delta \rho_s + \mathcal{O}(\Delta t^2).$$

One or several of the terms in the Kraus sum must thus be close to the identity. If there are several such terms, we can always use a unitary transformation on the $\{M_\mu\}$ to transfer all weight $\sim \mathbb{1}$ to a single measurement operator, say, M_1 , such that

$$M_1 \rho_s M_1^\dagger = \rho_s + \Delta t \delta \rho_{s,1} + \mathcal{O}(\Delta t^2).$$

Expanding M_1 in orders of Δt , we thus have

$$M_1 = \mathbb{1} - iK\Delta t + \mathcal{O}(\Delta t^2).$$

Here, the second term has been written in this form for later convenience, and K does not depend on Δt (but, possibly, on t). Decompose K into two parts,

$$H = \hbar(K + K^\dagger)/2 \quad \text{and} \quad J = i(K - K^\dagger)/2$$

where $H = H^\dagger$ and $J = J^\dagger$ (made hermitian by factor of "i")

$$\therefore K = H/\hbar - iJ.$$

With this, the Kraus terms for $\mu=1$ can be written as:

$$\begin{aligned} M_1 \rho_s M_1^\dagger &= (\mathbb{1} - iK\Delta t) \rho_s (\mathbb{1} + iK^\dagger \Delta t) + \mathcal{O}(\Delta t^2) \\ &= \rho_s - iK\Delta t \rho_s + i\rho_s K^\dagger \Delta t + \mathcal{O}(\Delta t^2) \\ &= \rho_s - \frac{i\Delta t}{\hbar} [H, \rho_s] - \Delta t (J \rho_s + \rho_s J) \end{aligned}$$

All remaining terms $\sum_{\mu>1} M_\mu \rho_s M_\mu^\dagger = \Delta t \delta \rho_s'$ lead to

$$M_\mu = \sqrt{\Delta t} L_\mu + \mathcal{O}(\Delta t^{3/2}) \quad (\mu > 1)$$

where L_μ is independent of Δt .

From the completeness condition, we infer that

$$\begin{aligned}
 \mathbb{1} &\stackrel{!}{=} \sum_{\mu} M_{\mu}^+ M_{\mu} = M_1^+ M_1 + \sum_{\mu>1} M_{\mu}^+ M_{\mu} \\
 &= (\mathbb{1} + iK^+ \Delta t - iK \Delta t) + \sum_{\mu>1} \Delta t L_{\mu}^+ L_{\mu} + O(\Delta t^2) \\
 &= \mathbb{1} - 2J \Delta t + \sum_{\mu>1} \Delta t L_{\mu}^+ L_{\mu} + O(\Delta t^2) \\
 \therefore J &= \frac{1}{2} \sum_{\mu>1} L_{\mu}^+ L_{\mu}
 \end{aligned}$$

Overall:

Lindblad Master Equation in Standard Form

$$\frac{d}{dt} \rho_s = \frac{1}{\Delta t} \left(\sum_{\mu} M_{\mu} \rho_s M_{\mu}^+ - \rho_s \right) = \underbrace{-\frac{i}{\hbar} [H, \rho_s]}_{\text{Liouvillian term}} + \underbrace{\sum_{\mu>1} (L_{\mu} \rho_s L_{\mu}^+ - \frac{1}{2} \rho_s L_{\mu}^+ L_{\mu} - \frac{1}{2} L_{\mu}^+ L_{\mu} \rho_s)}_{\substack{\equiv \sum_{\mu>1} \mathbb{D}[L_{\mu}] \rho_s \\ \text{"damping terms"}}} \\
 H: \text{System Hamiltonian} \\
 \text{(plus Lamb shift)}$$

Here, the Lindblad damping superoperator \mathbb{D} is defined as:

$$\mathbb{D}[L] \rho \equiv L \rho L^+ - \frac{1}{2} (L^+ L \rho + \rho L^+ L).$$

Sometimes, L is referred to as a "Lindblad operator" or a "jump operator."

How can we interpret the Lindblad master equation?

One instructive way to interpret the master equation above is to employ an "environment simulator." This simulator is based on the insight that the effect of any operation

$$\rho \rightarrow \rho' = \Phi(\rho) = \sum_{k=1}^{N_k} M_k \rho M_k^+$$

can always be mimicked by entangling the system with an auxiliary system of dimension $\dim \mathcal{H}_E \leq N_k$ and performing an appropriate

measurement on \mathcal{H}_E . Specifically, in the case described by the $\{M_\mu\}$ above ($1 \leq \mu \leq N$), consider a Hilbert space \mathcal{H}_E with orthonormal basis $\{|1_E\rangle, |2_E\rangle, \dots, |N_E\rangle\}$.

Define a unitary map U_{SE} on $\mathcal{H}_S \otimes \mathcal{H}_E$ with the property

$$\begin{aligned} U_{SE} |\psi_s, 1_E\rangle &= M_1 |\psi_s\rangle \otimes |1_E\rangle + \sum_{\mu \geq 1} M_\mu |\psi_s\rangle \otimes |\mu_E\rangle \\ &= \left(\mathbb{1} - \frac{i}{\hbar} (H\Delta t - J\Delta t) \right) |\psi_s\rangle \otimes |1_E\rangle + \sum_{\mu \geq 1} \sqrt{\Delta t} L_\mu |\psi_s\rangle \otimes |\mu_E\rangle. \end{aligned}$$

Note: U_{SE} is not fully defined by this relation. For consistency, we should check that U_{SE} as given does not alter the norm of states, i.e.,

$$\|U_{SE} |\psi_s\rangle \otimes |1_E\rangle\|^2 = \langle \psi_s | M_1^\dagger M_1 | \psi_s \rangle + \sum_{\mu \geq 1} \langle \psi_s | M_\mu^\dagger M_\mu | \psi_s \rangle = 1$$

since $\sum_\mu M_\mu^\dagger M_\mu = \mathbb{1}$ and $\langle \psi_s | \psi_s \rangle = 1$.

Finally, perform a measurement in \mathcal{H}_E with an observable of the form

$$A_E = \sum_\mu a_\mu |\mu_E\rangle \langle \mu_E| \quad \text{with non-degenerate spectrum.}$$

Then, the unconditional post-measurement state obtained from $U_{SE} |\psi_s\rangle \otimes |1_E\rangle$ is:

$$\begin{aligned} \tilde{\rho} &= \sum_\mu |\mu_E\rangle \langle \mu_E| (U_{SE} |\psi_s, 1_E\rangle \langle \psi_s, 1_E| U_{SE}^\dagger) |\mu_E\rangle \langle \mu_E| \\ &= |1_E\rangle \langle 1_E| \left(\mathbb{1} - \frac{i}{\hbar} (H\Delta t - J\Delta t) \right) |\psi_s\rangle \langle \psi_s| \left(\mathbb{1} + \frac{i}{\hbar} (H\Delta t - J\Delta t) \right) |1_E\rangle \langle 1_E| \\ &\quad + \sum_{\mu \geq 1} |\mu_E\rangle \langle \mu_E| (\Delta t L_\mu |\psi_s\rangle \langle \psi_s| L_\mu^\dagger) |\mu_E\rangle \langle \mu_E| + O(\Delta t^2) \\ &= |1_E\rangle \langle 1_E| \left(\rho_s - \frac{i\Delta t}{\hbar} [H, \rho_s] - \Delta t (J\rho_s + \rho_s J) \right) |1_E\rangle \langle 1_E| + \sum_{\mu \geq 1} |\mu_E\rangle \langle \mu_E| \Delta t L_\mu \rho_s L_\mu^\dagger |\mu_E\rangle \langle \mu_E| + O(\Delta t^2) \end{aligned}$$

$$\Rightarrow \text{tr}_E \tilde{\rho} = \sum_\mu M_\mu \rho_s M_\mu^\dagger.$$

In other words: the time evolution of ρ_s under the operation

$$\rho_s \mapsto \Phi_{\Delta t}(\rho_s) = \sum_\mu M_\mu \rho_s M_\mu^\dagger$$

can be simulated by coupling the system

to a finite dimensional auxiliary system, entangling the two systems via \mathcal{U}_{SE} and performing an "unread" measurement on B .

For the study of quantum trajectories in chapter 3, it is useful to note the slightly different situation where the measurement on B is read out. In this case, we work with the conditional post-measurement states obtained from $\rho = |\psi_s, l_E\rangle\langle\psi_s, l_E|$:

measurement result	conditional post-measurement state
a_1	$\rho_1 = \frac{M_1 \psi_s\rangle\langle\psi_s M_1^\dagger}{\text{tr}_s(\psi_s\rangle\langle\psi_s M_1^\dagger M_1)} \otimes l_E\rangle\langle l_E = \phi_s\rangle\langle\phi_s \otimes l_E\rangle\langle l_E $ <p>with $\phi_s\rangle = \frac{1}{\sqrt{P_1}} M_1 \psi_s\rangle = \frac{1}{\sqrt{P_1}} (1 - \frac{i}{\hbar} H \Delta t - J \Delta t) \psi_s\rangle$</p> <p>and probability p_1 given by:</p> $p_1 = \text{tr}_s(\psi_s\rangle\langle\psi_s M_1^\dagger M_1) = \langle\psi_s M_1^\dagger M_1 \psi_s\rangle$ $= 1 - \sum_{\mu>1} \langle\psi_s M_\mu^\dagger M_\mu \psi_s\rangle = 1 - \Delta t \sum_{\mu>1} \langle\psi_s L_\mu^\dagger L_\mu \psi_s\rangle \sim \Theta(1)$
$a_\mu (\mu>1)$	$\rho_\mu = \frac{M_\mu \psi_s\rangle\langle\psi_s M_\mu^\dagger}{P_\mu} \otimes l_E\rangle\langle l_E = \chi_{\mu s}\rangle\langle\chi_{\mu s} \otimes l_E\rangle\langle l_E $ <p>with $\chi_{\mu s}\rangle = \frac{1}{\sqrt{P_\mu}} M_\mu \psi_s\rangle = \frac{1}{\sqrt{P_\mu}} = \frac{\sqrt{\Delta t}}{\sqrt{P_\mu}} L_\mu \psi_s\rangle$</p> <p>and probability $p_\mu = \langle\psi_s M_\mu^\dagger M_\mu \psi_s\rangle = \Delta t \langle\psi_s L_\mu^\dagger L_\mu \psi_s\rangle \sim \Theta(\Delta t)$</p>

Thus, if the measurement on E is read out, a pure system state $|\psi_s\rangle$ is mapped to another pure system state:

$$|\psi_s\rangle \xrightarrow{P_1 \sim \Theta(1)} \frac{1}{\sqrt{P_1}} \left(1 - \frac{i}{\hbar} H \Delta t - J \Delta t\right) |\psi_s\rangle$$

close to $|\psi_s\rangle$ for small Δt , non-unitary

$$|\psi_s\rangle \xrightarrow{P_\mu \sim \Theta(\Delta t)} \frac{1}{\sqrt{P_\mu/\Delta t}} L_\mu |\psi_s\rangle \quad \text{"jump" to new state}$$

Note that the state obtained when the measurement outcome is a_i , results from evolution under a non-hermitian "Hamiltonian"

$$H_{nh} = H - i\hbar J$$

We will see in chap. 3 how these statements convert into the quantum trajectory framework describing stochastic dynamics in Hilbert space.

Lindblad operators are not unique:

Consider a master equation

$$\frac{d}{dt}\rho_s = -\frac{i}{\hbar}[H, \rho_s] + \sum_{\mu} D[L_{\mu}]\rho_s .$$

Then, the following two transformations leave the master equation invariant:

1. unitary transformations among the Lindblad operators:

$$L_{\mu} \rightarrow L'_{\mu} = \sum_{\nu} u_{\mu\nu} L_{\nu} \quad \text{for } (u_{\mu\nu}) \text{ unitary},$$

2. inhomogeneous transformations of the type

$$L_{\mu} \rightarrow L'_{\mu} = L_{\mu} + c_{\mu} \quad (c_{\mu} \in \mathbb{C})$$

$$H \rightarrow H' = H + \frac{\hbar}{2i} \sum_{\mu} (c_{\mu}^* L_{\mu} - c_{\mu} L_{\mu}^+) + b \quad (b \in \mathbb{R})$$

Proof:

- 1: The suggested unitary transformation only affects the damping terms of the Master equation.

$$\begin{aligned} \sum_{\mu} D[L'_{\mu}]\rho &= \sum_{\mu} \left[L'_{\mu} \rho L'_{\mu}^+ - \frac{1}{2} L'_{\mu}^+ L'_{\mu} \rho - \frac{1}{2} \rho L'_{\mu} L'_{\mu}^+ \right] \\ &= \sum_{\mu, \nu, \lambda} u_{\mu\nu} u_{\mu\lambda}^* \left(L_{\nu} \rho L_{\lambda}^+ - \frac{1}{2} L_{\nu}^+ L_{\lambda} \rho - \frac{1}{2} \rho L_{\nu} L_{\lambda}^+ \right) \\ &= \sum_{\nu} \left(L_{\nu} \rho L_{\nu}^+ - \frac{1}{2} L_{\nu}^+ L_{\nu} \rho - \frac{1}{2} \rho L_{\nu} L_{\nu}^+ \right) = \sum_{\nu} D[L_{\nu}]\rho \end{aligned}$$

summation
on μ gives
 $\delta_{\nu\lambda}$

2: Consider the right-hand side of the master equation:

$$\begin{aligned}
 -\frac{i}{\hbar} [H', \rho] + \sum_{\mu} \mathbb{D}[L'_{\mu}] \rho &= -\frac{i}{\hbar} \left[H + \frac{\hbar}{2i} \sum_{\mu} (c_{\mu}^* L_{\mu} - c_{\mu} L_{\mu}^+) + b, \rho \right] + \sum_{\mu} \mathbb{D}[L_{\mu} + c_{\mu}] \rho \\
 &= -\frac{i}{\hbar} [H, \rho] - \frac{1}{2} \sum_{\mu} [c_{\mu}^* L_{\mu} - c_{\mu} L_{\mu}^+, \rho] \\
 &\quad + \sum_{\mu} \left\{ (L_{\mu} + c_{\mu}) \rho (L_{\mu}^+ + c_{\mu}^*) - \frac{1}{2} (L_{\mu}^+ + c_{\mu}^*) (L_{\mu} + c_{\mu}) \rho - \frac{1}{2} \rho (L_{\mu}^+ + c_{\mu}^*) (L_{\mu} + c_{\mu}) \right\} \\
 &= -\frac{i}{\hbar} [H, \rho] - \frac{1}{2} \sum_{\mu} [c_{\mu}^* L_{\mu} - c_{\mu} L_{\mu}^+, \rho] + \sum_{\mu} \mathbb{D}[L_{\mu}] \rho \\
 &\quad + \rho c_{\mu} L_{\mu}^+ + c_{\mu}^* L_{\mu} \rho - \frac{1}{2} c_{\mu} L_{\mu}^+ \rho - \frac{1}{2} c_{\mu}^* L_{\mu} \rho - \frac{1}{2} \rho c_{\mu} L_{\mu}^+ - \frac{1}{2} \rho c_{\mu}^* L_{\mu} \\
 &= -\frac{i}{\hbar} [H, \rho] + \sum_{\mu} \mathbb{D}[L_{\mu}] \rho
 \end{aligned}$$

Note:

- Due to the invariance under the inhomogeneous transformations of the second type, we can always choose finite dimensional Lindblad operators to be traceless by letting $c_{\mu} = -\frac{1}{N} \text{tr } L_{\mu}$ so that $\text{tr } L'_{\mu} = \text{tr } (L_{\mu} + c_{\mu}) = \text{tr } L_{\mu} - \frac{\text{tr } L_{\mu}}{N} \text{tr } \mathbb{1} = 0$. This does not work if $\text{tr } L_{\mu} = \infty$, as is the case for $L_{\mu} = a^* a$, for example.

- When writing the damping terms as $\frac{d}{dt} \rho = \dots + \sum_{\mu} \mathbb{D}[L_{\mu}] \rho$, each operator L_{μ} must carry dimension of $1/\sqrt{\text{time}}$. Rescaling $L_{\mu} = c_{\mu} L'_{\mu}$ with $c_{\mu} \in \mathbb{C}$ and dimension $1/\sqrt{\text{time}}$, we obtain dimensionless operators L'_{μ} . In terms of these new operators, the damping terms read

$$\sum_{\mu} \mathbb{D}[L_{\mu}] \rho = \sum_{\mu} \underbrace{|c_{\mu}|^2}_{\in \mathbb{R}^+} \mathbb{D}[L'_{\mu}] \rho$$

Where $|c_{\mu}|^2$ can be interpreted as a rate. In the examples we will encounter in chapter 2, we will see that $|c_{\mu}|$ assumes the roles of relaxation rate or rate of pure dephasing, for instance.