Quantum Noise and Decoherence

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Abstract

Introductory courses on quantum mechanics usually present free particles and other closed systems but no composite systems. The goal here is to introduce quantum mechanics of many systems, explore why measuring disturbs the observed system, and figure out where the classical limit in the everyday life comes from. Quantum noise and decoherence play an important role. Tobias Osborne from the Leibniz Universität Hanover gave a series of 13 lectures covering this topic in 2015. His lectures were available on YouTube at the time this transcript has been assembled and may as "Theory of Quantum Noise and Decoherence" still be available today.

1 Introduction to Quantum Mechanics

1.1 Composite Quantum Systems and Measurements

Quantum mechanics goes beyond free particles and closed systems and also covers composite system with many subsystems. In contrast to classical physics one cannot copy quantum information due to the no-cloning theorem. Thus, if one wants to gain information about some closed quantum system, one has to interact with it and this will unavoidably have some effect on the system. The act of measuring disturbs the system. In everyday classical physics one also encounters such effects. Gaining information from the stock market and acting on it, for example, will cause disturbances as other traders react on this action. Also the observer effect in social psychology shows this phenomenon when the participants of an experiment know that they are observed and therefore behave differently. In quantum mechanics, however, is the fact that the measurement disturbs the system fundamental.

When one looks at a quantum system with the eyes as the everyday apparatus for measurements, the system looks classical. Thus, the question is where does the classical limit come from. The reason, as will turn out, is quantum noise and decoherence which are a consequence of the measuring process and the fact that this process disturbs the system.

1.2 Kinematics of Isolated Quantum Systems

Physical experiments are interpreted here as consisting of two steps where preparation is followed by measurement. In classical physics there is never a real need to discuss measurement because one can copy information freely. In quantum mechanics the measurement always disturbs the system as mentioned above. Preparation consists of all steps performed to bring the system in a certain state. In more detail, preparation is the set of actions that determines all probability distributions of any possible measurement. Different preparations can lead to identical probability distributions. A state describes all the details (and no more) relevant for subsequent measurements, or, in other words, a state is the data sufficient to describe the probability distributions of all subsequent measurements.

Quantum mechanics is an example of a statistical theory meaning that one can only at best describe probability distributions of possible outcomes of measurements. It is therefore not a deterministic theory leading to many philosophical question which, however, will be ignored here. Mathematically the division of preparation and measurement is represented as observables which are more fundamental than states where *observables* are hermitian elements of the observable algebra \mathcal{A} (here in form of $n \times n$ matrices). A \mathbb{C} algebra is a closed set under addition and multiplication as well as multiplication by scalars (elements of \mathbb{C}). Each element $A \in \mathcal{A}$ has an adjoint A^{\dagger} . An element $E \in \mathcal{A}$ is *positive* if there is a $X \in \mathcal{A}$ such that $E = X^{\dagger}X$. Here \mathcal{A} will always be the bounded operators on some Hilbert space \mathfrak{H} . The set of these bounded operators is written as $\mathcal{B}(\mathfrak{H})$. The simplest example (apart from the trivial system) is the qubit where the set of all observables \mathcal{A}_{h} is

$$\mathcal{A}_{\mathrm{h}} \subset \mathcal{A} \cong \mathsf{M}_{2}(\mathbb{C}) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \middle| a, b, c, d \in \mathbb{C} \right\} \qquad \qquad \mathcal{A}_{\mathrm{h}} \equiv \left\{ X \in \mathcal{A} \middle| X^{\dagger} = X \right\}$$
(1.1)

and is called the set of hermitian 2×2 matrices.

Observables are an idealization while in an experiment one has some detector such as a photon counter making click. One can break down any detector in a sequence of click or no click objects. The voltage on a wire looks like a continuous signal but can also be seen as a sequence of clicks averaged over time bins. Therefore, here all detections are considered clicks.

Further, measurements themselves (not observables) are described by assigning to each outcome of a device an effect $E \in \mathcal{A}$ which satisfies

$$0 \le E \le \mathbb{I} \tag{1.2}$$

where $A \leq B$ holds if and only if B - A is positive defined above as $B - A = X^{\dagger}X$ for some X in \mathcal{A} . An example is the photon counter where $E = |0\rangle \langle 0|$ corresponds to no click and consequently $F = \mathbb{I} - E = \mathbb{I} - |0\rangle \langle 0|$ corresponds to some clicks. That is how measurements are described. There is a box doing the measurement which delivers classical information such as there was a click or there was no click. To each possible outcome an effect is assigned. The outcome is not always deterministic.

A state ω on \mathcal{A} is a positive normalized linear functional on \mathcal{A} . That is

$$\omega: \mathcal{A} \to \mathbb{C} \text{ is linear} \qquad \qquad \omega(X^{\dagger}X) \ge 0 \qquad \qquad \omega(\mathbb{I}) = 1 \qquad (1.3)$$

because states are supposed to assign probabilities to outcomes. Thus, an ω has to eat measurements and give probabilities. One can do no experiment at all, and the effect is I satisfying (1.2). The emphasis here is to the minimal structure, and describing states with Hilbert spaces gives only a subset of states. The missing states are the *mixed* states. In the real world there are no closed systems but there is noise and other imperfections leading to those mixed states.

If there is a detector that clicks then the question is what the empiric probability is that one measures a click. The *probability* of outcome E measured on a state ω is defined as

$$P(E) = \omega(E) \tag{1.4}$$

where $\omega(E)$ is usually written as $\langle E \rangle$ in quantum mechanics.

If somebody demands to measure the observable A then one has to design an apparatus which assigns an effect E for every possible outcome of the observable A. Thus, observables have to be linked to effects. One labels the outcomes of an experiment corresponding to an observable $A \in \mathcal{A}$ by an index α where α can be continuous. One assigns to each α an effect E_{α} so that the probability P_{α} of the outcome corresponding to α is $P_{\alpha} \equiv \omega(E_{\alpha})$. To ensure $\sum_{\alpha} P_{\alpha} = 1$ it is required that $\sum_{\alpha} E_{\alpha} = \mathbb{I}$. (The use of the sum for continuous α is not correct but most cases in the following will use finite indices α .)

A collection $\{E_{\alpha}\}_{\alpha}$ of effects such that $\sum_{\alpha} E_{\alpha} = \mathbb{I}$ is called POVM (positive operator-valued measure). The precise connection between observable A and effect E_{α} is via

$$A = \sum_{\alpha} a_{\alpha} E_{\alpha} \tag{1.5}$$

which is the eigenvalue-eigenvector decomposition with the eigenvalues a_{α} and the spectral projection E_{α} . Every observable gives rise to a POVM, but not every POVM comes from an observable. It is a more general concept. This is a case where this extra generality is very useful, for example, as for homodyne and heterodyne detection in quantum optics.

For finite-dimensional systems such as qubits one can always represent states $\omega : \mathcal{A} \to \mathbb{C}$ as *density* operators via

$$\omega(A) = \operatorname{tr}(\rho A) \tag{1.6}$$

where the density operator ρ satisfies $\operatorname{tr}(\rho) = 1$ and $\rho \geq 0$ due to (1.3). A state is *pure* if it cannot be written as $\omega = (1-\rho)\omega' + \rho\omega''$ with $0 < \rho < 1$ and $\omega' \neq \omega''$. For finite-dimensional systems one can prove that this definition implies that a density operator corresponds to a pure state if and only if the density operator is a projection. This gives the connection to the Hilbert space. However, this is not true for all infinite-dimensional systems because $\omega(A) = \operatorname{tr}(\rho A)$ cannot be used when the trace becomes infinity. Thus, the representation (1.3) is always valid while the representation with the density operator (1.6) is especially useful for finite-dimensional systems.

For finite-dimensional quantum systems ω is pure if and only if one can write $\omega(\cdot) \equiv \operatorname{tr}(\rho \cdot)$ with the density operator being a projection $\rho = |\psi\rangle \langle \psi|$ where $|\psi\rangle \in \mathfrak{H}$. Rays in Hilbert spaces are another way of talking about projections but $|\psi\rangle \langle \psi|$ is a more elegant way to say that a phase cancels.

For the qubit as an example all states ω may be represented by 2×2 matrices satisfying $\rho \ge 0$ and $tr(\rho) = 1$

$$\rho = \frac{1}{2} \begin{pmatrix} 1+x_3 & x_1 - ix_2 \\ x_1 + ix_2 & 1-x_3 \end{pmatrix}$$

with $\underline{x} \in \mathbb{R}^3$. The condition $\operatorname{tr}(\rho) = 1$ is obviously fulfilled, and the condition $\rho \geq 0$ requires $|\underline{x}|^2 \leq 1$ because the eigenvalues of this matrix are $\lambda_{1,2} = 1 \pm \sqrt{x_1^2 + x_2^2 + x_3^2}$. Thus, $\underline{x} = (x_1, x_2, x_3)$ is an element of a ball with radius 1 in \mathbb{R}^3 called the Bloch sphere. This is a very significant result because the abstract constraint $\rho \geq 0$ is translated to something geometrical. Every qubit state corresponds to a point in the Bloch sphere, and every point in the Bloch sphere corresponds to a qubit state. Measurements on these states all have a geometrical interpretation. (However, there is no nice geometrical representation for qutrits.) Considering the effect of the spin pointing up

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2} (\mathbb{I} + \sigma^z)$$

where σ^z is the third of the Pauli matrices

$$\sigma^{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \qquad \sigma^{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \qquad \sigma^{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.7}$$

the probability is $P(E) = \frac{1}{2}(1+x_3)$ according to (1.4) and (1.6). One can find this number also from the Bloch sphere.

Another more general way to calculate the probability is by looking at pure states. A necessary but not sufficient condition for a pure state is $\rho^2 = \rho$. Thus, trace of ρ and trace of ρ^2 must be 1 leading to

$$\left(\frac{\mathbb{I} + \underline{r} \cdot \underline{\sigma}}{2}\right)^2 = \left(\frac{\mathbb{I} + \underline{r} \cdot \underline{\sigma}}{2}\right)$$

where $\underline{r} \in \mathbb{R}$. The left side of this equation has 16 terms and the right side 4. The result for these equations is |r| = 1. This means that the pure states in the graphical representation are the points on the surface of the Bloch sphere. Because $\operatorname{tr}(\rho)$ is a linear functional on the algebra, convex combinations of the states correspond exactly to convex combinations in the Bloch sphere. The points on the boundary are the points one cannot write as a convex combination of two other points. One can do these calculation for other dimensions but one gets a horrible disgusting surface.

1.3 Kinematics of Composite Quantum Systems

So far only isolated quantum systems have been described as illustrated in the figure on the right side with two connected steps. The preparation step is the object on the left where ω is a positive linear functional on \mathcal{A} and the measurement step is the object on the right where E is a positive element of \mathcal{A} .



The question is how to put them together to get composite systems such as the one shown on the right side. In other words, the question is what mathematical objects represent joint measurements on more than one quantum system. The observable algebra for a quantum system AB combining the two quantum systems A and B with observable algebra \mathcal{A} and \mathcal{B} , respectively, is the tensor product $\mathcal{A} \otimes \mathcal{B}$. The effect $E \otimes F$ in $\mathcal{A} \otimes \mathcal{B}$ means that E and F both occur.



Two qubits A and B as an example have each the 2×2 matrices as their observables. Thus, $\mathcal{A} \cong M_2(\mathbb{C})$, $\mathcal{B} \cong \mathsf{M}_2(\mathbb{C})$, and $\mathcal{A} \otimes \mathcal{B} \cong \mathsf{M}_2(\mathbb{C}) \otimes \mathsf{M}_2(\mathbb{C}) \cong \mathsf{M}_4(\mathbb{C})$, and the combined system of two systems with two possible outcomes is a single isolated system with four possible outcomes. When talking about subsystems one attaches a kind of locality structure to the questions one can ask. As soon as one zooms out one can see the combined subsystems as one single system. However, not all $M \in \mathcal{A} \otimes \mathcal{B}$ are of the form $E \otimes F$. The fact that not all yes-no questions one can ask about the combined system are of the form $E \otimes F$ has a kind of dual structure on the states, and this phenomenon is called quantum entanglement.

The states of a composite system combining A and B with algebras \mathcal{A} and \mathcal{B} are defined as

$$\omega: \mathcal{A} \otimes \mathcal{B} \to \mathbb{C} \text{ is linear} \qquad \qquad \omega(X^{\dagger}X) \ge 0 \qquad \qquad \omega(\mathbb{I} \otimes \mathbb{I}) = 1 \qquad (1.8)$$

similar to (1.3). If there is an underlying Hilbert space $\mathfrak{H} \equiv \mathfrak{H}_{A} \otimes \mathfrak{H}_{B}$ there is a simple set of states on $\mathcal{A} \otimes \mathcal{B}$ called product states coming from $|\phi_{A}\rangle \otimes |\phi_{B}\rangle$ where $|\phi_{A}\rangle \in \mathfrak{H}_{A}$ and $|\phi_{B}\rangle \in \mathfrak{H}_{B}$. However, there are more states than only product states, and these additional states are called *entangled* states. The fact that there are entangled states leads to the dramatic effects of quantum noise. Thus, the fact that there is superposition in products is the reason why there is decoherence. There is entanglement fighting with entanglement because noise comes from non-product states within the environment and the way quantum computers work comes from non-product states within a quantum system. Product states ω of the composite system AB are of the form

$$\omega(X \otimes Y) = \omega_{\mathcal{A}}(X)\,\omega_{\mathcal{B}}(Y) \qquad \forall X \in \mathcal{A} \quad \forall Y \in \mathcal{B}$$
(1.9)

where pure product states have density operators $\rho = |\phi_A\rangle \langle \phi_A| \otimes |\phi_B\rangle \langle \phi_B| = \rho_A \otimes \rho_B$. States which are not products are *correlated*. Note that there are mixed states which cannot be written as a product but are not entangled.

As an example, the state $\rho = p |00\rangle \langle 00| + (1-p) |11\rangle \langle 11|$ of two qubits with $0 \le p \le 1$ ensures that both qubits are 0 with probability p or both qubits are 1 with probability 1 - p. This represents a correlated pair of coins. This is a classically correlated state and does not involve entanglement. Thus, a product at the level $\rho_{\rm A} \otimes \rho_{\rm B}$ is not the same as a product at the level $|\phi_{\rm A}\rangle \otimes |\phi_{\rm B}\rangle$.



There should be a legal state ω_{AE} of the subsystem A assuming a big quantum system E where one would like to look only at part A of it as in the figure on the left. That might be, for example, the local quantum state in a lab ignoring the rest of the universe. The state ω_{AE} when reduced to observables which are non-trivial only on A is of the form $X \otimes \mathbb{I}_{E}$. The corresponding state

$$\omega_{\rm A}(X_{\rm A}) = \omega_{\rm AE}(X_{\rm A} \otimes \mathbb{I}_{\rm E}) \tag{1.10}$$

is called a *reduced* state, and for density operators ρ_A for ω_A is defined via

$$tr(\rho_{A}X) = \omega_{A}(X \otimes \mathbb{I}_{E}) = tr(\rho_{AE}X_{A} \otimes \mathbb{I}_{E})$$

$$\rho_{A} = tr_{E}(\rho_{AE})$$

$$tr_{E} : \rho_{AE} \to \rho_{A} = \sum_{j} (\mathbb{I}_{A} \otimes |j_{E}\rangle)\rho_{AE}(\mathbb{I}_{A} \otimes |j_{E}\rangle)$$
(1.11)

where $|j_{\rm E}\rangle$ is an orthonormal basis of E. The trace tr_E is called the partial trace, and $\rho_{\rm A}$ is called the reduced density operator or the marginal.

Quantum entanglement and quantum noise are in an abstract sense the same thing. Quantum mechanics allows the existence of pure states of big systems which look mixed (not pure) in any reduced subsystem. That does not have an analog in probability theory because the composite system of two coins, for example, has the pure states head-head, head-tail, tail-head, tail-tail and each of these assign a definite

state to the subsystems. Quantum mechanics on the other hand allows pure states that do not assign a definite state to the subsystems. For quantum noise this means that the overall system can be completely pure at zero temperature evolving in a unitary fashion with no noise whatsoever but nonetheless if one looks only at a part of it the system looks very noisy.

A useful tool here is the Schmidt decomposition which states that for any vector $|\psi\rangle \in \mathfrak{H}_A \otimes \mathfrak{H}_B$ with $d = \min(\dim(\mathfrak{H}_A), \dim(\mathfrak{H}_B))$ there exists an orthonormal basis $\{|e_j\rangle\}_{j=1}^{d_A}$ and $\{|f_j\rangle\}_{j=1}^{d_B}$ of \mathfrak{H}_A and \mathfrak{H}_B , respectively, such that

$$\left|\psi\right\rangle = \sum_{j=1}^{d} \sqrt{p_j} \left|e_j\right\rangle_{\mathcal{A}} \left|f_j\right\rangle_{\mathcal{B}}$$
(1.12)

with $0 \le p_j \le 1$ and $\sum_j p_j = |||\psi\rangle||^2$ where the values $\sqrt{p_j}$ are called Schmidt coefficients. This is a constructive statement because there exists an algorithm to work out this decomposition. Product states are exactly of this form where $p_1 = 1$ and $p_j = 0$ for $j \ne 1$, and the algorithm allows to determine whether a state is a product state or not.

As an example the Schmidt decomposition shows that the superposition of two qubits

$$\left|\psi\right\rangle_{\rm AB} = \frac{1}{2} \left(\left|00\right\rangle + \left|01\right\rangle + \left|10\right\rangle + \left|11\right\rangle\right)_{\rm AB} = \left(\frac{\left|0\right\rangle + \left|1\right\rangle}{\sqrt{2}}\right)_{\rm A} \otimes \left(\frac{\left|0\right\rangle + \left|1\right\rangle}{\sqrt{2}}\right)_{\rm B}$$

is a product state. However, the superposition of two qubits

$$\left|\psi\right\rangle_{\rm AB} = \frac{1}{2} \Big(\left|00\right\rangle + \left|11\right\rangle \Big)_{\rm AB}$$

is an EPR type state and cannot be written as a product state because it is already in the form (1.12) of the Schmidt decomposition.

A state $|\psi\rangle$ of AB is *entangled* if its Schmidt decomposition involves two or more terms. That is very distinct from the notion of correlated state. The question of whether a correlated state is entangled is a hard question and nobody knows the answer. A handy result is, however, that if $|\psi\rangle_{AB}$ is a state of AB with Schmidt decomposition (1.12) then

$$\rho_{\rm A} = \sum_{j=1}^{d} p_j \left| e_j \right\rangle \left\langle e_j \right| \tag{1.13}$$

showing how the reduced state can be worked out from a pure state of a composite system.

1.4 Dynamics of Quantum Systems

The dynamics of a system has to do with time. If one knows how to represent a measurement at time t_0 then the fundamental question is how to represent the same measurement some time $t > t_0$ later. In addition to the preparation step first and the measurement step last an evolution step \mathcal{E} is inserted between these

ω <u>E</u> E

first and the measurement step last an evolution step \mathcal{E} is inserted between these two steps as illustrated in the figure on the right side.

There are two ways to turn this back into a kinematic question. One possibility is to combine the evolution step with the preparation step called the Schrödinger picture such that the new question is how evolution leads to a different effective state ω' , and the other possibility is to combine it with the measurement step called the Heisenberg picture such that the new question is how evolution leads to a measurement of a different effective observable E'. There are also various interaction pictures possible combining different parts of the evolution with preparation and measurement.

The first task is to explore evolution in time for closed systems and reversible dynamics without interactions with the environment. An evolution certainly should neither create nor destroy probabilities but should preserve probability. Evolution also ought to be linear. If one flips a coin, does a different preparation depending on the outcome and subjects that to an evolution, then this should be the same as first evolving the system and then flipping a coin. Thus, evolution is a linear transformation of observables such that $\mathcal{U} : \mathcal{A} \to \mathcal{A}$ and $\mathcal{U}(\mathcal{A}) \in \mathcal{A}$ (Heisenberg picture) or of states such that $\mathcal{U}^* : \mathcal{S}(\mathcal{A}) \to \mathcal{S}(\mathcal{A})$ and $\mathcal{U}^*(\rho) \in \mathcal{S}(\mathcal{A})$ where $\mathcal{S}(\mathcal{A})$ are the states of \mathcal{A} (Schrödinger picture) subject to

$$\operatorname{tr}\left(\rho \,\mathcal{U}(A)\right) = \operatorname{tr}\left(\mathcal{U}^*(\rho) A\right) \qquad \qquad \mathcal{U}(\mathbb{I}) = \mathbb{I} \qquad \qquad \mathcal{U}(X^{\dagger}X) = Y^{\dagger}Y \quad \forall X \in \mathcal{A}$$
(1.14)

in order to ensure that both pictures lead to the same evolution, to preserve probabilities and to evolve effects into effects. The third condition is equivalent with $\mathcal{U}(X^{\dagger}X) \geq 0$. This is the bare minimum an evolution should satisfy.

The closed systems and reversible dynamics are exactly those evolutions that are represented as unitary operators. In the Heisenberg picture this means $\mathcal{U}(A) \equiv U^{\dagger}AU$ for some unitary operator $U \in \mathcal{B}(\mathfrak{H})$ but this is only true for finite-dimensional systems. In infinite dimensions there exist reversible dynamics that might not be representable as unitaties $U \in \mathcal{B}(\mathfrak{H})$. This is an issue with an infinite tensor product of qubits.

If \mathcal{U} depends homogeneously on a parameter $t \in \mathbb{R}$ (called "time") such that $\mathcal{U}_{t+s} \equiv \mathcal{U}_t(\mathcal{U}_s)$ for all $s, t \in \mathbb{R}$ then

$$\frac{d}{dt}U_t = -i H U_t \tag{1.15}$$

where H is the Hamiltonian. This is the Schrödinger equation for the situation in closed systems.



The aim is to study dynamics of composite quantum systems. A system A that may be an atom in some trap is embedded in a bigger system E called the environment. This can model the universe E where A is whatever one can control. One can usually separate an experiment into a part A one can

control and a part E one cannot control. The universe is assumed to undergo reversible evolution \mathcal{U}_t as in the figure on the left side although black holes may turn out to be irreversible. Assuming that the universe is reversible then the question is how does the evolution restricted to A look like, and the answer to the question whether \mathcal{U}_t restricted to A is also reversible is that this is not always the case. That is, for example, how thermodynamical processes work. There is some reservoir E and a closed system A, and then A is opened and starts interacting with the reservoir. The subsystem A can change because particles can flow in, and A' may become completely irreversible.

Open systems are systems that interact with other systems such as the environment. Irreversible dynamics usually occur when one considers only part of a larger system undergoing reversible dynamics. The most general irreversible dynamics allowed by quantum mechanics can be axiomatically characterized in order to define what a legal evolution \mathcal{E} called *channel* in quantum mechanics is. A channel \mathcal{E} converting systems with observable algebra \mathcal{A} to systems with observable algebra \mathcal{B} is a linear operator $\mathcal{E} : \mathcal{B} \to \mathcal{A}$ in the Heisenberg picture (looking as if going in the wrong direction) which is

(i)
$$\mathcal{E}(\mathbb{I}_{\mathcal{B}}) = \mathbb{I}_{\mathcal{A}}$$

(ii) $\forall E \in \mathcal{B} \otimes (M)_n(\mathbb{C}) \text{ and } E \ge 0 \Rightarrow \mathcal{E} \otimes \mathcal{I}_n(E_{\mathcal{A},n}) \ge 0 \ \forall n \in \mathbb{N}$ (1.16)

where \mathcal{I}_n is the identity channel for an *n*-level system. Condition (*i*) requires \mathcal{E} to be unit preserving meaning that probabilities are preserved, and condition (*ii*) defines what completely positive (CP) means.

The figure on the right side shows this situation in the Heisbenberg picture where the channel \mathcal{E} is part of the measurement. Thus, \mathcal{E} better has the property that it takes an observation one can make on \mathcal{B} and gives an observation one can make on \mathcal{A} . Even though times goes from left to right the actual evolution \mathcal{E} maps \mathcal{B} to \mathcal{A} . Therefore (i) requires that \mathcal{E} maps $\mathbb{I}_{\mathcal{B}}$ to $\mathbb{I}_{\mathcal{A}}$.

The explanation for (ii) is that if one adds stuff in and does nothing to them as illustrated in the figure on the right side then that should lead to legal measurements. One does the original measurement completely isolated from the environment. There is another laboratory next door that does not interact with





this experiment at all. This is modeled as in the figure where the experiment is done in one lab and the lab next door does nothing. This may look obvious but there exist channels such as the transpose channel $A \to A^T$ that is unit preserving and takes positive operators to positive operators but is not completely positive. Therefore condition (*ii*) is needed.

The two conditions (i) and (ii) in (1.16) are the bare minimum required for a valid evolution of a quantum system. Unitary operations for closed systems satisfy these requirements. Thus, $\mathcal{E}(X) = U^{\dagger}(X) U$ should be a legal evolution. With $U^{\dagger} \mathbb{I} U = \mathbb{I}$ condition (i) is satisfied, and since the channel $\mathcal{E} \otimes \mathcal{I}(E)$ becomes $(U^{\dagger} \otimes \mathbb{I}_n) E(U \otimes \mathbb{I}_n) = (U^{\dagger} \otimes \mathbb{I}_n) X^{\dagger} X(U \otimes \mathbb{I}_n) = X'^{\dagger} X' \geq 0$ for some X' also (ii) is satisfied.

The axiomatic approach is not the only possibility to characterize valid evolutions and there is an alternate approach to defining the most general dynamical process allowed in quantum mechanics. One can enumerate the allowed operations.

Visualized with the figures on the right side the three possible cases are:

(1) Tensor with system in specific state: $\omega_A \rightarrow \omega_A \otimes \sigma_B \forall \sigma_B$ (Schrödinger picture)

This operation is not resulting from unitary dynamics because there is a state of a smaller system being transformed to a state of a bigger system.

- (2) Unitary transformations: $\mathcal{U}(X) \equiv U X U^{\dagger}$ (Schrödinger picture) This is the case for a closed system in quantum mechanics.
- (3) Reduction to a subsystem: If one has state ω_{AB} on $\mathcal{A} \otimes \mathcal{B}$ then one can build the effective or reduced state ω_A via $\omega_A(X_A) = \omega_{AB}(X_A \otimes \mathbb{I}_B)$

$$(\omega_{A} \xrightarrow{A} \rightarrow (\omega_{AB} \xrightarrow{B} \rightarrow (\omega_{AB} \xrightarrow{B} U \xrightarrow{A} B)$$



unitary evolution can be added in a second step. As a third step – not shown in the figure – a third qubit C might be added adjoined with another unitary evolution only involving B and C in a fourth step. Lastly, one might throw away A by just ignoring it and so on.

The kind of operations one can achieve by combining these three valid evolution steps correspond exactly to the axiomatic approach (1.16). Unfortunately this is only true for finite-dimensional systems but is still a powerful result.

This is the theorem by Stinespring: Let $\mathcal{E} : \mathsf{M}_n(\mathbb{C}) \to \mathsf{M}_m(\mathbb{C})$ be a completely positive map. Then there is an $\ell \in \mathbb{N}$ and an operator $V : \mathbb{C}^m \to \mathbb{C}^n \otimes \mathbb{C}^\ell$ in the Heisenberg picture such that $\mathcal{E}(X) = V^{\dagger}(X \otimes \mathbb{I}_{\ell})V$ and the vectors of the form $(X \otimes \mathbb{I})V |\phi\rangle$ with $|\phi\rangle \in \mathbb{C}^m$ span $\mathbb{C}^n \otimes \mathbb{C}^\ell$. Decomposition is unique up to unitary transformations on \mathbb{C}^ℓ . The operator V is not an unitary but an isometry as it satisfies $V^{\dagger}V = \mathbb{I}$.

An isometry (satisfying $V^{\dagger}V = \mathbb{I}$ but $VV^{\dagger} = \mathbb{I}$ not necessarily) is really just an unitary acting on a bigger space where one ignores part of the bigger space. The isometry V takes some m-dimensional vector to some

m		n		m	n
	V		\cong	0>	

 $n \otimes \ell$, and one can always write that as an unitary U with some input state $|0\rangle$ (assuming that the numbers n, ℓ, m and the dimension of $|0\rangle$ match) as illustrated in the figure on the right.

$$-\mathcal{I}^{\dagger} = \mathbf{U}_{\mathbf{x}}$$

The theorem states that every completely positive map on a finitedimensional system \mathcal{E} can be represented as a unitary. In more detail, every transformation \mathcal{E}^{\dagger} allowed by quantum mechanics described in the

Schrödinger picture can be written as tensoring in an additional system in state zero some unitary operation followed by a reduction to a subsystem as shown in the figure on the left side. The three steps tensoring in a new ancella subsystem in a state $|\phi\rangle$, performing a unitary operation U, and reducing to a subsystem are exactly the three allowed operations listed above. The reduction is shown as the lower outgoing line with a cross.

The theorem is very remarkable. If one demands the bare minimum (1.16) required by quantum mechanics that it satisfies the two conditions (i) and (ii) then any such map can be written as a composition of three of these allowed operations. This is what allows physicists to forget about the two conditions (i)and (ii) in (1.16) and describe all allowed operations in quantum mechanics as combinations of unitary evolutions and reductions of subsystems. Thus, the system is prepared in some state, it is uncoupled with the environment, interacts with the environment and then one throws away part of the system. Sadly, however, this is only true for finite-dimensional systems as already mentioned above. There are processes in infinite-dimensional systems that cannot be written this way.

2 Quantum Systems with Many Particles

2.1 Fock Spaces with Creation and Annihilation Operators

The next topic is how one can model the environment. So far systems interacting with the environment have been described by preparing the system and the environment in some state, allowing it to evolve according to the Schrödinger equation and throwing out the environment. Thus, one has to consider systems with many particles. The precise question to be answered is how one can describe systems comprised of a possibly indefinite number of particles where indefinite means that particles can be created and destroyed. Here the environment is simply modeled as a bunch of photons such that the environment is the electromagnetic field in some thermal state.

To describe the composition of n quantum systems $A_1, A_2, ..., A_n$ with observable algebras $\mathcal{A}_1, \mathcal{A}_2, ..., \mathcal{A}_n$ the tensor product $\mathcal{A}_1 \otimes \mathcal{A}_2 \otimes ... \otimes \mathcal{A}_n$ is used to describe all possible observables. The corresponding Hilbert space for the system $A_1A_2...A_n$ is $\mathfrak{H}_{A_1A_2...A_n} = \mathfrak{H}_{A_1} \otimes \mathfrak{H}_{A_2} \otimes ... \otimes \mathfrak{H}_{A_n}$ where \mathfrak{H}_{A_j} is the Hilbert space of A_j .

However, this is not sufficient for an indefinite number of particles. To discuss an indefinite number of particles each with the same single-particle Hilbert space \mathfrak{H} the Fock space defined as

$$\mathfrak{F}(\mathfrak{H}) \cong \bigoplus_{n \ge 0} \mathfrak{H}^{(n)} \tag{2.1}$$

is introduced where $\mathfrak{H}^{(0)} = \mathbb{C}$ and $\mathfrak{H}^{(n)} = \mathfrak{H} \otimes ... \otimes \mathfrak{H}$ (*n* times). The Fock space is infinite-dimensional because *n* is unbound. Vectors representing states are lists of vectors of the form $(|\alpha_0\rangle, |\alpha_1\rangle, |\alpha_2, ...\rangle$ where $|\alpha_0\rangle \equiv \alpha_0 \in \mathbb{C}$, $|\alpha_1\rangle \in \mathfrak{H}$, $|\alpha_2\rangle \in \mathfrak{H} \otimes \mathfrak{H}$, and so on for the other $|\alpha_j\rangle$ which eventually become 0. Note that these vectors are not normalized.

Note also that this space is still to big for many practical purposes because this space describes distinguishable particles but photons are identical. If there are two identical particles and one swaps them then this is the same state. One defines the Fock space for identical particles by starting from the Fock space of distinguishable particles (2.1) and identify all the states that are the same. The projections

$$P_{\pm}^{(n)} |f_1\rangle |f_2\rangle \dots |f_n\rangle = \frac{1}{n!} \sum_{\pi \in S_n} \varepsilon_{\pi}^{(\pm)} |f_{\pi^{-1}(1)}\rangle |f_{\pi^{-1}(2)}\rangle \dots |f_{\pi^{-1}(n)}\rangle$$

where S_n is the symmetric group of permutations π of the set $\{1, ..., n\}$ and $\varepsilon_{\pi}^{(+)}$ is always +1 while $\varepsilon_{\pi}^{(-)}$ is +1 or -1 depending on whether the number of transpositions is even or odd. With this the Bose- and the Fermi-Fock space are

$$\mathfrak{F}_{\pm}(\mathfrak{H}) \cong \bigoplus_{n \ge 0} P_{\pm}^{(n)} \mathfrak{H}^{(n)}$$

$$\tag{2.2}$$

respectively. In the following mainly the Bose-Fock space $\mathfrak{F}_+(\mathfrak{H})$ will be used because photons are bosons. However, also fermions interact with the electromagnetic field.

An example of a single-particle Hilbert space is $\mathfrak{H} \cong L^2(\mathbb{R})$ for the mode of a standing wave of light. The Hilbert space for a single photon in a cavity as in the figure on the right side can also be $\ell^2(\mathbb{N})$ or any vector space with vectors $|\psi\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$. This



is already an infinite configuration space. With an indefinite number of photons in the cavity there are even more possible states and $\mathfrak{F}_{+}(\mathfrak{H})$ is big. If only the lowest mode is occupied then states live in a subspace $\mathfrak{F}_{+}(\mathbb{C})$ which also has an infinite dimension.

For $|f\rangle \in \mathfrak{H}$ the two operators $a(|f\rangle)$ and $a^{\dagger}(|f\rangle)$ on $\mathfrak{F}(\mathfrak{H})$ are defined via

$$\begin{split} \mathfrak{H}^{(0)} &: a(|f\rangle) |f_0\rangle = 0 \text{ for } |f_0\rangle \in \mathfrak{H}^{(0)} \cong \mathbb{C} \\ \mathfrak{H}^{(1)} &: a^{\dagger}(|f\rangle) |f_0\rangle \equiv |||f_0\rangle|| |f\rangle \\ \mathfrak{H}^{(n)} &: a(|f\rangle) (|f_1\rangle |f_2\rangle \dots |f_n\rangle) \equiv \sqrt{n} \langle f|f_1\rangle |f_2\rangle \dots |f_n\rangle \in \mathfrak{H}^{(n-1)} \\ &a^{\dagger}(|f\rangle) (|f_1\rangle |f_2\rangle \dots |f_n\rangle) \equiv \sqrt{n+1} |f\rangle |f_1\rangle |f_2\rangle \dots |f_n\rangle \in \mathfrak{H}^{(n+1)} \end{split}$$

and are the building blocks for the *annihilation* and *creation* operators working on distinguishable states, and the actual annihilation and creation operators are defined as

$$a_{\pm}(|f\rangle) \equiv P_{\pm} a(|f\rangle) P_{\pm}$$

$$a_{\pm}^{\dagger}(|f\rangle) \equiv P_{\pm} a^{\dagger}(|f\rangle) P_{\pm}$$
(2.3)

obeying the relations

$$\left[a_{\pm}(|f\rangle), a_{\pm}(|g\rangle)\right]_{\mp} = \left[a_{\pm}^{\dagger}(|f\rangle), a_{\pm}^{\dagger}(|g\rangle)\right]_{\mp} = 0 \qquad \left[a_{\pm}(|f\rangle), a_{\pm}^{\dagger}(|g\rangle)\right]_{\mp} = \langle f | g \rangle \mathbb{I} \qquad (2.4)$$

where $[A, B]_{\mp} = AB \pm BA$. This is so general that one can talk about fermions and bosons at the same time.

2.2 Continuous Quantum Variables

The Hilbert space $\mathfrak{H} = \mathbb{C}$ is useful to describe a single mode of light in a cavity as the simplest bosonic quantum system. The Fock space is

$$\mathfrak{F}_+(\mathbb{C}) \equiv \bigoplus_{n \ge 0} P_+^{(n)} \mathfrak{H}^{(n)} \equiv \bigoplus_{n \ge 0} \mathbb{C} \cong \ell^2(\mathbb{N})$$

according to (2.2) with $P_{+}^{(n)} = 1$ where $\mathfrak{H}^{(n)}$ is one-dimensional because $\mathfrak{H}^{(n)} = \mathbb{C} \otimes ... \otimes \mathbb{C} \equiv \mathbb{C}$. Using $|n\rangle$ as the basis vector for the n^{th} subspace $P_{+}^{(n)}\mathfrak{H}^{(n)}$ an arbitrary state $|\psi\rangle \in \mathfrak{F}_{+}(\mathbb{C})$ has the form

$$|\psi\rangle = \sum_{n\geq 0} c_n |n\rangle$$
 such that $\sum_{n\geq 0} |c_n|^2 < 0$

and this is the state of a single harmonic oscillator. An infinite-dimensional quantum system with Fock space $\mathfrak{F}_+(\mathbb{C})$ is called a continuous quantum variable.

A qubit has two levels. A pure state can be specified as two complex numbers and a mixed state needs three real numbers which is basically the same as two complex numbers up to a normalization. Thus, one never has to worry about how to represent the state of qubits. If one has a harmonic oscillator, one has to specify its state somehow. One way is to write down the whole list of complex numbers but, as this is not possible for an infinite list, one can either use a finite list and ignore the rest or one can try to find an algorithm $n \to c_n$ for the complete list.

A continuous quantum variable is a quantum system with a Hilbert space $\mathfrak{H} \cong \mathfrak{F}_+(\mathbb{C})$. There is only one annihilation operator and one creation operator (2.3) with simple commutation relations (2.4)

$$a \equiv a(|1\rangle) \qquad \qquad a^{\dagger} \equiv a^{\dagger}(|1\rangle) \qquad \qquad [a,a] = [a^{\dagger},a^{\dagger}] = 0 \qquad \qquad [a,a^{\dagger}] = \mathbb{I} \qquad (2.5)$$

since the Hilbert space has only one state. With

$$|n\rangle \equiv \frac{1}{\sqrt{n!}} (a^{\dagger})^{n} |0\rangle \qquad \qquad a^{\dagger} a |n\rangle = n |n\rangle$$

$$a |n\rangle = \sqrt{n} |n-1\rangle \qquad a^{\dagger} |n\rangle = \sqrt{n+1} |n+1\rangle \quad \langle n | m\rangle = \delta_{n,m} \quad \forall n, m \in \mathbb{N}$$

$$(2.6)$$

where n is the number operator the harmonic oscillator is completely described.

The *displacement* operator also called Weyl operator is defined as

$$D(a,\alpha) \equiv e^{\alpha a^{\dagger} - \alpha^* a} \tag{2.7}$$

for $\alpha \in \mathbb{C}$. The mathematical reason for defining the displacement operator is that a and a^{\dagger} are unbounded operators and it is not clear whether they are continuous and whether expressions with them converge. By exponentiating them they become unitary operators which obviously are bounded. One can do all calculations with them and differentiate with respect to α when needing expressions with a and a^{\dagger} . There is also a physical reason because these displacement operators correspond to linear optics transformations such as phase shifters and beam splitters. They closely correspond to what one does in experiments. These displacement operators are unitary operators, and $D^{-1}(a, \alpha) = D(a, -\alpha) = D^{\dagger}(a, \alpha)$ is a kind of proof. They can be written in the form

$$D(a,\alpha) = e^{-\frac{|\alpha|^2}{2}} e^{\alpha a^{\dagger}} e^{\alpha^* a}$$

as can be shown using the Baker-Campbell-Hausdorff formula. Because there is only one mode of light, the displacement operators will be written simply as $D(\alpha) \equiv D(a, \alpha)$ in the following, and the identities

(i)
$$D^{\dagger}(\alpha) D(\alpha) = a + \alpha$$

(ii) $D(\alpha)D(\beta) = e^{(\alpha\beta^* - \alpha^*\beta)/2} D(\alpha + \beta)$
(2.8)

are useful.

With $D(\alpha)$ one can build states. The state

$$|\alpha\rangle = D(\alpha) |0\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$
(2.9)

for $\alpha \in \mathbb{C}$ is called a *coherent* state. These are the ones that get prepared in experiments involving linear optics. One can prove that a Fock state except for 0 is not a coherent state. The coherent states have mathematical properties. One is that they are overcomplete such that

$$\langle n \mid \left(\int d^2 \alpha \mid \alpha \rangle \langle \alpha \mid \right) \mid m \rangle = \pi \delta_{n,m}$$

where $\int d^2 \alpha = \int (d \operatorname{Re}(\alpha)) (d \operatorname{Im}(\alpha))$. They have

$$\mathbb{I} = \frac{1}{\pi} \int d^2 \alpha \, \left| \alpha \right\rangle \left\langle \alpha \right| \tag{2.10}$$

as the completeness relation. Because of this completeness relations an arbitrary state $|\psi\rangle \in \mathfrak{F}_+(\mathbb{C})$ can be expressed as a linear combination of coherent states as long as one can compute the inner product $f(\alpha) = \langle \alpha | \psi \rangle$ between this state and an arbitrary coherent state. This gives

$$\mathbb{I} |\psi\rangle = \frac{1}{\pi} \int d^2 \alpha \, \left(\langle \alpha |\psi \rangle \right) |\alpha\rangle = \frac{1}{\pi} \int d^2 \alpha \, \left(f(\alpha) \right) |\alpha\rangle \tag{2.11}$$

and knowing $f(\alpha)$ is the same as knowing $|\psi\rangle$. Coherent states are overcomplete meaning that there is more than one way for representing arbitrary states, and this creates problems.

The figure on the right side shows an overcomplete basis $\{e_1, e_2, e_3\}$ of \mathbb{R}^2 . There is an infinite number of ways to specify point P in \mathbb{R}^2 because it can be specified as a linear combination of any two vectors e_1 , e_2 , e_3 but also of any two linear independent linear combinations of them. This leads to a redundant specification of any point.

Similarly here, states are represented redundantly, and more than one function f will give the same state. This is a blessing and a curse. It is a blessing because one might find a nice function f instead of an ugly one, and it is a curse because one might have to show that two integrals $f(\alpha) |\alpha\rangle$ and $g(\alpha) |\alpha\rangle$ are equal.

So far, pure states have been used but mixed states are needed for systems that are in contact with the environment and hence exchange information with the environment. This is more difficult for infinitedimensional systems than for finite-dimensional systems because one has to deal with an infinite list of numbers, and formula (2.11) has to be generalized to mixed states. Since mixed states are usually represented as density operators, the goal is to represent operators on an infinite-dimensional space. This leads to infinite-dimensional matrices, and the displacement operators help to do that.

The orthogonality and completeness of the displacement operators needs to be proven. However, as the coherent states are overcomplete also the displacement operators are overcomplete. In a first step $tr(D(\alpha))$ is calculated although this is not something one can observe in an experiment. This gives

$$\operatorname{tr}\left(D(\alpha)\right) = \frac{1}{\pi} \int d^2\beta \operatorname{tr}\left(\left|\beta\right\rangle \left\langle\beta\right| D(\alpha)\right) = \frac{1}{\pi} \int d^2\beta \left\langle0\left|e^{(\alpha+\beta)^{\dagger}\alpha - (\alpha+\beta)\alpha^*}\right|0\right\rangle$$
$$= \frac{e^{-|\alpha|^2/2}}{\pi} \int d^2\beta \, e^{-\beta\alpha^* + \beta^*\alpha} = \pi \, \delta^2(\alpha)$$

after inserting the identity from the completeness relation (2.10). Hence

$$\operatorname{tr}\left(D^{\dagger}(\beta) D(\alpha)\right) = \pi \,\delta^2(\beta - \alpha) \tag{2.12}$$

follows. One can look at this as analogous to the inner product $(D(\beta), D(\alpha))$ but of operators and not of vectors. Since mixed states are represented as density operators and density operators are bounded operators the really important result comes next. Under the assumption that A is a bounded operator on the Hilbert space \mathfrak{H} then

$$A = \frac{1}{\pi} \int d^2 \alpha \operatorname{tr} \left(A D^{\dagger}(\alpha) \right) D(\alpha) = \frac{1}{\pi} \int d^2 \alpha \, \chi(\alpha) D(\alpha)$$
(2.13)

and this result could be called the operator overcompleteness relation looking similar to (2.11). Any operator can be expressed as a linear combination of displacement operators but it is not a unique linear combination because of the overcompleteness. One can turn the relation in (2.13) around and ask what is the operator given some $\chi(\alpha)$.

The proof for (2.13) works as

$$\begin{split} \langle n \, | \, A \, | \, m \rangle \stackrel{?}{=} \frac{1}{\pi} \int d^2 \alpha \, \sum_{\ell} \langle \ell \, | \, A \, D^{\dagger}(\alpha) \, | \, \ell \rangle \, \langle n \, | \, D(\alpha) \, | \, m \rangle \\ \stackrel{?}{=} \frac{1}{\pi} \int d^2 \alpha \, \sum_{\ell,k} \langle \ell \, | \, A \, | k \rangle \, \langle k \, | \, D^{\dagger}(\alpha) \, | \, \ell \rangle \, \langle n \, | \, D(\alpha) \, | \, m \rangle \\ \stackrel{1}{=} \frac{1}{\pi} \int d^2 \alpha \, \langle k \, | \, D^{\dagger}(\alpha) \, | \, \ell \rangle \, \langle n \, | \, D(\alpha) \, | \, m \rangle \stackrel{\text{suppose}}{=} \delta_{k,m} \delta_{\ell,n} \end{split}$$

$$\Rightarrow \frac{1}{\pi} \int d^{2} \alpha \sum_{\ell,k} \left\langle \ell \left| A \right| k \right\rangle \left\langle k \left| D^{\dagger}(\alpha) \right| \ell \right\rangle \left\langle n \left| D(\alpha) \right| m \right\rangle = \sum_{\ell,k} \left\langle \ell \left| A \right| k \right\rangle \delta_{k,m} \delta_{\ell,n} = \left\langle n \left| A \right| m \right\rangle$$

where $\frac{1}{\pi} \int d^2 \alpha \, \langle k \, | \, D^{\dagger}(\alpha) \, | \, \ell \rangle \, \langle n \, | \, D(\alpha) \, | \, m \rangle = \delta_{k,m} \delta_{\ell,n}$ follows from

$$\operatorname{tr}(A)\mathbb{I} = \frac{1}{\pi} \int d^2 \alpha \, D(\alpha) \, A \, D^{\dagger}(\alpha)$$

which can be proved using

$$\frac{1}{\pi} \int d^2 \alpha \, \left\langle \mu \,|\, D(\alpha) \,|\, \beta \right\rangle \left\langle \gamma \,|\, D^{\dagger}(\alpha) \,|\, \nu \right\rangle = \left\langle \gamma \,|\, \beta \right\rangle \left\langle \mu \,|\, \nu \right\rangle$$

where $|\mu\rangle$, $|\nu\rangle$, $|\beta\rangle$, $|\gamma\rangle$ are coherent states.

All states are represented by density operators ρ such that $\rho \ge 0$ and $\operatorname{tr}(\rho) = 1$ in finite dimensions but not all states have this form in infinite dimensions. However, states interesting for physics are in this form. One calls $\chi(\alpha)$ with

$$\chi_{\rho}(\alpha) = \operatorname{tr}\left(\rho D(\alpha)\right) \tag{2.14}$$

the characteristic function of ρ . This is interesting because one can estimate $\chi_{\rho}(\alpha)$ by experiments, and if one knows $\chi_{\rho}(\alpha)$ one can reconstruct ρ from $\chi(\alpha)$ as

$$\rho = \frac{1}{\pi} \int d^2 \alpha \, \chi^*(\alpha) \, D(\alpha)$$

because of $A = \frac{1}{\pi} \int d^2 \alpha \operatorname{tr} (A D^{\dagger}(\alpha)) D(\alpha)$ from the completeness relation (2.13). The fact that ρ is a hermitian operator places some constraints on the shape of the characteristic function.

This described how one represents single modes of continuous variables. For multiple modes the Hilbert space is defined as $\mathfrak{H}_n = \mathfrak{H} \otimes \mathfrak{H} \otimes \ldots \otimes \mathfrak{H}$ (*n* times) for *N* distinguishable continuous quantum variables. (If the continuous quantum variables are indistinguishable one has to compensate for the symmetry.) The displacement operators have *n* complex numbers with $\underline{\alpha} \in \mathbb{C}^n$ and are defined as

$$D(\underline{\alpha}) \equiv D(\alpha_1) \otimes D(\alpha_2) \otimes \dots \otimes D(\alpha_n) = \bigotimes_{j=1}^n D(\alpha_j)$$
$$= e^{\sum_{j=1}^n \alpha_j a_j^{\dagger} - \alpha_j^* a_j}$$
(2.15)

where a_j^{\dagger} and a_j are the creation and annihilation operators of these modes with the commutation relations $[a_j, a_k^{\dagger}] = \delta_{jk} \mathbb{I}$. Given the coherent states $|\underline{\alpha}\rangle = D(\underline{\alpha}) |0\rangle \otimes ... \otimes |0\rangle$ completeness is

$$\mathbb{I} \otimes \mathbb{I} \otimes \ldots \otimes \mathbb{I} = \frac{1}{\pi^n} \int d^2 \alpha_1 d^2 \alpha_2 \ldots d^2 \alpha_n \, \left| \alpha_1 \right\rangle \left\langle \alpha_1 \right| \otimes \left| \alpha_2 \right\rangle \left\langle \alpha_2 \right| \otimes \ldots \otimes \left| \alpha_n \right\rangle \left\langle \alpha_n \right|$$

for the multiple modes.

2.3 Gaussian States

Gaussian states are states of continuous quantum variables and are defined by a very special mathematical property. Their physical property is that they show up in experiments all the time. They are a good model for the kinds of quantum states one encounters in a linear optical apparatus, for example. The Hilbert space for n continuous quantum variables is $\mathfrak{H} \equiv \mathfrak{F}_+(\mathbb{C}) \otimes ... \otimes \mathfrak{F}_+(\mathbb{C})$ (n times) for bosons and this is also $\mathfrak{F}_+(\mathbb{C}^n)$.

However, there are different conventions how one specifies displacement operators in quantum optics, and a very common one used in the literature has to be presented before continuing. For $\underline{\alpha} \in \mathbb{C}^n$ the displacement operators have been introduced as

$$D(\alpha) = e^{\alpha_1 a_1^{\dagger} - \alpha_1^* a_1} \otimes \dots \otimes e^{\alpha_n a_n^{\dagger} - \alpha_n^* a_n}$$

above. It is also convenient to define canonical operators with their commutation relations

analogous to position and momentum operator. Thus, one can write everything with \hat{q}_j and \hat{p}_j instead of a_j and a_j^{\dagger} . Since Gaussian states are usually expressed in this notation, it will be used in the following as well.

With $\underline{\xi} \cong (x_1, ..., x_n; p_1, ..., p_n) \in \mathbb{R}^{2n}$ the displacement operators become

$$D(\underline{\xi}) = e^{i\underline{\xi}\,p^T}\underline{\underline{\sigma}}\,\underline{\hat{R}} = e^{i\sum_{j=1}^n p_j\hat{q}_j - x_j\hat{p}_j} \qquad \underline{\underline{\sigma}} = \begin{pmatrix} 0 & -\mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix} \qquad \underline{\hat{R}} \equiv (\hat{q}_1, \hat{q}_2, ..., \hat{q}_n; \hat{p}_1, \hat{p}_2, ..., \hat{p}_n)$$
(2.16)

where p_j is a number and \hat{p}_j an operator. This is completely equivalent to (2.15) such that $D(\underline{\alpha}) \equiv D(\underline{\xi})$ if one sets

$$\alpha_j = \frac{x_j + i\,p_j}{\sqrt{2}}$$

for the coefficients. One can express the characteristic function as

$$\chi_{\rho}(\xi) = \operatorname{tr}\left(\rho D(\xi)\right)$$

in terms of $\underline{\xi}$. In the notation with $\underline{\alpha}$ the characteristic function $\chi_{\rho}(\underline{\alpha}) = \operatorname{tr}(\rho D(\underline{\alpha}))$ is a function of n complex numbers, and in this other notation the characteristic function $\chi_{\rho}(\underline{\xi})$ is a function of 2n real numbers.

A Gaussian state ρ is a state whose characteristic function is a Gaussian such that

$$\chi_{\rho}(\underline{\xi}) \equiv e^{-i\underline{m}^T\underline{\sigma}\underline{\xi} - \frac{1}{4}(\underline{\sigma}\underline{\xi})^T\underline{\gamma}(\underline{\sigma}\underline{\xi})}$$
(2.17)

where \underline{m} is the vector of first moments called displacement vector defined as

$$[\underline{m}]_j = \operatorname{tr}\left(\rho\,\hat{R}_j\right)$$

and $\underline{\gamma}$ is the matrix of second moments

$$[\underline{\gamma}]_{jk} = 2\operatorname{tr}\left(\rho\left[\hat{R}_j - m_j\right]\left[\hat{R}_k - m_k\right]\right) + i[\underline{\sigma}]_{jk} = \operatorname{tr}\left(\rho\left(\hat{R}_j\hat{R}_k + \hat{R}_k\hat{R}_j\right)\right) - 2m_jm_k$$
(2.18)

called covariance matrix. For Gaussians in probability theory first and second moments determine all the higher moments.

At this point it is not clear whether states satisfying (2.17) exist, and whether all characteristic functions defined by this equation are really states. Thus, this is just a definition but one has to prove first that it is a good definition. If this is a good definition and states are defined by this characteristic function then the state of an infinite-dimensional Hilbert space is defined in terms of some $4n^2 + 2n$ numbers because one needs only the vector of first moments \underline{m} and the matrix of second moments γ .

As a first example of a Gaussian state the density operator and the characteristic function are

$$\rho = \bigotimes_{j=1}^{n} |0\rangle \langle 0| \qquad \qquad \chi(\underline{\xi}) = e^{-\frac{1}{4}\underline{\xi}^{T}\underline{\xi}} = e^{-\frac{1}{4}(\underline{\sigma}\underline{\xi})^{T}(\underline{\sigma}\underline{\xi})}$$

for the vacuum state using $\underline{\underline{\sigma}}^T \underline{\underline{\sigma}} = \mathbb{I}$. This is a minimum uncertainty state such that $(\Delta q_j)(\Delta p_j) = \frac{1}{2}$, and the first moments are $\underline{\underline{m}} = 0$ and $\underline{\gamma} = \mathbb{I}$.

The vacuum state is a coherent state and it turns out that all the coherent states are Gaussian. They form an overcomplete basis for the Hilbert space but the linear combination of two Gaussian states is not necessarily a Gaussian state. (It actually often is not.) Density operator and characteristic function for a coherent state are

$$\rho = |\underline{\alpha}\rangle \langle \underline{\alpha}| \equiv D(\underline{\alpha}) |0\rangle \langle 0| D^{T}(\underline{\alpha}) \qquad \qquad \chi(\underline{\xi}) = e^{-i(a_{1},a_{2},\dots,a_{n};b_{1},b_{2},\dots,b_{n})} \underline{\underline{\sigma}} \underline{\xi} - \frac{1}{4} \underline{\xi}^{T} \underline{\xi}$$

where $\alpha_j = (a_j + i b_j)/\sqrt{2}$. There is a shift such that the vector of first moments is not zero, and the matrix of second moments is still the identity as in the case of the vacuum.

Not all possible matrices can serve as a covariance matrix because γ must satisfy the conditions

$$\underline{\underline{\gamma}} - i \underline{\underline{\sigma}} \ge 0 \qquad \qquad \underline{\underline{\gamma}}^T = \underline{\underline{\gamma}} \tag{2.19}$$

and, if it fulfills these conditions, it corresponds to a state. To prove it

$$\underline{z}^{\dagger}(\underline{\gamma} - i\underline{\sigma})\underline{z} = 2\operatorname{tr}\left(\rho\sum_{jk} z_{j}^{*}(\hat{R}_{j} - m_{j})(\hat{R}_{k} - m_{k})z_{k}\right) = \operatorname{tr}(\rho A^{\dagger}A)$$

using $\operatorname{tr}(\rho A^{\dagger}A) \geq 0$ for all A and (2.18) where $\underline{z} \in \mathbb{C}^{2n}$ and $A = \sum (\hat{R}_j - m_j) z_j$. This proves that given a state ρ whose characteristic function is a Gaussian then the covariance matrix must satisfy (2.19) but one also has to show that a state corresponding to a covariance matrix satisfying (2.19) is a Gaussian state. A flavor of the argument for the statement that every covariance matrix corresponds to a valid quantum state is based on the idea to fix the first and second moments and to build the set of all states matching them. The state in this set with the largest entropy is the Gaussian state. The result is that there exists a system of coupled harmonic oscillators whose thermal state $\rho = e^{-\beta \hat{H}}/Z$ has (2.17) as its characteristic function for given \underline{m} and $\underline{\gamma}$ satisfying $\underline{\gamma} - i \underline{\sigma} \geq 0$.

Actually, as a more general statement, thermal states $e^{-\beta \hat{H}}/Z$ of quadratic Hamiltonians

$$\hat{H} = \sum_{jk} \hat{R}_j \, h_{jk} \, \hat{R}_k$$

are always Gaussian. The exact formula for h_{jk} given the displacement vector and the covariance matrix is not so intuitive.

2.4 Bipartite Gaussian States

So far general Gaussian states have been studied. In the following the focus will be on bipartite Gaussian states which one can therefore put into two groups. There are two parties assumed which will be called Alice and Bob as usual. Both have n modes such that they have together 2n modes. The modes of Alice

are numbered 1, ..., n and the modes of Bob are numbered 1', ..., n'. Gaussian states of the combined system will be examined, and the question is what joint states can they share. A trivial observation is that Alice and Bob can certainly share a Gaussian state on Alice's modes and a Gaussian state of Bob's modes. It will turn out that not only separable or product states are allowed but one can also express some interesting entangled states in terms of Gaussian states, and the general question is what kind of joint states ρ_{AB} are Gaussian.

The reduced state of a Gaussian state is also Gaussian. If ρ_{AB} is Gaussian then also

$$\rho_{\rm A} \equiv {\rm tr}_{\rm B}(\rho_{\rm AB})$$

is Gaussian. The proof is straightforward as the characteristic function of the reduced state of Alice is

$$\chi_{\mathbf{A}}(\underline{\xi}) = \operatorname{tr}_{\mathbf{A}}\left(\rho_{\mathbf{A}} D_{\mathbf{A}}(\underline{\xi})\right) = \operatorname{tr}_{\mathbf{AB}}\left(\rho_{\mathbf{AB}} D_{\mathbf{AB}}(\underline{\xi}_{\mathbf{A}}, \underline{0}_{\mathbf{B}})\right) = \operatorname{tr}_{\mathbf{AB}}\left(\rho_{\mathbf{AB}} D_{\mathbf{A}}(\underline{\xi}_{\mathbf{A}}) \otimes \mathbb{I}_{\mathbf{B}}\right) \\ - e^{-i\underline{m}^{T}} \underline{\underline{\sigma}}(\underline{\xi}_{\mathbf{A}}, \underline{0}_{\mathbf{B}}) - \frac{1}{4}(\underline{\underline{\sigma}}(\underline{\xi}_{\mathbf{A}}, \underline{0}_{\mathbf{B}}))^{T} \underline{\underline{\gamma}}_{\mathbf{AB}}(\underline{\underline{\sigma}}(\underline{\xi}_{\mathbf{A}}, \underline{0}_{\mathbf{B}}))$$

because of $D(\underline{\xi}_{A}, \underline{0}_{B}) = D(\underline{\xi}_{A}) \otimes \mathbb{I}_{B}$. One just puts in zeros for Bob's modes. Hence $\chi_{A}(\underline{\xi})$ has first moments given by the first moments of $(\hat{q}_{1}, \hat{q}_{2}, ..., \hat{q}_{n}; \hat{p}_{1}, \hat{p}_{2}, ..., \hat{p}_{n})$ in Alice's system (ignoring first moments $(\hat{q}_{1'}, ..., \hat{q}_{n'}; \hat{p}_{1'}, ..., \hat{p}_{n'})$ of Bob's system), and the covariance matrix for Alice is found by restricting the covariance matrix of the combined system to the submatrix with respect to the index set of modes $\{1, ..., n\}$ of Alice.

To illustrate this the two-mode squeezed state is used as an example. Assuming there are two modes A and B with $\hat{R} = (\hat{q}_A, \hat{q}_B; \hat{p}_A, \hat{p}_B)$ then $\rho = |\psi_r\rangle \langle \psi_r|$ is called a two-mode squeezed state illustrated in the figure on the right side if



$$\gamma_{\equiv AB} = \begin{pmatrix} \cosh(2r) & \sinh(2r) & 0 & 0\\ \sinh(2r) & \cosh(2r) & 0 & 0\\ 0 & 0 & \cosh(2r) & -\sinh(2r)\\ 0 & 0 & -\sinh(2r) & \cosh(2r) \end{pmatrix}$$

is the covariance matrix. This corresponds to the pure state

$$|\psi_r\rangle = \sqrt{1 - \left(\tanh\left(\frac{r}{2}\right)\right)^2} \sum_{n=1}^{\infty} \left(\tanh\left(\frac{r}{2}\right)\right)^n |n\rangle_{\mathcal{A}} |n\rangle_{\mathcal{B}}$$

where $|n\rangle_{\rm A}$ and $|n\rangle_{\rm B}$ are Fock states. (Here *r* is called the squeezing parameter or $\tanh\left(\frac{r}{2}\right)$ depending on the terminology.) This looks like a maximally entangled state. The reduced density operator for *A* has the covariance matrix

$$\begin{pmatrix} \cosh(2r) & 0\\ 0 & \cosh(2r) \end{pmatrix}$$

by restricting $\underline{\gamma}_{AB}$.

This shows how to find the covariance matrix of a subsystem by restricting the covariance matrix of a gaussian state. The other question is whether a Gaussian state always comes from a bigger Gaussian state, and the answer is yes for the bipartite case but not always for the tripartite case. Extending a Gaussian state means to find a Gaussian state ρ_{AB} given the Gaussian state ρ_A such that $\rho_A = \text{tr}_B(\rho_{AB})$ if it exists. In other words, the question is whether one can infer that a smaller system comes from a Gaussian state of a bigger system. The answer is trivial because there is always $\rho_{AB} = \rho_A \otimes \rho_B$ where ρ_B is any Gaussian state. The question becomes much richer when putting constraints on how to extend the system. One can ask, for example, whether there are extensions such that the extended Gaussian state is pure. There is an infinite number of extensions, and this is called purification.

The question becomes much richer with three modes A, B, C with Gaussian modes AB and BC. One might assume that there is always a Gaussian state ρ_{ABC} given Gaussian states ρ_{AB} and ρ_{BC} but this is not always the case. It actually can happen that there is no ρ_{ABC} at all such that $tr_C(\rho_{ABC}) = \rho_{AB}$ and $tr_A(\rho_{ABC}) = \rho_{BC}$. That comes from the fact that there can be entangled states. Thus, the task of extending states is not easy but the state of reducing states is easy.

2.5 Quasi-Free Boson Systems

The goal is to understand the dynamics of a system A embedded in an environment E. One can understand the dynamics of A by integrating the Schrödinger equation for the whole system but this is a inconceivably difficult problem because the environment is enormous and it very quickly happens as time passes that A will become correlated and entangled with E. The task becomes harder and harder as time progresses. Thus, the goal is to understand the dynamics of A while ignoring or neglecting E. There is the possibility of doing this within the framework of quantum mechanics but one has to employ the technology of completely positive maps because if one looks only at A ignoring E then A will become noisy. The noise will come in from every degree of freedom of E that interacts with A.

The reason for studying continuous quantum variables up to now is that system A could be comprised of some continuous quantum variables but the environment E is pretty much for sure comprised of continuous quantum variable such as the environment coming from the electromagnetic field. Thus, before the environment can be ignored or neglected one should know it. This means that the environment E has to be modeled, and E here is mostly the electromagnetic field. Once E at time t = 0 is understood its interactions with A will be approximated and then E can be thrown away. This approach leads to the Lindblad equation.

A Gaussian model is also called quasi-free. A collection $L = \{1, ..., n\}$ of n modes with \hat{q}_j , \hat{p}_j for j = 1, ..., n obeying the canonical commutation relations $[\hat{q}_j, \hat{p}_k] = i \, \delta_{jk} \mathbb{I}$ and a system with Hamiltonian

$$\hat{H} = \frac{1}{2} \sum_{j,k=1}^{n} \left(\hat{q}_j \left[\underline{\underline{V}}_q \right]_{jk} \hat{q}_k + \hat{p}_j \left[\underline{\underline{V}}_p \right]_{jk} \hat{p}_k \right)$$
(2.20)

is assumed where the potential energy is the term with \hat{q} , and the kinetic energy is the term with \hat{p} . (Note that *n* does not have to be a small number but can be 10^{23} or larger and that \hat{H} is not the most general quadratic Hamiltonian.) The model with this Hamiltonian is capable of describing physics of non-relativistic and relativistic collections of harmonic oscillators interacting in an arbitrary way. It is pretty general in the sense that it captures everything from the Klein-Gordon equation through to phonon propagation in solids.

The Hamiltonian (2.20) is written in the form

$$\hat{H} = \frac{1}{2} \underline{\hat{R}}^T \underline{\underline{H}} \underline{\hat{R}} \qquad \underline{\hat{R}}^T = (\hat{q}_1, \dots, \hat{q}_n, \hat{p}_1, \dots, \hat{p}_n) \qquad \underline{\underline{H}} = \begin{pmatrix} \underline{\underline{V}}_q & 0\\ 0 & \underline{\underline{V}}_p \end{pmatrix}$$
(2.21)

in order to gain a concise notation, and it may also be expressed in terms of annihilation and creation operators as

$$\begin{split} \hat{H} &= \frac{1}{2} \hat{\underline{b}}^{\dagger} \underline{\underline{H}}' \hat{\underline{b}} & \hat{\underline{b}} &= (\hat{b}_1, \dots, \hat{b}_n, \hat{b}_1^{\dagger}, \dots, \hat{b}_n^{\dagger}) & \underline{\underline{H}}' &= \left(\underline{\underline{\underline{B}}}_{\underline{\underline{A}}} \quad \underline{\underline{\underline{B}}}_{\underline{\underline{B}}}\right) \\ \underline{\underline{A}} &= \frac{\underline{\underline{V}}_q + \underline{\underline{V}}_p}{2} & \underline{\underline{B}} &= \frac{\underline{\underline{V}}_q - \underline{\underline{V}}_p}{2} & \hat{b}_j &= \frac{\hat{q}_j + i\,\hat{p}_j}{\sqrt{2}} \end{split}$$

where \hat{H} not only couples \hat{b}_j^{\dagger} and \hat{b}_k as well as \hat{b}_j and \hat{b}_k^{\dagger} but also \hat{b}_j and \hat{b}_k as well as \hat{b}_j^{\dagger} and \hat{b}_k^{\dagger} . The first two types of terms with \hat{b}_j^{\dagger} and \hat{b}_k as well as \hat{b}_j and \hat{b}_k^{\dagger} conserve total particle number but the other types \hat{b}_j and \hat{b}_k^{\dagger} as well as \hat{b}_j^{\dagger} and \hat{b}_k^{\dagger} do not and generate squeezing between the modes.

The model (2.20) is diagonalized by a transformation preserving the canonical commutation relations. (The trick is not do diagonalize \hat{H} as a matrix and to make the transformation on the states but to make the transformation on the operators.) One defines \hat{R}'_i such that they obey

$$[\hat{R}'_{j}, \hat{R}'_{k}] = -i [\sigma]_{jk} \mathbb{I} \qquad \underline{\sigma} = \begin{pmatrix} 0 & -\mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}$$
(2.22)

and one looks for a transformation from the original $\underline{\hat{R}}$ to the new $\underline{\hat{R}}'$ which still obey these canonical commutation relations. The hope is that this transformation will turn out to be unitary.

Starting from a general linear function with a matrix $\underline{S} \in M_{2n}(\mathbb{R})$

$$\hat{R}'_j = \sum_k [\underline{\underline{S}}]_{jk} \, \hat{R}_k$$

one has to figure out what constraints have to be imposed on it due to (2.22). Substituting this into the commutation relations gives

$$[\hat{R}'_{j}, \hat{R}'_{k}] = \sum_{j',k'} [\underline{\underline{S}}]_{jj'} [\underline{\underline{S}}]_{kk'} [\hat{R}'_{j'}, \hat{R}'_{k'}] = -i \sum_{j',k'} [\underline{\underline{S}}]_{jj'} [\underline{\underline{\sigma}}]_{j'k'} [\underline{\underline{S}}]_{kk'} \mathbb{I} = -i [\underline{\underline{\sigma}}]_{jk} \mathbb{I} \quad \Rightarrow \quad \underline{\underline{S}} \underline{\underline{\sigma}} \underline{\underline{S}}^{T} = \underline{\underline{\sigma}} \quad (2.23)$$

and matrices \underline{S} satisfying this equation are called symplectic transformations.

The Lie group called symplectic group is certainly not empty because the identity belongs to it. The set of matrices $\{\underline{S} \in \mathsf{M}_{2n}(\mathbb{R}) \mid \underline{S} \underline{\sigma} \underline{S}^T = \underline{\sigma}\}$ is denoted by $\mathsf{Sp}(2n, \mathbb{R})$. The theorem of Williamson states that one can use symplectic matrices to bring other matrices into normal form. It formally states that given $\underline{\underline{M}} \in \mathsf{M}_{2n}(\mathbb{R})$ with $\underline{\underline{M}}^T = \underline{\underline{M}}$ and $\underline{\underline{M}} > 0$ there exists $\underline{\underline{S}} \in \mathsf{Sp}(2n, \mathbb{R})$ and $\underline{\underline{D}} = \operatorname{diag}(\mu_1, \mu_2, ..., \mu_n) \in \mathsf{M}_n(\mathbb{R})$ with $\mu_j > 0$ such that $\underline{\underline{M}} = \underline{\underline{S}}^T(\underline{\underline{D}} \otimes \underline{\underline{D}})\underline{\underline{S}}$ where μ_j are called the symplectic eigenvalues determined as

$$\mu_j = \sqrt{\lambda_j (i \,\underline{\underline{\sigma}M})^2}$$

by diagonalizing $\underline{\sigma M}$. The value $\lambda_j(\underline{X})$ is the j^{th} eigenvalue of \underline{X} when listed in descending order. One can find \underline{S} which diagonalizes \underline{M} as

$$\underline{\underline{S}} = \begin{pmatrix} \frac{1}{\sqrt{\underline{\underline{D}}}} & 0\\ 0 & \frac{1}{\sqrt{\underline{\underline{D}}}} \end{pmatrix} \underline{\underline{O}} \sqrt{\underline{\underline{M}}}$$

where \underline{O} must satisfy

$$\begin{pmatrix} \frac{1}{\sqrt{\underline{D}}} & 0\\ 0 & \frac{1}{\sqrt{\underline{D}}} \end{pmatrix} \underline{\underline{O}} \sqrt{\underline{\underline{M}}} \underline{\underline{\sigma}} \sqrt{\underline{\underline{M}}} \underline{\underline{O}}^T \begin{pmatrix} \frac{1}{\sqrt{\underline{D}}} & 0\\ 0 & \frac{1}{\sqrt{\underline{D}}} \end{pmatrix} = \underline{\underline{\sigma}}$$

because of (2.23). Multiplying with the inverse of the term with \underline{D} on both sides gives

$$\underline{\underline{O}}\sqrt{\underline{\underline{M}}}\,\underline{\underline{\sigma}}\sqrt{\underline{\underline{M}}}\,\underline{\underline{O}}^{T} = \begin{pmatrix} 0 & -\underline{\underline{D}}\\ \underline{\underline{D}} & 0 \end{pmatrix}$$
(2.24)

as an equivalent condition which \underline{O} must satisfy. This condition is in general a hard problem but the full general case is not needed here.

For $\underline{\underline{M}} = \underline{\underline{H}}$ in (2.21) one can find $\underline{\underline{O}}$ satisfying (2.24) by choosing $\underline{\underline{Q}}$ such that

$$\underline{\underline{Q}}^T \sqrt{\underline{\underline{V}}_q} \, \underline{\underline{V}}_p \sqrt{\underline{\underline{V}}_q} \, \underline{\underline{Q}} = \underline{\underline{D}}^2$$

and build

$$\underline{\underline{O}} = \begin{pmatrix} \underline{\underline{Q}}^T & 0 \\ \hline 0 & \underline{\underline{D}} \\ \underline{\underline{Q}}^T \\ \underline{\underline{D}} \\ \underline{\underline{Q}}^T \\ \underline{\underline{V}}_{q} \\ \underline{\underline{V}}_{p} \end{pmatrix}$$

which can be solved at least by a computer. The matrix $\sqrt{\underline{\underline{V}}_q} \underline{\underline{V}}_p \sqrt{\underline{\underline{V}}_q}$ is symmetric, $\underline{\underline{Q}}$ is orthogonal, and one can compute $\underline{\underline{O}}$ and $\underline{\underline{S}}$. One can show that

$$\underline{\underline{S}} = \begin{pmatrix} \frac{1}{\sqrt{\underline{D}}} & 0\\ 0 & \frac{1}{\sqrt{\underline{D}}} \end{pmatrix} \underline{\underline{O}} \begin{pmatrix} \sqrt{\underline{\underline{V}}_{q}} & 0\\ 0 & \sqrt{\underline{\underline{V}}_{p}} \end{pmatrix}$$
(2.25)

satisfies

$$\begin{pmatrix} \underline{\underline{V}}_{q} & 0\\ 0 & \underline{\underline{V}}_{p} \end{pmatrix} = \underline{\underline{S}}^{T} \begin{pmatrix} \underline{\underline{D}} & 0\\ \overline{0} & \underline{\underline{D}} \end{pmatrix} \underline{\underline{S}}$$
(2.26)

and the linear function \underline{S} in (2.23) has been found.

Defining $\hat{R}'_j = \sum_k [\underline{\underline{S}}]_{jk} \hat{R}_k$ one can diagonalize \hat{H} in (2.20)

$$\hat{H} = \frac{1}{2} (\underline{\hat{R}}')^T \begin{pmatrix} \underline{\underline{D}} & 0\\ 0 & \underline{\underline{D}} \end{pmatrix} \underline{\hat{R}'} = \sum_{j=1}^n \mu_j \left(\hat{a}_j^{\dagger} \hat{a}_j + \frac{1}{2} \right) \qquad \qquad \hat{a}_j = \frac{\hat{q}_j + i\,\hat{p}_j}{\sqrt{2}} \tag{2.27}$$

showing that there is a transformation to a collection of independent harmonic oscillators. This justifies the name quasi-free because the initial complicated quadratic model is not a sum of independent harmonic oscillators but it is a unitary transformation away from it.

One can now go back and express the original model in terms of creation and annihilation operators. The question is how to do that. The characteristic function of a general ρ behaves under the transformation $\hat{R}'_{j} = \sum_{k} [\underline{S}]_{jk} \hat{R}_{k}$ as

$$\chi_{\rho}(\underline{\xi}) = \operatorname{tr}\left(\rho e^{i\underline{\xi}^{T}}\underline{\underline{\sigma}}\underline{\hat{R}}\right) = \operatorname{tr}\left(\rho e^{i\underline{\xi}^{T}}\underline{\underline{\sigma}}\underline{\underline{[S]}}^{-1}\underline{\hat{R}'}\right) = \operatorname{tr}\left(\rho e^{i(\underline{S}\,\underline{\xi})^{T}}\underline{\underline{\sigma}}\underline{\hat{R}'}\right) = \chi_{\rho}'(\underline{\underline{S}}\,\underline{\xi})$$

and hence the result for the inverse transformation is

$$\underline{\underline{m}} = \underline{\underline{S}}^{-1} \underline{\underline{m}}' \qquad \qquad \underline{\underline{\gamma}} = \underline{\underline{S}}^{-1} \underline{\underline{\gamma}}' (\underline{\underline{S}}^{-1})^T \qquad (2.28)$$

for the first and second moments, respectively. Thus, this linear transformation can be undone.

The thermal state of the model with the Hamiltonian \hat{H} in (2.20)

$$\rho = \frac{e^{-\beta \hat{H}}}{\operatorname{tr}\left(e^{-\beta \hat{H}}\right)} \tag{2.29}$$

is Gaussian. The statement (2.27) above is actually more powerful than the statement (2.29) because it not only tells what the ground state is but also all the excited states. In practice however the statement (2.29) is used because the environments one encounters are fields in thermal states. One assumes that the system has been cooled down and is isolated from the environment but as time progresses it slowly interacts with the environment, and this environment can be assumed in some thermal equilibrium. Because the thermal state (2.29) is Gaussian one knows everything about the system when knowing \underline{m} and γ .

To show that ρ is Gaussian one transforms it

$$\rho = \bigotimes_{j=1}^{n} \frac{e^{-\beta(\mu_j \, a_j^{+} a_j + \frac{1}{2})}}{Z_j} = \det\left(1 - e^{-\beta \underline{D}}\right) \cdot \sum_{m_1, \dots, m_n} e^{-\beta \, \mu_j m_j} \left|m_1, \dots, m_n\right\rangle \left\langle m_1, \dots, m_n\right\rangle$$

where $Z_j = \text{tr}\left(e^{-\beta(\mu_j a_j^{\dagger} a_j + \frac{1}{2})}\right)$. Since the characteristic function for a tensor product is a product of the characteristic functions. Thus, it is enough to understand a single mode. The characteristic function is proportional as in

$$\chi_{\rho}'(\underline{\xi}) \propto e^{-\frac{1}{4}\underline{\xi}^{T} \begin{pmatrix} \overline{\underline{\gamma}} & 0\\ \overline{0} & \underline{\underline{\gamma}} \end{pmatrix} \underline{\xi}} \quad \text{with} \quad \underline{\underline{\gamma}} = 4 \operatorname{diag} \left(\frac{e^{\beta \,\mu_{j}} + 1}{e^{\beta \,\mu_{j}} - 1} \right)$$

but this calculation is rather tricky. Finally, one gets

$$\underline{\underline{\gamma}}(\beta) = \underline{\underline{S}}^{-1} \begin{pmatrix} \overline{\underline{\gamma}} & 0\\ \overline{\underline{0}} & \underline{\underline{\gamma}} \end{pmatrix} (\underline{\underline{S}}^{-1})^T = \begin{pmatrix} \underline{\underline{\gamma}}_q(\beta) & 0\\ 0 & \underline{\underline{\gamma}}_p(\beta) \end{pmatrix}$$
(2.30)

with

$$\begin{split} \underline{\underline{\gamma}}_{\underline{q}}(\beta) &= \frac{1}{\sqrt{\underline{\underline{V}}_{q}}} \left(\sqrt{\underline{\underline{V}}_{q}} \, \underline{\underline{V}}_{p} \sqrt{\underline{\underline{V}}_{q}} \right)^{\frac{1}{2}} \left(\mathbb{I} + \underline{\underline{G}} \right) \frac{1}{\sqrt{\underline{\underline{V}}_{q}}} \\ \underline{\underline{\gamma}}_{\underline{p}}(\beta) &= \sqrt{\underline{\underline{V}}_{q}} \left(\sqrt{\underline{\underline{V}}_{q}} \, \underline{\underline{V}}_{p} \sqrt{\underline{\underline{V}}_{q}} \right)^{-\frac{1}{2}} \left(\mathbb{I} + \underline{\underline{G}} \right) \sqrt{\underline{\underline{V}}_{q}} \\ \underline{\underline{G}} &= 2 \left(e^{\beta \left(\sqrt{\underline{\underline{V}}_{q}} \, \underline{\underline{V}}_{p} \sqrt{\underline{\underline{V}}_{q}} \right)} - \mathbb{I} \right)^{-1} \end{split}$$
(2.31)

where $\underline{\gamma}(\beta)$ is the covariance matrix in the thermal state with inverse temperature β in the original variables. In practice many of the matrices \underline{V} are much simpler, and \underline{V}_p is almost always the identity matrix. In the end one can actually work out every single entry of $\underline{\gamma}(\beta)$ both non-relativistically and relativistically.

2.6 The Master Equation

The dynamics of a system S interacting with an environment E is described as

$$\mathcal{E}_{\rm S}(\rho_{\rm S}) = \operatorname{tr}_{\rm E} \left(U_{\rm SE} \left(\rho_{\rm S}(0) \otimes \rho_{\rm E}(0) \right) U_{\rm SE}^{\dagger} \right)$$
(2.32)

in complete generality. The dynamics $\mathcal{E}_{\rm S}(\rho_{\rm S})$ is described by a completely positive map where the unitary dynamics $U_{\rm SE}$ couples the system and the environment and $\rho_{\rm S}(0)$ and $\rho_{\rm E}(0)$ are the initial states of the system and the environment, respectively.

There are several assumptions in this equation. One is that system and environment at time t = 0 are decoupled such that $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$ but that system and environment interact some time later. Three justifications for this assumption are that the system could have been insulated from the environment by design at time t = 0, that system and environment are only weakly coupled, or that system and environment are decoupled but one wants to turn on a coupling. (If one relaxes this assumption then things become much more complicated.)

Equation (2.32) also has some defects. One is that the unitary operator $U_{\rm SE}$ between the system and the environment is presumably a gigantic matrix that couples the degrees of freedom of the system and the possibly infinite degrees of freedom of the environment. One would have to describe the full dynamics of the system and the environment if one wants to describe the dynamics of the system. This is not only practically difficult to do but also physically undesirable because it should not be necessary to know the position of every mode in the environment if one has only access to the system and knows just a few things about the system.

The Hilbert space for the system and the environment is $\mathfrak{H}_S \otimes \mathfrak{H}_E$ where \mathfrak{H}_S is often assumed to be finitedimensional and usually \mathfrak{H}_E is taken to be an infinite number of harmonic oscillators. This describes the kinematics. For the dynamics describing how the system and the environment evolve according to the Schrödinger equation the Hamiltonian is a sum of the three terms $H_{tot} = H_S + H_E + V$ for the system, for the environment and for the interactions between them where $H_S + H_E = H_0$ represents the free part. Further as initial conditions, the environment (reservoir) is in thermal equilibrium at temperature T

$$\rho_{\rm E}(0) = \frac{e^{-\frac{H_{\rm E}}{k_{\rm B}T}}}{\operatorname{tr}\left(e^{-\frac{H_{\rm E}}{k_{\rm B}T}}\right)} \equiv \frac{e^{-\beta H_{\rm E}}}{\operatorname{tr}\left(e^{-\beta H_{\rm E}}\right)}$$
(2.33)

at time 0. The total state of system and environment at time t with its time evolution according to the Schrödinger equation become

$$\rho_{\rm tot}(t) = e^{-i H_{\rm tot} t} \left(\rho_{\rm S}(0) \otimes \rho_{\rm E}(0) \right) e^{i H_{\rm tot} t} \qquad \frac{d}{dt} \rho_{\rm tot}(t) = -i \left[H_0 + V, \rho_{\rm tot}(t) \right]$$
(2.34)

and the state of the system alone is $\rho_{\rm S}(t) = {\rm tr}_{\rm E}(\rho_{\rm tot}(t))$ using equation (2.32).

The next assumption is that the dynamics of $H_0 = H_S + H_E$ is solvable, and this means that H_E is a quasi-free Hamiltonian. One moves to the rotating frame of the interaction picture and defines

$$V_{\rm int}(t) = e^{-i H_0 t} V e^{i H_0 t} \qquad \qquad \rho_{\rm int,tot}(t) = e^{i H_0 t} \rho_{\rm tot}(t) e^{-i H_0 t}$$

with the goal to make the remaining dynamics a bit easier to describe. The Schrödinger equation

$$\frac{d}{dt}\rho_{\text{int,tot}}(t) = i\left(e^{-iH_0 t}\left[H_0, \rho_{\text{tot}}(t)\right]e^{iH_0 t}\right) - i\left(e^{-iH_0 t}\left[H_0 + V, \rho_{\text{tot}}(t)\right]e^{iH_0 t}\right) \\
= -i\left[V_{\text{int}}(t), \rho_{\text{int,tot}}(t)\right]$$
(2.35)

shows the dynamics in the rotating frame where the expression "rotating frame" means that unitary operations $\pm e^{-iH_0 t}$ look like a kind of rotation.

The equation (2.35) can be solved

$$\rho_{\rm tot}(t) = \int_0^t \frac{d}{ds} \rho_{\rm tot}(s) \, ds + \rho_{\rm tot}(0) = -i \int_0^t \frac{d}{ds} \Big[V(s), \rho_{\rm tot}(s) \Big] + \rho_{\rm tot}(0)$$

where the subscripts "int" have been dropped. Substituting this into (2.35) gives a Dyson series (a fixed-point iteration) where

$$\frac{d}{dt}\rho_{\text{tot}}(t) = -i\left[V(t), \rho_{\text{tot}}(0)\right] - \int_0^t dt_1\left[V(t), \left[V(t_1), \rho_{\text{tot}}(t_1)\right]\right]$$

is the result after the first iteration. The reason to stop after one iteration is that V(t) is assumed to be a small perturbation and the first non-trivial effects come at second order. One can get rid of the environment in the following by starting with

$$\frac{d}{dt}\rho_{\rm S}(t) = -i\,\mathrm{tr}_{\rm E}\left(\left[V(t),\rho_{\rm tot}(0)\right]\right) - \int_0^t dt_1\,\,\mathrm{tr}_{\rm E}\left(\left[V(t),\left[V(t_1),\rho_{\rm tot}(t_1)\right]\right]\right)$$

and using $\rho_{\text{tot}}(0) = \rho_{\text{S}}(0) \otimes \rho_{\text{E}}(0)$ after splitting V(t)

 $V(t) = V_{\rm S}(t) + V_{\rm SE}(t) \qquad \qquad V_{\rm S} = V_{\rm S} \otimes \mathbb{I}_{\rm E} \qquad \qquad {\rm tr}_{\rm E} \left(V_{\rm SE}(t) \, \rho_{\rm tot}(0) \right) = 0$

into a system piece and a system-environment piece as one can do by redefining H_0 .

Using the further assumption that V is weak stated as $V = \lambda H_{\rm I}$ for a small λ valid for the electromagnetic field interaction and the assumption (called the Born approximation) that sets $\rho_{\rm tot}(t_1) = \rho_{\rm S}(t_1) \otimes \rho_{\rm E}(t_1)$ the next steps can be computed. However, the Born approximation completely demolishes the entanglement between the system and the environment and is a terrible assumption because the system and the environment initially in a product state start interacting. As time passes electrons emit photons that are getting entangled and the entanglement between system and environment gets stronger and stronger. The system looks more and more getting mixed such that no definite state can be assigned to the system. However, the Born approximation implies that there is no entanglement between system and environment.

Thus, the Born approximation looks like a stupid assumption given what one knows about the physics of the situation. If one asks questions about the environment as well as the system this is a bad assumption. However, one is never going to interrogate the environment, and the only degrees of freedom accessible are the ones of the system. Thus, one can never see the entanglement between the system and the environment. On the other hand, something like the Born approximation is necessary because one has to get rid of the environment and if the environment can talk back this would also be a problem.

Applying these assumptions give

$$\frac{d}{dt}\rho_{\rm S}(t) = -i \left[V_{\rm S}(t), \rho_{\rm S}(0) \right] - \int_0^t dt_1 \, \operatorname{tr}_{\rm E} \left(\left[V_{\rm SE}(t), \left[V_{\rm SE}(t_1), \rho_{\rm S}(t_1) \otimes \rho_{\rm E}(t_1) \right] \right] \right)$$
(2.36)

and this is non-local in time making it quite difficult to solve. However, this is the starting point for many other calculations while here further assumptions are made. It is assumed that the physics of the bath is such that the system couples roughly equally to many closely spaced energy levels of the bath. If one draws the spectrum of the bath there are many closely spaced energy eigenvalues in any interval ΔE . This is a reasonable assumption which models most of the baths one encounters. The electromagnetic field, for example, consists of an infinite number of harmonic oscillators each with a slightly different energy. The spectrum is actually continuous. The state $\rho_{\rm S}(t)$ also should only depend on $\rho_{\rm S}(t')$ for t' near t. Thus, the equation (2.36) becomes

$$\frac{d}{dt}\rho_{\rm S}(t) = -i\left[V_{\rm S}(t), \rho_{\rm S}(0)\right] - \int_0^t dt_1 \,\operatorname{tr}_{\rm E}\left(\left[V_{\rm SE}(t), \left[V_{\rm SE}(t_1), \rho_{\rm S}(t) \otimes \rho_{\rm E}(0)\right]\right]\right) \tag{2.37}$$

and is called the Redfield equation.

The last assumption is called the Markov approximation and assumes the bath to be memoryless. It replaces the lower limit of the integral by $-\infty$ such that

$$\frac{d}{dt}\rho_{\rm S}(t) = -i\left[V_{\rm S}(t), \rho_{\rm S}(0)\right] - \int_{-\infty}^{t} dt_1 \operatorname{tr}_{\rm E}\left(\left[V_{\rm SE}(t), \left[V_{\rm SE}(t_1), \rho_{\rm S}(t) \otimes \rho_{\rm E}(0)\right]\right]\right)$$
(2.38)

and this is called the Born-Markov master equation. It requires $H_{\rm E}$ to have a continuous spectrum in the relevant energy ranges.

2.7 Example of the Radiative Decay of a Two-Level Atom

The following example shows a two-level atom that interacts with the electromagnetic field which is in its vacuum. When there is an excited atom one puts into an electromagnetic field in a vacuum then the atom decays after some time. Because all solutions of the Schrödinger equation are unitary operators, this situation is puzzling. The system is closed and undergoes unitary evolution but the atom always decays and never becomes reexcited. This is surprising because on one hand one has unitary dynamics for the whole system but on the other hand there is irreversible dynamics. The atom decays and goes to its ground state and the reverse process almost never occurs. Looking at the degrees of freedom this is no longer very surprising because there are two levels for the atom and an infinite number of levels for the environment. In the sense of statistical mechanics there are many more ways for the excitation to float into the environment than there are ways for the flow from the environment back to the atom.

The master equation can be applied to the radiative damping. Wigner and Weisskopf following Bohr and Einstein explained how radiative decay of an atom from an excited state could be explained in quantum mechanics. The environment is modeled as a free field with

$$H_{\rm E} = \sum_k \omega_k \, \hat{b}_k^\dagger \, \hat{b}_k$$

according to quantum field theory because the free field can be written as a collection of harmonic oscillators where ω_k is the energy of the k^{th} mode and \hat{b}_k^{\dagger} and \hat{b}_k are the bosonic creation and annihilation operators satisfying $[\hat{b}_k, \hat{b}_{\ell}^{\dagger}] = \delta_{k\ell}$. The system is the simplest quantum mechanical system namely a two-level atom representing a qubit with

$$H_{\rm S} = \omega_{\rm a} \, \frac{\sigma^2}{2}$$

stating basically that the ground state has energy zero and the excited state has an energy above zero. The interaction is a cartoon of dipole coupling

$$V = \sum_{k} \left(g_k \, \hat{b}_k + g_k \, \hat{b}_k^{\dagger} \right) \left(\sigma^+ + \sigma^- \right)$$

where $\sigma^+ = |0\rangle \langle 1|$ and $\sigma^- = |1\rangle \langle 0|$. The coupling constants g_k are proportional to the dipole matrix element for the transition. They depend on the structure of mode k

$$g_k \sim \frac{1}{\sqrt{V_k}}$$

where V_k is the volume of mode k although the derivation works for fairly general sets of g_k . Therefore, V in the interaction picture becomes

$$V_{\rm int}(t) = \sum_{k} \left(g_k \, \hat{b}_k \, e^{-i\,\omega_k \, t} + g_k \, \hat{b}_k^{\dagger} \, e^{i\,\omega_k \, t} \right) \left(\sigma^+ \, e^{i\,\omega_a \, t} + \sigma^- \, e^{-i\,\omega_a \, t} \right)$$

with some phases on top of the original V with $\omega_{\rm a} \sim 10^{15} \, {\rm s}^{-1}$.

Two of the four terms of V_{int} are ignored in the approximation

$$V_{\rm int}(t) \approx \sum_{k} \left(g_k \, \hat{b}_k \, \sigma^+ \, e^{-i \left(\omega_k - \omega_{\rm a}\right) t} + g_k \, \hat{b}_k^\dagger \, \sigma^- \, e^{i \left(\omega_k - \omega_{\rm a}\right) t} \right) \tag{2.39}$$

because the terms with $\omega_k + \omega_a$ represent very fast frequencies relative to $\omega_k - \omega_a$ and fast frequencies tend to self-average out. This is called the rotating wave approximation. Now the initial state is chosen as the vacuum state $\rho_{\rm E}(0) = |\Omega\rangle \langle \Omega|$ such that $\rho_{\rm SE}(0) = \rho_{\rm S}(0) \otimes |\Omega_{\rm E}\rangle \langle \Omega_{\rm E}|$. Thus, there are no photons in the field, and the terms with \hat{b}_k applied to the vacuum cancel as $\hat{b}_k |\Omega_{\rm E}\rangle = 0$ for all k. The interaction of the system with the environment is weak, but $g_k \hat{b}_k^{\dagger}$ eventually creates a degree of freedom in the environment and as time progresses this degree of freedom might act back on the atom. However, this is one of the assumptions that the bath is so designed that these excitations fly away and never interact with the atom. If the atom is in the excited state $|1\rangle$ at the bottom of the Bloch sphere then there is an amplitude for a process such that $|1\rangle$ gets mapped down to $|0\rangle$ and a photon is created and flies away. Once the atom is in state $|0\rangle$ it stays there forever because there is no process to take it back.

In order to derive the equations of motion one starts from the rotating wave approximation for $V_{int}(t)$ in (2.39). One splits this equation into

$$V^{+}(t) = \sum_{k} \left(g_k \, \hat{b}_k \, \sigma^+ \, e^{-i \left(\omega_k - \omega_a\right) t} \right) \qquad \qquad V^{-}(t) = \sum_{k} \left(g_k \, \hat{b}_k^\dagger \, \sigma^- \, e^{i \left(\omega_k - \omega_a\right) t} \right)$$

and inserts it into the Born approximation

$$\frac{d}{dt}\rho_{\rm S}(t) = -\int_0^t dt_1 \,\operatorname{tr}_{\rm E}\left(\left[V_{\rm int}(t), \left[V_{\rm int}(t_1), \rho_{\rm S}(t_1) \otimes |\Omega_{\rm E}\rangle \left\langle \Omega_{\rm E}\right|\right]\right)\right)$$

where the split of $V_{int}(t) = V^+(t) + V^-(t)$ gives four possible combinations as a complication but some of these terms vanish when acting on the vacuum as a simplification. Also the expansion of the commutator gives additional terms, and together this gives sixteen terms leading to sixteen similar calculations

$$\frac{d}{dt}\rho_{\rm S}(t) = -\int_0^t dt_1 \left(\mathbb{I}_{\rm S} \otimes \langle \Omega_{\rm E} |\right) \left(V^+(t)V^+(t_1) \left(\rho_{\rm S}(t_1) \otimes \mathbb{I}_{\rm E}\right) + V^+(t)V^-(t_1) \left(\rho_{\rm S}(t_1) \otimes \mathbb{I}_{\rm E}\right) + V^-(t)V^-(t_1) \left(\rho_{\rm S}(t_1) \otimes \mathbb{I}_{\rm E}\right) + \dots - V^+(t_1) \left(\rho_{\rm S}(t_1) \otimes \mathbb{I}_{\rm E}\right) V^+(t) + \dots \right) \left(\mathbb{I}_{\rm S} \otimes |\Omega_{\rm E}\rangle\right)$$

using the identity $\operatorname{tr}_{\mathrm{E}}(W(\rho_{\mathrm{S}} \otimes |\Omega_{\mathrm{E}}\rangle \langle \Omega_{\mathrm{E}}|)) \equiv (\mathbb{I} \otimes \langle \Omega_{\mathrm{E}}|) W(\rho_{\mathrm{S}} \otimes \mathbb{I}) (\mathbb{I} \otimes |\Omega_{\mathrm{E}}\rangle)$. This shows five of the sixteen terms. Some cancel such that

$$\frac{d}{dt}\rho_{\rm S}(t) = -\int_0^t dt_1 \left(\mathbb{I}_{\rm S} \otimes \langle \Omega_{\rm E} |\right) \left(V^+(t) V^-(t_1) \left(\rho_{\rm S}(t_1) \otimes \mathbb{I}_{\rm E}\right) + \dots \right) \left(\mathbb{I}_{\rm S} \otimes |\Omega_{\rm E}\rangle\right)$$

because of $V^+(\mathbb{I} \otimes |\Omega_{\rm E}\rangle) = 0$ and $(\langle \Omega_{\rm E} | \otimes \mathbb{I})V^- = 0$. Only four terms remain, and the first one is

$$\begin{aligned} (\mathbb{I}_{\mathrm{S}} \otimes \langle \Omega_{\mathrm{E}} |) V^{+}(t) V^{-}(t_{1}) (\rho_{\mathrm{S}}(t_{1}) \otimes \mathbb{I}_{\mathrm{E}}) (\mathbb{I}_{\mathrm{S}} \otimes |\Omega_{\mathrm{E}}\rangle) \\ &= \sum_{k,\ell} g_{k} g_{\ell} e^{-i (\omega_{k} - \omega_{\mathrm{a}}) t + i (\omega_{\ell} - \omega_{\mathrm{a}}) t_{1}} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle \\ &= \sum_{k} g_{k}^{2} e^{i (\omega_{k} - \omega_{\mathrm{a}}) (t_{1} - t)} \sigma^{+} \sigma^{-} \rho_{\mathrm{S}}(t_{1}) \langle \Omega_{\mathrm{E}} | \hat{b}_{k} \hat{b}_{\ell}^{\dagger} | \Omega_{\mathrm{E}}\rangle$$

because $\langle \Omega_{\rm E} | \hat{b}_k \hat{b}_{\ell}^{\dagger} | \Omega_{\rm E} \rangle$ is just a delta function. Note that the environment is no longer present in this equation. The other three terms can be calculated similarly.

The final result including the other three terms is

$$\frac{d}{dt}\rho_{\rm S}(t) = -\int_0^t dt_1 \left\{ \Gamma(t-t_1) \left[\sigma^+ \sigma^- \rho_{\rm S}(t_1) - \sigma^- \rho_{\rm S}(t_1) \sigma^+ \right] + \left[-\sigma^- \rho_{\rm S}(t_1) \sigma^+ + \sigma^+ \sigma^- \rho_{\rm S}(t_1) \right] \overline{\Gamma}(t-t_1) \right\}$$
(2.40)

where $\Gamma(\tau) = \sum_k g_k^2 e^{-i(\omega_k - \omega_a)\tau}$. This equation is not memoryless because of $t - t_1$ but it involves only the system density operator and nothing from the environment anymore. This equation is also no longer completely positive because of the approximation truncating the Taylor expansion.

One can surprisingly recover complete positivity by making more approximations. To make the Markov approximation the sum is replaced by an integral in a first step such that

$$\Gamma(\tau) = \sum_{k} g_k^2 e^{-i(\omega_k - \omega_a)\tau} \qquad \Rightarrow \qquad \Gamma(\tau) = \int_0^\infty d\omega \,\rho(\omega) \, g^2(\omega) \, e^{-i(\omega - \omega_a)\tau}$$

where $\rho(\omega)$ is the density of states assumed to be smooth but infinite while $\chi(\omega) = \rho(\omega) g^2(\omega)$ is firstly assumed to be finite and secondly assumed to be slowly varying over a frequency range $\omega \approx \omega_a$.

If $\chi(\omega) = \rho(\omega) g^2(\omega)$ is slowly varying then the Fourier transformed $\hat{\chi}(\omega)$ after a phase-shift looks like a delta function as illustrated in the figure on the right side and $\Gamma(\tau)$ can be approximated as

$$\Gamma(\tau) = \Gamma_0 \int_0^\infty d\omega \, e^{-i \, (\omega - \omega_{\mathbf{a}}) \, \tau} \, \chi(\omega) = \Gamma_0 \, \hat{\chi}(\omega) \, e^{i \, \omega_{\mathbf{a}}}$$
$$\cong \Gamma_0 \, \delta(\tau) \, e^{i \, \omega_{\mathbf{a}} \, \tau}$$



to complete the Markov approximation. This turns the equation (2.40) into a memoryless equation

$$\frac{d}{dt}\rho_{\rm S}(t) \cong -\left(\int_{-\infty}^{t} dt_1 \,\Gamma(t-t_1)\right) \left[\sigma^+ \sigma^- \rho_{\rm S}(t_1) - \sigma^- \rho_{\rm S}(t_1) \,\sigma^+\right] \\ + \left[-\sigma^- \rho_{\rm S}(t_1) \,\sigma^+ + \sigma^+ \sigma^- \rho_{\rm S}(t_1)\right] \left(\int_{-\infty}^{t} \overline{\Gamma}(t-t_1) \,dt_1\right)$$

changing also the lower integration boundary to $-\infty$.

2.8 Bosonic Solutions of the Lindblad Equation

The left integral is just a complex number written as $\frac{\gamma}{2} + i \Delta \omega_a$ with real and imaginary part such that

$$\frac{d}{dt}\rho = -i\left(\frac{\Delta\omega_{\rm a}}{2}\right)\left[\sigma^2,\rho\right] + \gamma \mathcal{D}[\sigma^-](\rho)$$
(2.41)

with the definition $\mathcal{D}[A](\rho) = A\rho A^{\dagger} - \frac{1}{2}(A^{\dagger}A\rho + \rho A^{\dagger}A)$. This is a memoryless equation where the original Hamiltonian shows up as σ^2 with a frequency factor $\frac{\Delta \omega_a}{2}$. The term $-i(\frac{\Delta \omega_a}{2})[\sigma^2, \rho]$ represents the unitary part of the dynamics and $\gamma \mathcal{D}[\sigma^-](\rho)$ the non-unitary part. This equation is called the Lindblad equation and has the remarkable property that it generates a completely positive map. For finite-dimensional systems any evolution equation in quantum mechanics that is continuous and memoryless gives rise to a Lindblad equation. For infinite-dimensional systems this is still controversial.

In order to solve equation (2.41) with its 2×2 matrices the frequency shift is set to zero $\Delta \omega_a = 0$ because the unitary part is not the interesting part of the dynamics as it just generates a rotation on the Bloch sphere. The goal is to solve the equation of motion

$$\begin{aligned} \frac{d}{dt} \begin{pmatrix} p & \bar{x} \\ x & 1-p \end{pmatrix} &= \gamma \left\{ \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} p & \bar{x} \\ x & 1-p \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p & \bar{x} \\ x & 1-p \end{pmatrix} - \frac{1}{2} \begin{pmatrix} p & \bar{x} \\ x & 1-p \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\} \\ &= \gamma \begin{pmatrix} 1-p & -\frac{1}{2}\bar{x} \\ -\frac{1}{2}x & -(1-p) \end{pmatrix} \end{aligned}$$

where the equation with p and the equation with x nicely decouple. This lead to the two equations

$$\frac{dp}{dt} = \gamma(1-p) \qquad \qquad \frac{dx}{dt} = -\frac{\gamma}{2}x$$

and the other two equations are the same. Their solution is

$$p(t) = 1 - e^{-\gamma t} \left(1 - p(0) \right) \qquad x(t) = x(0) e^{-\frac{\gamma}{2}t} \qquad \rho(t) = \begin{pmatrix} 1 - e^{-\gamma t} \left(1 - p(0) \right) & \bar{x}(0) e^{-\frac{\gamma}{2}t} \\ x(0) e^{-\frac{\gamma}{2}t} & e^{-\gamma t} \left(1 - p(0) \right) \end{pmatrix}$$

where all the four exponential terms converge to zero and the off-diagonal terms representing coherence therefore decay exponentially quickly in time.

On the Bloch sphere in the figure on the right side all states move to $|0\rangle$. Thus, this atom will be with very high probability in its ground state

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

darker and darker. The total Hamiltonian after the rotating wave approximation is

after a characteristic decay time depending on γ . The quantum of energy in the atom if there was one propagates to the environment, flies away with the speed of light and never comes back.

This is a prototype for every other calculation one can do with decoherence processes. There is an environment that acts as a gigantic measuring instrument and sucks out coherence sending the system to a fixed point. This fixed point $\lim_{t\to\infty} \rho(t) = \rho_{\rm SS}$ is called the steady state and is $\rho_{\rm SS} = |0\rangle \langle 0|$ in the case of the two-level atom in the example.

Another example is a cavity in the form of a box with mirrors and light in it drawn on the right side. One of the mirrors is not perfect and the others are as perfect as one can make them. Thus, whatever electromagnetic field was initially in the box will decay after some time, and the situation is as in an elevator with mirrors where one sees a long tunnel getting

$$H = \omega_{\rm C} \, \hat{a}^{\dagger} \hat{a} + \sum_k \omega_k \, \hat{b}_k^{\dagger} \hat{b}_k + \sum_k g_k \left(\hat{a}^{\dagger} \hat{b}_k + \hat{a} \, \hat{b}_k^{\dagger} \right)$$

where the three terms correspond to $H_{\rm S}$, $H_{\rm E}$ and $V_{\rm int}$, respectively. Assuming weak coupling the solution after the Born-Markov approximation becomes

$$\frac{d}{dt}\rho = \gamma(\bar{n}+1)\mathcal{D}[\hat{a}]\rho + \gamma\,\bar{n}\,\mathcal{D}[\hat{a}^{\dagger}]\rho \qquad (2.42)$$

where \bar{n} means the number of photons outside the cavity at cavity frequency $\omega_{\rm C}$. There is an additional second term coming from the fact that if one assumes the environment is not in the vacuum state but in some thermal state then there is a chance for the environment to incoherently stuff a photon back into the box. The total initial state is

$$\rho_{\rm SE}(0) \equiv \rho_{\rm S}(0) \otimes \left(\frac{e^{-\beta H_{\rm E}}}{\operatorname{tr}(e^{-\beta H_{\rm E}})}\right)$$

where the cavity as the system contains some photons and the environment is in some thermal state.

To compare (2.42) with (2.41) the environment is assumed to be in a vacuum $\rho_{\rm E} = |\Omega\rangle \langle \Omega|$ such that equation (2.42) becomes

$$\frac{d}{dt}\rho = \gamma \,\mathcal{D}[\hat{a}]\rho$$

and looks very similar to (2.41) with $\Delta \omega_a = 0$. However, this is an infinite-dimensional equation because ρ represents an infinite number of degrees of freedom as there is a harmonic oscillator inside the box and not a spin. One can still solve it using the characteristic function $\chi(\xi) = \operatorname{tr}(\rho D(\xi))$ and gets

$$\frac{d}{dt}\chi(\xi) = \gamma \operatorname{tr}\left(\rho\left(\hat{a}^{\dagger}D(\xi)\hat{a} - \frac{1}{2}D(\xi)\hat{a}^{\dagger}\hat{a} - \frac{1}{2}\hat{a}^{\dagger}\hat{a}D(\xi)\right)\right)$$



leading to the equations of motion

$$\partial_t \chi(\xi) = \frac{\gamma}{2} \left(-|\xi|^2 - \overline{\xi} \,\overline{\partial}_{\xi} - \xi \,\partial_{\xi} \right) \chi(\xi)$$

because every derivative with respect to ξ or $\overline{\xi}$ brings down factors of \hat{a} and \hat{a}^{\dagger} . One can actually solve this equation and gets

$$\chi(\xi) = e^{\frac{K(t)}{2}|\xi|^2} \qquad K(t) = 1 - e^{-\gamma t} \left(1 - K(0)\right)$$

by guessing that $\chi(\xi)$ is a quadratic function. The function K(t) equals the function p(t) for the two-level atom example above, and both are Fokker-Planck type equations. This is not a surprise because $\chi(\xi)$ more and more looks like the characteristic function of the vacuum. All photons have left the cavity and the box is in a vacuum state. The case where the environment is in a thermal state instead of the vacuum state is a bit more complicated and is not covered here.

2.9 Quasi-Free Fermion Systems

So far systems embedded in a environment which is comprised of bosonic degrees of freedom have been studied. The natural system to consider for fermions is a block of conducting material (usually a resistor) and in it is some kind of impurity or quantum dot like a cavity for electrons. It turns out that one can model the passage of the electrons through that quantum dot with a formalism essentially identical with the one derived above for cavities and other open quantum systems. As a bonus one gets to solve all fermion systems quasi for free.

As the environment in the bosonic case has been modeled as a bath of harmonic oscillators one considers for the fermionic case the most general model with a quadratic Hamiltonian

$$\hat{H} = \frac{1}{2} \sum_{j,k=1}^{n} \left(\hat{f}_{j}^{\dagger}[\underline{A}]_{jk} \hat{f}_{k} - \hat{f}_{j}[\underline{A}]_{jk} \hat{f}_{k}^{\dagger} + \hat{f}_{j}[\underline{B}]_{jk} \hat{f}_{k} - \hat{f}_{j}^{\dagger}[\underline{B}]_{jk} \hat{f}_{k}^{\dagger} \right)$$
(2.43)

in terms of two $n \times n$ matrices <u>A</u> and <u>B</u>. This Hamiltonian can be written as

$$\hat{H} = \frac{1}{2} \underline{\hat{f}}^T \underline{\underline{H}} \underline{\hat{f}} \qquad \underline{\underline{H}} = \begin{pmatrix} \underline{\underline{B}} & -\underline{\underline{A}} \\ \underline{\underline{A}} & -\underline{\underline{B}} \end{pmatrix} \qquad \underline{\hat{f}} = (\hat{f}_1, ..., \hat{f}_n; \hat{f}_1^{\dagger}, ..., \hat{f}_n^{\dagger}) \qquad (2.44)$$

in a compact form. This is the most general model with creation and annihilation operators \hat{f}_j^{\dagger} and \hat{f}_j , respectively, for *n* spinless fermions. The anticommutation relations are

$$\left\{\hat{f}_{j},\hat{f}_{k}^{\dagger}\right\} = \delta_{jk} \qquad \left\{\hat{f}_{j},\hat{f}_{k}\right\} = \left\{\hat{f}_{j}^{\dagger},\hat{f}_{k}^{\dagger}\right\} = 0 \qquad (2.45)$$

as expected for fermions. To ensure $\hat{H} = \hat{H}^T$ requires that matrix $\underline{\underline{A}}$ is real and symmetric and that matrix $\underline{\underline{B}}$ is real and antisymmetric. (There is actually a possibility to make these two matrices complex when one puts a fermion into an magnetic field.)

One can solve this model exactly the same way as for the bosonic case by doing some canonical rotations of the operators. Before that can be done the fermionic position and momentum operators have to be defined because the operators \hat{f}_j are not hermitian. Introducing Majorana operators

$$\underline{\hat{c}} = \underline{\underline{\Omega}}\,\underline{\hat{f}} \qquad \underline{\underline{\Omega}} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I} & \mathbb{I} \\ -i\mathbb{I} & i\mathbb{I} \end{pmatrix} \qquad \underline{\underline{\Omega}}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I} & i\mathbb{I} \\ \mathbb{I} & -i\mathbb{I} \end{pmatrix}$$
(2.46)

which are very much like the position and momentum operators. Two of these operators are

$$\hat{c}_1 = \frac{1}{\sqrt{2}} \left(\hat{f}_1 + \hat{f}_1^{\dagger} \right)$$
 $\hat{c}_{n+1} = \frac{1}{\sqrt{2}} \left(-i \, \hat{f}_1 + i \, \hat{f}_1^{\dagger} \right)$

as examples where \hat{c}_1 is like the position \hat{x} and \hat{c}_{n+1} like the momentum \hat{p} . Note also that the Majorana operators are hermitian operators obeying anticommutation relations $\{\hat{c}_j, \hat{c}_k\} = \delta_{jk}$.

The Hamiltonian becomes

$$\hat{H} = \frac{i}{2} \hat{\underline{c}}^T \begin{pmatrix} 0 & \underline{V} \\ -\underline{\underline{V}}^T & \overline{0} \end{pmatrix} \hat{\underline{c}} \qquad \qquad \underline{\underline{V}} = \underline{\underline{A}} + \underline{\underline{B}}$$
(2.47)

where $\underline{\underline{V}}$ is not hermitian because $\underline{\underline{A}}$ is symmetric but $\underline{\underline{\underline{B}}}$ is antisymmetric. Thus, one cannot expect to diagonalize $\underline{\underline{V}}$ in terms of orthogonal matrices but one can use singular value decomposition

$$\underline{\underline{V}} = \underline{\underline{O}}_1 \underline{\underline{D}} \underline{\underline{O}}_2^T \qquad \qquad \underline{\underline{D}} = \operatorname{diag}(\sigma_1, \sigma_2, ..., \sigma_n) \qquad \qquad \sigma_1 \ge \sigma_2 \ge ... \ge \sigma_n$$

with two orthogonal matrices $\underline{O}_1, \underline{O}_2 \in O(n)$. One gets \underline{O}_1 by diagonalizing the symmetric matrix $\underline{\underline{V}} \underline{\underline{V}}^T$ and \underline{O}_2 by diagonalizing the symmetric matrix $\underline{\underline{V}} \underline{\underline{V}}^T \underline{\underline{V}}$. The canonical transformation

$$\underline{\hat{c}}' = \begin{pmatrix} \hat{c}_1' \\ \vdots \\ \hat{c}_{2n}' \end{pmatrix} = \begin{pmatrix} \underline{\underline{O}}_1^T & 0 \\ 0 & \underline{\underline{O}}_2^T \end{pmatrix} \begin{pmatrix} \hat{c}_1 \\ \vdots \\ \hat{c}_{2n} \end{pmatrix}$$

preserves the anticommutation relations. The Hamiltonian in the new Majorana operators

$$\begin{aligned} \hat{H} &= \frac{i}{2} \, \hat{\underline{c}}^T \begin{pmatrix} 0 & \underline{V} \\ -\underline{\underline{V}}^T & \overline{0} \end{pmatrix} \hat{\underline{c}} = \frac{i}{2} \, (\hat{\underline{c}}')^T \begin{pmatrix} \underline{\underline{O}}_1 & 0 \\ 0 & \underline{\underline{O}}_2 \end{pmatrix} \begin{pmatrix} 0 & \underline{\underline{V}} \\ -\underline{\underline{V}}^T & \overline{0} \end{pmatrix} \begin{pmatrix} \underline{\underline{O}}_1^T & 0 \\ 0 & \underline{\underline{O}}_2^T \end{pmatrix} (\hat{\underline{c}}') \\ &= \frac{i}{2} \, (\hat{\underline{c}}')^T \begin{pmatrix} 0 & \underline{\underline{D}} \\ -\underline{\underline{D}} & \overline{0} \end{pmatrix} (\hat{\underline{c}}') \end{aligned}$$
(2.48)

is not diagonal but is as good as diagonal.

Defining $\underline{\hat{b}} = \underline{\Omega}^{-1} \underline{\hat{c}}'$ which are not hermitian operators but creation and annihilation operators brings the Hamiltonian into the form

$$\hat{H} = \frac{1}{2} \hat{\underline{b}}^T \begin{pmatrix} 0 & -\underline{\underline{D}} \\ \underline{\underline{D}} & 0 \end{pmatrix} \hat{\underline{b}} = \sum_{j=1}^n \sigma_j \left(\hat{b}_j^{\dagger} \hat{b}_j - \frac{1}{2} \right)$$
(2.49)

with $\underline{\hat{b}}^T = (\hat{b}_1, ..., \hat{b}_n; \hat{b}_1^{\dagger}, ..., \hat{b}_n^{\dagger})$ where the left term shows that there is a bunch of *n* decoupled fermion oscillators.

Fermion oscillators are much simpler than boson oscillators such that one can easily determine the ground state. The Hilbert space for a fermion oscillator has only two dimensions and the Hamilton operator looks like

$$\hat{H} = \hat{b}^{\dagger}\hat{b} \cong \begin{pmatrix} 0 & 0\\ 0 & 1 \end{pmatrix}$$

with the two states $|0\rangle$ (upper row and left column in the matrix) with one fermion in the system and $|1\rangle$ (lower row and right column in the matrix) with one fermion in the system. The ground state is the empty state $|0\rangle$ with $\hat{b} |0\rangle = 0$, and the only other state is $|1\rangle = \hat{b}^{\dagger} |0\rangle$ because one cannot have more than one fermion in the same mode.

Many-body fermion systems such as the one in (2.49) have a Hilbert space which grows with the number of particles but is finite-dimensional and not infinite-dimensional as for the boson systems. The dimension is 2^n for a system with *n* fermions. The Hamiltonian (2.49) shows as mentioned above *n* independent oscillators. The ground state is unique if all σ_j are bigger than zero but some σ_j may be zero. Thus, the ground state space of \hat{H} is $2^{n-\operatorname{rank}(\underline{V})}$ -fold degenerate. In the following \underline{V} is assumed to have full rank.

The ground state is the empty vacuum in terms of the operators \hat{b}_j such that $\hat{b}_j |\Omega\rangle = 0$ for j = 1, ..., n. This looks odd because it is different what one learns about fermions especially those in a metal. A metal has a description in terms of a Fermi sea which is full of fermions. This is not in contradiction with this because the operators \hat{b}_j are not the original fermion operators but some superpositions of them. Using the operators \hat{f}_j instead shows that this ground state has many particles in it. The gap between the ground state and the first excited state is

$$\Delta E = \sqrt{\lambda_{\min}(\underline{\underline{V}}\,\underline{\underline{V}}^T)} = \sqrt{\lambda_{\min}\left((\underline{\underline{A}} + \underline{\underline{B}})(\underline{\underline{A}} - \underline{\underline{B}})\right)} \tag{2.50}$$

since all eigenvalues of the model \hat{H} can be calculated. The first eigenvalue $\hat{H} |\Omega\rangle = E_0 |\Omega\rangle$ is

$$E_0 = -\frac{1}{2} \sum_{j=1}^n \sigma_j$$

and the next eigenvalues are $E_j = E_0 + \sigma_j$ for the single-particle state $\hat{b}_j^{\dagger} |\Omega\rangle$ and $E_{j < k} = E_0 + \sigma_j + \sigma_k$ for the two-particle state $\hat{b}_j^{\dagger} \hat{b}_k^{\dagger} |\Omega\rangle$. Finally, the eigenvalue is

$$E_{12\dots n} = \frac{1}{2} \sum_{j=1}^{n} \sigma_j$$

for the *n*-particle state $\hat{b}_1^{\dagger} \hat{b}_2^{\dagger} ... \hat{b}_n^{\dagger} |\Omega\rangle$. The ground state energy is negative, and the eigenvalues grow from the *j*-particle state to the *j* + 1-particle state because the values σ_j are assumed positive as stated above. For the gap between the ground state and the first excited state the single-particle state with the lowest energy is used as indicated by λ_{\min} in (2.50) meaning the minimal eigenvalue.

The result of the above calculations is that practically every quadratic fermion model one can encounter has been diagonalized. This includes metal, the Dirac equation, Majorana fermions and superconducting wires, and this result is completely general as it does not restrict the model with the exception that it must be quadratic.

It is clear what is meant by the fact that a bosonic model is Gaussian but it is less clear what is meant by the statement that this ground state is Gaussian because firstly there is no characteristic function and secondly there are Grassmann numbers involved. The statement that the ground state is Gaussian means that it is determined by its second moments. The covariance matrix for a fermion model is defined as the $2n \times 2n$ matrix

$$\left[\underline{\underline{\Gamma}'}\right]_{jk} = \langle \Omega \mid \left[\underline{\hat{b}}\right]_j \left[\underline{\hat{b}}\right]_k \mid \Omega \rangle \qquad \qquad \underline{\underline{\Gamma}'} = \begin{pmatrix} 0 & \mathbb{I} \\ 0 & 0 \end{pmatrix}$$
(2.51)

with j, k = 1, ..., 2n similarly to the bosonic case. Because $\underline{\hat{b}}$ contains elements \hat{b}_{ℓ} and \hat{b}_{ℓ}^{\dagger} the covariance matrix contains four types of terms $[\underline{\hat{b}}]_j [\underline{\hat{b}}]_k$. It has the simple form shown in (2.51) because only terms $\hat{b}_j \hat{b}_k^{\dagger}$ are non-zero.

The covariance matrix in terms of $\hat{\underline{c}}$ is defined as

$$\begin{bmatrix} \underline{\Gamma} \end{bmatrix}_{jk} = \langle \Omega \mid [\underline{\hat{c}}]_j \mid \underline{\hat{c}} \rceil_k \mid \Omega \rangle = \begin{pmatrix} \underline{\underline{O}}_1 & 0\\ 0 & \underline{\underline{O}}_2 \end{pmatrix} \begin{pmatrix} \underline{\Omega} \end{pmatrix} \underline{\underline{\Gamma}}' \begin{pmatrix} \underline{\Omega} \end{pmatrix}^T \begin{pmatrix} \underline{\underline{O}}_1^T & 0\\ 0 & \underline{\underline{O}}_2^T \end{pmatrix}$$
$$= \frac{1}{2} \begin{pmatrix} \mathbb{I} & i \underline{\underline{O}}_1 \underline{\underline{O}}_2^T\\ -i \underline{\underline{O}}_2 \underline{\underline{O}}_1^T & \mathbb{I} \end{pmatrix}$$
(2.52)

and in terms of \hat{f}

$$\langle \Omega | \left[\underline{\hat{f}} \right]_{j} \left[\underline{\hat{f}} \right]_{k} | \Omega \rangle = \left(\underline{\underline{\Omega}}^{-1} \right) \underline{\underline{\Gamma}} \left(\underline{\underline{\Omega}}^{-1} \right)^{T} = \frac{1}{4} \begin{pmatrix} \underline{\underline{V}}^{T} - \underline{\underline{V}} & 2 \mathbb{I} + \underline{\underline{V}}^{T} + \underline{\underline{V}} \\ 2 \mathbb{I} - (\underline{\underline{V}}^{T} + \underline{\underline{V}}) & \underline{\underline{V}} - \underline{\underline{V}}^{T} \end{pmatrix}$$
 (2.53)

where $\underline{\underline{V}} = \underline{\underline{O}}_1 \underline{\underline{O}}_2^T$.

Gaussian models for bosons and for fermions are easy in the sense that one can determine everything about their eigenvalues and eigenvectors. One can usually not say much about models which are not Gaussian but these quadratic models are often used as a starting point. One can solve them completely and add a small perturbation for other models to be solved using perturbation theory. Note that the ground state $|\Omega\rangle$ is not necessarily empty but may contain fermions. The average number of fermions in terms of the original variables in the ground state is

$$\sum_{j=1}^{n} \langle \Omega \,|\, \hat{n}_{j} \,|\, \Omega \rangle = \sum_{j=1}^{n} \langle \Omega \,|\, \hat{f}_{j}^{\dagger} \hat{f}_{j} \,|\, \Omega \rangle = \frac{n}{2} - \sum_{j=1}^{n} \frac{1}{4} \left(\underline{\underline{V}}^{T} + \underline{\underline{V}} \right)_{jj} = \frac{1}{2} \operatorname{tr}(\mathbb{I}) - \frac{1}{2} \left(\underline{\underline{O}}_{1} \underline{\underline{O}}_{2}^{T} \right)$$

containing $\frac{n}{2}$ particles plus something that can vary between $\pm \frac{n}{2}$ depending on $\underline{\underline{O}}_1$ and $\underline{\underline{O}}_2$. Thus, it can vary between no fermions and the situation where every single fermion mode is occupied. One can see this when free fermions are hopping in the presence of a reservoir kept at a chemical potential μ .

2.10 Example of the Tunneling of Fermions Through a Quantum Dot

As an example the master equation describing the tunneling of fermions through a quantum dot between two fermion reservoirs is derived. This is the closest

analogy for fermions in an optical cavity. An optical cavity is actually coupled to two reservoirs with the in-modes and the out-modes as shown in the figure on the right side. The in-modes and the out-modes are usually both in the vacuum for bosons.



The situation is different for the fermions as illustrated in the figure on the left side. There are two fermionic reservoirs where one has a higher chemical potential than the other. It is assumed that the quantum dot has a single bound state with energy \mathcal{E}_{c} and that it is connected via tunnel junctions to the fermion reservoirs. There is a bias voltage V_{SD}

across source and drain. Both reservoirs are at thermal equilibrium at temperature T but with different chemical potentials $\mu_{\rm S}$ and $\mu_{\rm D}$. The Hamiltonian is

$$\hat{H}_{\text{QD+leads}} = \sum_{k} \mathcal{E}_{k}^{\text{S}} \hat{a}_{k}^{\dagger} \hat{a}_{k} + \mathcal{E}_{\text{c}} \hat{c}^{\dagger} \hat{c} + \sum_{p} \mathcal{E}_{p}^{\text{D}} \hat{b}_{p}^{\dagger} \hat{b}_{p} + \sum_{k} \left((T_{k}^{\text{S}}) \hat{c}^{\dagger} \hat{a}_{k} + (T_{k}^{\text{S}})^{*} \hat{a}_{k}^{\dagger} \hat{c} \right) + \sum_{p} \left((T_{p}^{\text{D}}) \hat{b}_{p}^{\dagger} \hat{c} + (T_{p}^{\text{D}})^{*} \hat{c}^{\dagger} \hat{b}_{p} \right)$$

$$(2.54)$$

with one term for the quantum dot and two terms for the reservoirs. The three terms in the first line are \hat{H}_0 and the two terms in the second line are \hat{V} . The operators \hat{a}_k , \hat{c} , \hat{b}_p are fermion operators for source, dot, drain, respectively, but note that the operators \hat{c} are not Majorana here. The anticommutation relations are $\{\hat{a}_k, \hat{a}_\ell^\dagger\} = \delta_{k\ell}, \{\hat{c}, \hat{c}^\dagger\} = \mathbb{I}, \{\hat{b}_p, \hat{b}_q^\dagger\} = \delta_{pq}$, and all others vanish. The matrices T_k^S and T_p^D are the tunneling coefficients, and they contain small numbers because the transitions from the source to the dot and from the dot to the drain are classically forbidden. It is assumed that the fermions tunnel one by one from one lead to the other. The energies $\mathcal{E}_k^S = \frac{k^2}{2m}$ and $\mathcal{E}_p^D = \frac{p^2}{2m}$ are the non-relativistic kinetic energies in the momentum basis because these are free fermions moving in the reservoirs. The quantum dot is the system and the two leads are the environment.

This model with the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ is quadratic and can be diagonalized but it will not be solved analytically because it does not give insight in how the equation of motion is determined. The derivation of the Born-Markov master equation will be exactly followed as if the particles were bosons. The resulting solution is only an approximation but it is easier to use than the analytic solution. It also allows to describe the dynamics of the dot alone while the exact solution gives all the modes of the source, the drain and the dot, and it is not easy to extract the dynamics of the dot.

The setup used is as follows for the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$. The ground state at time t = 0where the tunnel junctions are very high is $\rho_{\rm in} = |\Omega_{\rm S}\rangle \langle \Omega_{\rm S}| \otimes |\Omega_{\rm dot}\rangle \langle \Omega_{\rm dot}| \otimes |\Omega_{\rm D}\rangle \langle \Omega_{\rm D}|$ where $|\Omega_{\rm S}\rangle \langle \Omega_{\rm S}|$ and $|\Omega_{\rm D}\rangle \langle \Omega_{\rm D}|$ are filled with fermions due to the chemical potential. The state for the dot alone is

$$\rho_{\rm dot}(t) = \operatorname{tr}_{\rm S,D}\left(e^{-i\,t\,\hat{H}}\,\rho_{\rm in}\,e^{-i\,t\,\hat{H}}\right)$$

when the time goes on. This works when there is a huge resistance between the source and the drain. The Born-Markov master equation for the dot alone requires that there is a small rate hopping into the dot and there is a small rate hopping out of the dot. Outside this regime the approach shown here will not work and another description of the model is needed but is not introduced here. In the interaction picture \hat{H}_0 is the free part and

$$\hat{V}(t) = \sum_{j=1}^{2} \left(\hat{c}^{\dagger} \hat{Y}_{j}(t) e^{i\mathcal{E}_{c} t} + \hat{c} \, \hat{Y}_{j}^{\dagger}(t) e^{-i\mathcal{E}_{c} t} \right) \qquad \hat{Y}_{1}(t) = \sum_{k} T_{k}^{S} \hat{a}_{k} \, e^{-i\mathcal{E}_{k}^{S} t} \qquad \hat{Y}_{2}(t) = \sum_{p} T_{p}^{D} \hat{b}_{p} \, e^{-i\mathcal{E}_{p}^{D} t}$$

is the interaction part in the rotating frame where the free dynamics is trivialized. Now one can follow the standard method introduced above for the bosonic case. This leads to an equation of motion for the density operator ρ of the bound state of the quantum dot.

The reservoir correlation functions needed are

$$I_{jN}(t) = \int_0^t dt_1 \, \langle \hat{Y}_j^{\dagger}(t) \, \hat{Y}_j(t_1) \rangle \, e^{-i \, \mathcal{E}_c \, (t-t_1)} \qquad \qquad I_{jA}(t) = \int_0^t dt_1 \, \langle \hat{Y}_j(t_1) \, \hat{Y}_j^{\dagger}(t) \rangle \, e^{-i \, \mathcal{E}_c \, (t-t_1)}$$

where N stands for normal order and A stands for antinormal order. The antinormal ordered correlation function is there because fermions can have a Fermi sea. It is assumed that the leads (also called "Fermi reservoirs") are in thermal equilibrium. Because of j = 1, 2 and N or A there are four cases but only one is shown because the others are similar. One finds

$$I_{1N}(t) = \sum_{k} \bar{n}_{k}^{S} \left| T_{k}^{S} \right|^{2} \int_{0}^{t} dt_{1} e^{i(\mathcal{E}_{k}^{S} - \mathcal{E}_{c})(t - t_{1})}$$
(2.55)

because

$$\langle \hat{Y}_{1}^{\dagger}(t) \, \hat{Y}_{1}(t_{1}) \rangle = \sum_{k,\ell} (T_{k}^{\mathrm{S}})^{*} (T_{\ell}^{\mathrm{S}}) \, e^{i\mathcal{E}_{k}^{\mathrm{S}}t - i\mathcal{E}_{\ell}^{\mathrm{S}}t_{1}} \, \langle \hat{a}_{k}^{\dagger} \, \hat{a}_{\ell} \rangle = \sum_{k} \left| T_{k}^{\mathrm{S}} \right|^{2} e^{i\mathcal{E}_{k}^{\mathrm{S}}(t - t_{1})} \, \bar{n}_{k}^{\mathrm{S}}$$

due to $\langle \hat{a}_k^{\dagger} \hat{a}_\ell \rangle = \bar{n}_k^{\rm S} \delta_{k\ell}$ in thermal equilibrium.

In the next step the reservoir is approximated by introducing a density of state $\rho(\omega)$ and the sum is replaced by an integral. (If the reservoir has a discrete number of energy levels then the reservoir and the system will feed information back and forth and it is impossible for the reservoir to loose information.) The correlation function (2.55) becomes

$$I_{1N}(t) = \int_0^\infty d\omega \,\rho(\omega) \,\bar{n}^{\rm S}(\omega) \left| T^{\rm S}(\omega) \right|^2 \int_{-t}^0 d\tau \, e^{-i(\omega - \mathcal{E}_{\rm c})\tau}$$

where the second integral is highly oscillatory and can therefore be approximated by a delta function because the only dominant contributions come from $\omega \approx \mathcal{E}_{c}$. For Fermi reservoirs

$$\bar{n}^{\mathrm{S}}(\omega) = \left(1 + e^{\frac{\omega - \omega_{\mathrm{f}}}{k_{\mathrm{B}}T}}\right)^{-1}$$

where $\omega_{\rm f}$ is the Fermi energy. With the assumptions that $\mathcal{E}_{\rm c} < \omega_{\rm f}$ and that T is small in the order of 1 K such that the average occupation of the reservoir is close to 1 the Markov approximation is applied. The result is

$$I_{1N}(t) = \int_0^\infty d\omega \,\rho(\omega) \,\bar{n}^{\rm S}(\omega) \left| T^{\rm S}(\omega) \right|^2 \int_{-t}^0 d\tau \, e^{-i(\omega - \mathcal{E}_{\rm c})\tau} \approx \pi \,\rho(\mathcal{E}_{\rm c}) \left| T^{\rm S}(\mathcal{E}_{\rm c}) \right|^2 = \frac{\gamma_{\rm L}}{2}$$

and this means that the number $\frac{\gamma_{\rm L}}{2}$ replacing $I_{1\rm N}(t)$ is dominated by the energy $\mathcal{E}_{\rm c}$ of the dot. The other correlation functions lead to similar numbers.

The equation of motion is

$$\frac{d}{dt}\rho_{\rm dot}(t) = \frac{\gamma_{\rm L}}{2} \left(2\,\hat{c}^{\dagger}\,\rho_{\rm dot}(t)\,\hat{c} - \hat{c}\,\hat{c}^{\dagger}\,\rho_{\rm dot}(t) - \rho_{\rm dot}(t)\,\hat{c}\,\hat{c}^{\dagger} \right)
+ \frac{\gamma_{\rm R}}{2} \left(2\,\hat{c}\,\rho_{\rm dot}(t)\,\hat{c}^{\dagger} - \hat{c}^{\dagger}\,\hat{c}\,\rho_{\rm dot}(t) - \rho_{\rm dot}(t)\,\hat{c}^{\dagger}\,\hat{c} \right)$$
(2.56)

and the Hilbert space for the quantum dot is $\mathcal{H}_{dot} \cong \mathbb{C}^2$ where $|0\rangle$ means no electron in the bound state and $|1\rangle$ means one electron in the bound state. Superpositions of no electron and one electron are not possible thanks to the superselection rules. This equation can be solved easily and depends only on one number. The average occupancy of the bound state is

$$\langle \hat{n}(t) \rangle_{\rho} = \operatorname{tr} \left(\hat{c}^{\dagger} \hat{c} \rho \right)$$

and this is the probability that the electron is in the bound state. Differentiating gives

$$\frac{d}{dt} \langle \hat{n}(t) \rangle = \operatorname{tr} \left(\hat{c}^{\dagger} \hat{c} \frac{d}{dt} \rho(t) \right) = \gamma_{\mathrm{L}} \operatorname{tr} \left(\hat{c}^{\dagger} \hat{c} \hat{c}^{\dagger} \rho \, \hat{c} \right) - \gamma_{\mathrm{R}} \operatorname{tr} \left(\hat{c}^{\dagger} \hat{c} \, \hat{c}^{\dagger} \hat{c} \, \rho \right)$$
$$= \gamma_{\mathrm{L}} \operatorname{tr} \left((\mathbb{I} - \hat{n}) (\mathbb{I} - \hat{n}) \right) - \gamma_{\mathrm{R}} \operatorname{tr} \left(\hat{n}^{2} \, \rho \right)$$
$$= \gamma_{\mathrm{L}} \left(1 - \langle \hat{n}(t) \rangle \right) - \gamma_{\mathrm{R}} \langle \hat{n}(t) \rangle$$

using (2.56) with the facts that $\hat{c}^{\dagger}\hat{c}^{\dagger} = \hat{c}\hat{c} = 0$, $\hat{c}^{\dagger}\hat{c} = \hat{n}$ and $\hat{n}^2 = \hat{n}$.

The inhomogeneous linear first-order differential equation to solve is

$$\frac{dy}{dt} = \gamma_{\rm L}(1-y) - \gamma_{\rm R} y = -(\gamma_{\rm L} + \gamma_{\rm R})y + \gamma_{\rm L}$$

after substituting $y(t) = \langle \hat{n}(t) \rangle$. The fixed point (or equilibrium value) is $0 = -(\gamma_{\rm L} + \gamma_{\rm R})y_* + \gamma_{\rm L}$ such that $y_* = \langle \hat{n} \rangle = \gamma_{\rm L}/(\gamma_{\rm L} + \gamma_{\rm R})$. To get the full solution one solves the homogeneous part on the left side and gets its solution on the right side

$$\frac{dy}{dt} = -(\gamma_{\rm L} + \gamma_{\rm R})y \qquad \qquad y_{\rm h}(t) = c \, e^{-(\gamma_{\rm L} + \gamma_{\rm R})t}$$

such that

$$y(t) = c e^{-(\gamma_{\rm L} + \gamma_{\rm R})t} + \frac{\gamma_{\rm L}}{\gamma_{\rm L} + \gamma_{\rm R}}$$

is the solution of the inhomogeneous differential equation. If it is not in equilibrium it rapidly relaxes to the equilibrium value for the probability of the average number of electrons on the dot. With the boundary condition $\langle \hat{n}(0) \rangle = c + \gamma_{\rm L}/(\gamma_{\rm L} + \gamma_{\rm R})$ the full solution is

$$\langle \hat{n}(t) \rangle = \left[\langle \hat{n}(0) \rangle - \frac{\gamma_{\rm L}}{\gamma_{\rm L} + \gamma_{\rm R}} \right] e^{-(\gamma_{\rm L} + \gamma_{\rm R})t} + \frac{\gamma_{\rm L}}{\gamma_{\rm L} + \gamma_{\rm R}}$$
(2.57)

for the fermion cavity.

This is another example with the typical equation of motion

$$\frac{d}{dt}\rho_{\rm S} = \mathcal{D}[\hat{A}]\rho_{\rm S}$$

for the system alone. If one wants to describe the dynamics of the non-unitary dynamics of a system the process has to be completely positive. This requirement for complete positivity places huge constraints on the equation of motion if one assumes it to be Markovian such that the change in the state at time t can only depend on the state at time t and not on the history.

2.11 Quantum-Mechanical Model for Continuous Position Measurement

A model is described here for a system that might be subjected to multiple measurements of position \hat{x} . There is a system such as a particle in a harmonic oscillator that is isolated from the environment except at certain times when the system is measured with a process described by a completely positive map. The process is repeated n times by interacting with a measurement device and then one checks in which state the system is. Finally, one takes the limit $n \to \infty$.

There is a meter (or gauge) called M_1 and this measurement device is a harmonic oscillator. There are other meters called M_2 to M_n of the same kind. The system is initially closed off from the meters and the environment. At time t_1 the system interacts with the first meter M_1 , some time later at t_2 it interacts with the second meter M_2 and so on until it interacts at time t_n with the last meter M_n .



This is not such a bad model for how experiments are done. Optically, there is a perfect cavity which is the system in some state, and at t_1 the cavity is interrogated via an interaction. The measurement is the instantaneous interaction with the mode in the cavity with some measuring device. Then the cavity is closed again and after some time it is interrogated a second time and so on. Finally, one looks at the meters and looks at the result consisting most likely of a sequence of random numbers. The goal is to describe the state of the meters and the state of the system. The added twist is to do more and more measurements but weaker and weaker.

If one does the measurement of position with meter M_1 too strong one slams it almost into a position eigenstate. Later one does the second measurement and so on. If one does more and more essentially projective measurements one encounters the quantum Zeno effect. This effect refers to the expression "the watched pot never boils" in the quantum setting. If one keeps measuring the system in quantum mechanics with strength such that the measurement is almost projective (watching the pot in the analogy) then the system never evolves because it goes into an eigenstate of the observable and stays there. If on the other hand the measurement is too weak then, as one increases the number of measurements and decrease their strength, the system becomes effectively decoupled from the meters and evolves by itself according to its own internal dynamics. There is a Goldilock spot in between where the setup is not in the quantum Zeno regime and not in the completely decoupled regime but in an intermediate regime where the meters interfere with the system just enough such that there is some back action between the two. This intermediate regime turns out to be a really good model for how environments act with systems.

Thus, one models a sequence of instantaneous measurements at times $t_j = j \tau$, and the meter M_j for the j^{th} measurement is a quantum harmonic oscillator (a continuous quantum variable) with canonical operators \hat{x}_j and \hat{p}_j satisfying $[\hat{x}_j, \hat{p}_k] = i \delta_{jk}$ prepared in a known state. The total Hilbert space is

$$\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{env}} \otimes \mathcal{H}_{\text{sys}} = \mathcal{H}_{M_1} \otimes \mathcal{H}_{M_2} \otimes \ldots \otimes \mathcal{H}_{M_n} \otimes \mathcal{H}_{\text{sys}} = L^2(\mathbb{R}) \otimes \ldots \otimes L^2(\mathbb{R}) \otimes \mathcal{H}_{\text{sys}}$$

for this process, and this process is time-dependent such that energy will not be conserved because certain knobs will be twiddled. The time-dependent Hamiltonian

$$\hat{H}(t) = \hat{H}_0 + \sum_{j=1}^n \delta(t - j\tau) \,\hat{x}_{\text{sys}} \otimes \hat{p}_j \tag{2.58}$$

describes this measurement process. One allows the system to evolve according to its natural Hamiltonian \hat{H}_0 , and at instances $t = j \tau$ the system is instantaneously interrogated with the meter M_j .

As an excursus to explain the term $\hat{x}_{sys} \otimes \hat{p}_j$, this Hamiltonian for one system and one meter is due to von Neumann. To describe a measurement of an observable there must be a measuring device that corresponds to this hermitan operator. This measuring device should presumably also obey the rules of quantum mechanics and must therefore have a Hamiltonian. If \hat{A}_{sys} is a hermitian observable on \mathcal{H}_{sys} adjoined to an ancilla system (the meter) then the dynamics according to the Hamiltonian

$$\hat{H}_{\rm vN} = \hat{A}_{\rm sys} \otimes \hat{p}$$

will carry out a measurement of the operator \hat{A}_{sys} . At time t = 0 the combination of system and ancilla is assumed to be in a product state $|\Psi_0\rangle = |\psi_{sys}\rangle \otimes |x = 0\rangle$ where the state of the meter $|x = 0\rangle$ is a delta function and therefore a badly behaved object. Evolving this for a time t according to the Hamiltonian \hat{H}_{vN} gives

$$\left|\Psi_{t}\right\rangle = e^{-i\,\hat{H}_{\mathrm{vN}}\,t}\left|\Psi_{0}\right\rangle = \left(\sum_{j=1}^{m} \left|\alpha_{j}\right\rangle\left\langle\alpha_{j}\right| \otimes e^{-i\,\alpha_{j}\,t\,\hat{p}}\right)\left|\Psi_{0}\right\rangle$$

using the decomposition of $\hat{H}_{\rm vN}$

$$\hat{H}_{\rm vN} = \hat{A}_{\rm sys} \otimes \hat{p} = \sum_{j=1}^{m} (\alpha_j |\alpha_j\rangle \langle \alpha_j |) \otimes \hat{p}$$

in terms of eigenvalues and eigenvectors. Substituting $|\psi_{\rm sys}\rangle \otimes |x=0\rangle$ for $|\Psi_0\rangle$ results in

$$|\Psi_t\rangle = \sum_{j=1}^m \langle \alpha_j | \psi_{\rm sys} \rangle | \alpha_j \rangle_{\rm sys} | x = \alpha_j t \rangle_{\rm meter}$$

using the fact that $e^{-i\alpha_j t \hat{p}}$ is the translation operator shifting in position. The state after the interaction is an entangled state between the system and the meter. The quantity $|x = \alpha_j t\rangle_{\text{meter}}$ is called a pointer. Looking at the pointer there are m possible values for the meter depending on α_j and t. The meter is entangled with the system and has some information about the system. Thus, one measures the meter. (How this is done is not explained because otherwise one would need another process to do so and so on infinitely many times. This is called the measurement problem.) The meter (the value of this particle which is the meter) is in a superposition of values $\alpha_1 t$, $\alpha_2 t$ and so on. There are m possible outcomes depending on α_j and this will project the system in one of these posterior states $|\alpha_j\rangle$ (eigenstates of the hermitan operator). The probability that this occurs is $|\langle \alpha_j | \psi_{\text{sys}} \rangle|^2$. This is a way to measure a hermitian operator (an arbitrary observable) by reducing the problem to measuring a single harmonic oscillator (a single free particle). This ends the excursus on the von Neumann prescription to measure the hermitian observable \hat{A}_{sys} .

The Hamiltonian (2.58) involves this kind of measurement according to the theory of measurement of an observable by von Neumann n times. There is no interaction with the system except at that instances of time $t = j \tau$ when the system undergoes an interaction with the meter M_j .

To summarize the physics of the quantum mechanical model of continuous measurement explored here, the goal of this model is to gain some intuition why a system will decohere. In order for a system to lose coherence, information has to flow from it to the environment as time progresses. If there is no transfer of information from the system to the environment then the system undergoes its own internal unitary dynamics. If there is some initial state $\rho_{\text{init}} = |\Omega\rangle \langle \Omega|$ at time t = 0 which is pure then the question is what is the mechanism for how this initially pure state loses its purity and becomes some kind of mixed state $\rho(t)$. The mechanism is that the environment gains information about the system, and once the environment has gained information about the system it becomes correlated with the system. Information gain by the environment is equivalent to the loss of coherence of the system or, in other words, the system becomes entangled with the environment.

The Hamiltonian (2.58) introduced above describes the measurement process, and each meter M_j for j = 1, ..., n is assumed to be in a known initial state

$$|G_j\rangle = \frac{1}{(\phi\sigma)^{\frac{1}{4}}} \int_{-\infty}^{\infty} e^{-\frac{x_j^2}{2\sigma}} |x_j\rangle \ dx_j$$

which is a Gaussian state with width σ . For an ideal projective type measurement of the system via this von Neumann measurement prescription the meters have to be initialized in a delta function of position. The full initial state of the system and the meters is

$$\rho(0) = \rho_{\rm sys} \otimes |G_1\rangle \langle G_1| \otimes |G_2\rangle \langle G_2| \otimes \dots \otimes |G_n\rangle \langle G_n|$$

at time t = 0. (Note that ρ depends on σ .) If one prepares the meters and turns off the measurement apparatus the system would evolve according to its internal unitary dynamics generated by \hat{H}_0 and remain in its pure state. However, with meters turned on instantaneous interactions between the system and a meter take place at the stroboscopic times $t = j \tau$ and a little bit of information flows from the system to the corresponding meter and back because information flows bidirectional in quantum mechanics.

If $\rho_{\text{sys}}(t_j^-)$ is the system state just before the j^{th} measurement then the joint state of the system and the corresponding meters is

$$\rho_{M_j,\text{sys}}(t_j^+) = e^{-i\,\hat{x}_{\text{sys}}\otimes\hat{p}_j} \left[|G_j\rangle \langle G_j| \otimes \rho_{\text{sys}}(t_j^-) \right] e^{i\,\hat{x}_{\text{sys}}\otimes\hat{p}_j}$$

after the j^{th} measurement. The first and last term are just unitary evolution while the term in the middle couples the system with the j^{th} meter, and the system becomes entangled with the j^{th} meter. The meter M_j is measured in the basis $|x_j\rangle$ conditional the system state leading to

$$\rho_{\rm sys}(t_j^+, x_j) = \frac{(\langle x_j | \otimes \mathbb{I})(\rho_{M_j, \rm sys})(|x_j \rangle \otimes \mathbb{I})}{P(x_j)} \qquad \hat{Y}(y) = \frac{1}{(\pi \sigma)^{\frac{1}{4}}} e^{-\frac{(y\mathbb{I} - \hat{x})^2}{2\sigma}} \\
= \frac{\hat{Y}(x_j) \rho_{\rm sys}(t_j^-) \hat{Y}^{\dagger}(x_j)}{\operatorname{tr} \left(\rho_{M_j, \rm sys} \hat{Y}^{\dagger}(x_j) \hat{Y}(x_j)\right)}$$
(2.59)

where $P(x_j)$ is the probability required for the normalization. This is modeling the case of the selective measurement where one looks at the meter at time t_j .

In the case of the non-selective measurement one does not look at the meter. The system is measured and gets correlated with the meter variable but then the result of the measurement is thrown into the bin. This has still some back action on the system because of the interaction with the variable. In this case the state is the completely positive map

$$\rho_{\rm sys}(t_j^+) = \int dx_j \, \hat{Y}(x_j) \, \rho_{\rm sys}(t_j^-) \, \hat{Y}^{\dagger}(x_j)$$

where the meters are ignored and this is the same as averaging over all the outcomes of the selective measurements. This is the case where the meter or pointer variable is controlled by an environment that tries to gain access to the quantum system. Since the environment has the meters and not the physicists one has no access to the outcome of the measurement.

The environment behaves like a spy but unlike the classical case where a spy can take photographs of a secret document without leaving a trace behind here the secret document burns up when photographed. This is the physical explanation for how quantum cryptography works. It boils down to the fact that if somebody measures a quantum system then there is a back action on the system. As long as one can detect this back action one knows that an eavesdropper has intercepted the message. Information gain in quantum mechanics always leads to the disturbance of the system.

The above calculations show what happens just before and after this instance t_j in time of the j^{th} measurement, and it is assumed that the measurement process is so fast that no dynamics occur during the measurement but between the measurements there is some unitary dynamics. Thus, the next question is what happens between the measurements where the system evolves according to

$$U(\tau) = e^{-i\hat{H}_0\tau}$$

freely. If $\rho_{\text{sys}}(0)$ is the initial state at time t = 0 and one obtains the measurement outcomes $\bar{x}_1, \bar{x}_2, ..., \bar{x}_n$ then the state just after the j^{th} measurement is

$$\rho_{\rm sys}(\{\bar{x}_1,...,\bar{x}_j\},t_j^+) = \frac{\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)\rho_{\rm sys}(0)\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)^{\dagger}}{P(\{\bar{x}_1,...,\bar{x}_j\})} \\
= \frac{\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)\rho_{\rm sys}(0)\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)^{\dagger}}{\operatorname{tr}\left(\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)^{\dagger}\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)\rho_{\rm sys}(0)\right)} \tag{2.60}$$

with

$$P(\{\bar{x}_1, ..., \bar{x}_j\}) = \operatorname{tr}\left(\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)^{\dagger}\left(\prod_{k=1}^j Y(\bar{x}_k)U(\tau)\right)\rho_{\operatorname{sys}}(0)\right)$$

using (2.59) and the unitary free evolution due to \hat{H}_0 . The products are taken from increasing values of k on the left. This is the full selective evolution of the system during these n measurements. The state after j of those position measurement is (2.60) conditioned on getting the measurement outcomes $\bar{x}_1, ..., \bar{x}_j$. It shows that the system must have undergone this non-unitary process in order to end up in the state $\rho_{sys}(\{\bar{x}_1, ..., \bar{x}_j\}, t_j^+)$. From now on approximations are applied to explore this result further.

The sequence $\bar{x}_1, ..., \bar{x}_j$ is called a measurement trajectory and looks like some random walk as in the figure on the right side. Each of these measurement records as a kind of history of the measurement process leads to a trajectory in (2.60) as a conditional state that depends on these random numbers from the measurements.

In the case of the non-selective evolution where one cannot look at the meters and the environment has control over them, one averages over all possible outcomes of the measurements. This is much easier because one does not need to know the measurement outcomes. The state after the j^{th} measurement is

$$\rho_{\rm sys}(t_j^+) = \int \left(\prod_{k=1}^j d\bar{x}_k\right) \rho_{\rm sys}(\{\bar{x}_1, ..., \bar{x}_j\}, t_j^+) P(\{\bar{x}_1, ..., \bar{x}_j\})$$
(2.61)

and looks still quite complicated, but one can approximate it in a controlled way. The following steps are not rigorous but could be made rigorous.

For continuous measurement one studies the limit $n \to \infty$ and $\tau \to 0$ of this non-selective evolution by increasing the number of measurements and by reducing the time between measurements. To observe the system over a fixed interval of time t the number n of measurements and the gap τ between measurements are adapted in just the right rate by making $n\tau$ constant. Thus, an infinite number of measurements are done in a constant time. By doing so the equation (2.61) is turned into a differential equation.

In order to get the corresponding master equation the evolution equation is written as

$$\frac{d}{dt}\rho_{\rm sys}(t) = \lim_{\tau \to 0} \frac{\rho_{\rm sys}(t_n^+) - \rho_{\rm sys}(t_{n-1}^+)}{\tau}$$

for a density operator $\rho_{\text{sys}}(t)$. Because of the fact that $n\tau$ is constant the instances in time of $\rho_{\text{sys}}(t_n^+)$ and $\rho_{\text{sys}}(t_{n-1}^+)$ come closer together. One can define a Brownian motion process taking place in the entries of the density operator. Using (2.60) and (2.61) the limit becomes

$$\frac{d}{dt}\rho_{\rm sys}(t) = \lim_{\tau \to 0} \left[\frac{1}{\tau} \int_{-\infty}^{\infty} d\bar{x} \; \hat{Y}(\bar{x}) \, U(\tau) \, \rho_{\rm sys}(t_{n-1}^+) \, U^{\dagger}(\tau) \, \hat{Y}^{\dagger}(\bar{x}) - \frac{1}{\tau} \, \rho_{\rm sys}(t_{n-1}^+) \right]$$

and one can exploit the fact that $\hat{Y}(\bar{x})$ and $|G_i\rangle$ are Gaussians of width σ . The formula

$$\int_{-\infty}^{\infty} d\bar{x} \; \hat{Y}(\bar{x}) \, \hat{A} \, \hat{Y}^{\dagger}(\bar{x}) = \hat{A} - \frac{1}{2\sigma} \left[\hat{x}_{\text{sys}}, \left[\hat{x}_{\text{sys}}, \hat{A} \right] \right] + O\left(\frac{1}{\sigma^2} \right)$$

can be derived using the fact that \hat{Y} are bounded operators and expanding them around the identity. One sees the influence of σ because the larger σ is the less effect the second term has. With $\sigma = \infty$ on one hand the integral over \bar{x} would be nothing and leave the argument untouched such that the system just undergoes unitary evolution. With σ close to zero on the other hand the second term dominates and overwhelms the identity contribution.

The quantity σ measures the width of the pointer state of the meter. The larger σ is the wider is this state of the meter. If σ is infinity then the meter is essentially in a zero momentum eigenstate such that it is in an equal superposition of position over all space. The von Neumann measurement prescription does not give any information about the system because it is an eigenstate of momentum. In the other case where σ is close to zero then the wave function of the meter is almost a delta function such that nearly everything is distinguishable with respect to the von Neumann prescription. There is a kind of Goldilock position in between which is interesting.

Using the Taylor expansion $U(\tau) = \mathbb{I} - i \hat{H}_0 \tau + O(\tau^2)$ gives

$$\begin{aligned} \frac{d}{dt}\rho_{\rm sys}(t) &= \lim_{\tau \to 0} \left[\frac{1}{\tau} \left(\rho_{\rm sys}(t) - \frac{1}{2\sigma} \Big[\hat{x}_{\rm sys}, \Big[\hat{x}_{\rm sys}, \rho_{\rm sys}(t) \Big] \Big] - i \Big[\hat{H}_0, \rho_{\rm sys}(t) \Big] \tau \right) - \frac{1}{\tau} \rho_{\rm sys}(t) \right] \\ &= \lim_{\tau \to 0} \left[-\frac{1}{2\sigma\tau} \Big[\hat{x}_{\rm sys}, \Big[\hat{x}_{\rm sys}, \rho_{\rm sys}(t) \Big] \Big] - i \Big[\hat{H}_0, \rho_{\rm sys}(t) \Big] \Big] \end{aligned}$$

showing that σ is tied to τ . As long as the width of the initial states of these measurement or meter states scales as $\frac{1}{\tau}$ and gets wider the more measurements one does then there is a non-trivial limit. The differential equation becomes

$$\frac{d}{dt}\rho_{\rm sys}(t) = -i\left[\hat{H}_0, \rho_{\rm sys}(t)\right] - \frac{1}{4D}\left[\hat{x}_{\rm sys}, \left[\hat{x}_{\rm sys}, \rho_{\rm sys}(t)\right]\right]$$
(2.62)

with $\sigma \tau \to 2D$ constant. As long as one chooses each meter to be in a very very broad Gaussian initial state then one can end up in a non-trivial dynamics like this.

Three scalings are of interest:

Case 1: $\sigma > \frac{1}{|\tau|}$

As τ goes to zero the left term in (2.62) goes to infinity and overwhelms the right term. The left term dephases everything off the diagonal and projects the system on a position eigenstate where it remains. This is the quantum Zeno regime because one makes such a strong measurement of position at each instance of time that the system cannot undergo any evolution.

Case 2: $\sigma = \frac{1}{\tau} \Rightarrow \text{non-trivial}$

This is a balanced regime between the unitary dynamics and the quantum Zeno regime. The system undergoes dissipation and unitary evolution at the same time.

Case 3: $|\sigma| < \frac{1}{|\tau|}$

In this case which could be called the unitary regime the first term in (2.62) vanishes and the evolution is just the unitary evolution. The meters gain no information at all.

Depending on \hat{H}_0 the differential equation (2.62) can be solved or cannot be solved. When it is quadratic it can be solved but in general it cannot be solved. If one continuously monitors the position of the particle but one does it very weakly then the system undergoes unitary evolution but there is some back action due to the measurements which takes the form of a dissipation.

The free particle as the simplest possible system is used as an example. Given the Hamiltonian

$$\hat{H}_0 = \frac{\hat{p}_{\rm sys}^2}{2m}$$

the expectation value of position

$$\langle \hat{x}_{\rm sys} \rangle (t) = \operatorname{tr} \left(\rho_{\rm sys}(t) \, \hat{x}_{\rm sys}(t) \right) \qquad \qquad \frac{d}{dt} \, \langle \hat{x}_{\rm sys} \rangle (t) = \frac{\langle \hat{p}_{\rm sys} \rangle}{m} \qquad \qquad \frac{d}{dt} \, \langle \hat{p}_{\rm sys} \rangle (t) = 0$$

shows the expected unitary dynamics, and momentum is conserved. It looks as if there is no dissipation at all. Looking at the variance (the momentum distribution)

$$\langle (\Delta \hat{p}_{\rm sys})^2 \rangle (t) = \langle (\Delta \hat{p}_{\rm sys})^2 \rangle (0) + \frac{t}{2D}$$

shows that the momentum wave function starts to broaden linearly with time as time progresses. This measurement of position starts to have a back action on the momentum distribution. That is to be expected because measuring position makes momentum less certain according to the uncertainty principle.

2.12 Working with Superoperators

The equation of motions for a system in the presence of an environment have been determined for the reduced density operator system in several cases above by derivations and approximations. The density operator for the system alone got the very special form

$$\frac{d}{dt}\rho_{\rm sys}(t) = -i\left[\hat{H}_0, \rho_{\rm sys}(t)\right] - \gamma \sum_j \left\{ L_j^{\dagger} L_j, \rho_{\rm sys}(t) \right\} - 2L_j \,\rho_{\rm sys}(t) \,L_j^{\dagger} \tag{2.63}$$

with just the right number of approximations. There is some kind of system Hamiltonian contribution and some additional terms. This is a first-order differential equation in time which gives some effective dynamics when solved. Because this differential equation is first order in time and the right-hand side is homogeneous the solution can be expressed as an exponential

$$\rho_{\rm sys}(t) = e^{t\mathcal{L}} \left(\rho_{\rm sys}(0) \right)$$

where \mathcal{L} is a superoperator defined as

$$\mathcal{L}(\rho) = -i \left[\hat{H}_0, \rho \right] - \gamma \sum_j \left\{ L_j^{\dagger} L_j, \rho \right\} - 2L_j \rho L_j^{\dagger}$$

which eats a density operator and returns a hermitian operator.

This differential equation (2.63) is not different from an ordinary standard first-order differential equation of the form $\frac{dy}{dx} = -Ly$ for a function y(x) with $x \in \mathbb{R}$ and $y(x) \in \mathbb{R}$. It has the solution $y(x) = e^{-Lx}y(0)$. Equation (2.63) is just a matrix version of this differential equation where the matrix version has the form $\frac{dv}{dx} = -Lv$ and where $v \in \mathbb{C}^D$, $L \in M_D(\mathbb{C})$ and L is hermitian or normal, and its solution is $v(x) = e^{-Lx}v(0)$. Since ρ is a matrix and not a vector equation, equation (2.63) looks different but it is just an encoded form of the matrix version of the differential equation. The trick is to take the matrix ρ and string it out like a vector, and to vectorize ρ one does what also a computer would do in order to store a matrix in memory. One can draw a snake through the entries of the matrix and line it up as some big vector with the components $\rho_{00}, \rho_{10}, \rho_{20}, ..., \rho_{D-10}, \rho_{01}, ..., \rho_{D-1D-1}$ with D^2 entries. Then the left-hand side of (2.63) is in the form of the matrix version of the differential equation. The right-hand side consists of three linear operators with a corresponding matrix form to be vectorized the same way.

There is no unique way for vectorizing a matrix but the standard way is for ρ in a computational basis to create a ket-vector

by turning around $\langle k | \Rightarrow | k \rangle$. This depends on the basis. When mapping ρ to $| \rho \rangle$ this way then $\hat{H}_0 \rho$ becomes $(\hat{H}_0 \otimes \mathbb{I}) | \rho \rangle = |\hat{H}_0 \rho \rangle$ and $| \rho \hat{H}_0 \rangle = \mathbb{I} \times \hat{H}_0^T | \rho \rangle$.

Applying this to the equation of motion (2.63) gives

$$\frac{d}{dt}|\rho\rangle = \left\{-i\left(\hat{H}_0\otimes\mathbb{I} - \mathbb{I}\times\hat{H}_0^T\right) - \gamma\sum_j\left(L_j^{\dagger}L_j\otimes\mathbb{I} + \mathbb{I}\otimes L_j^{\dagger}\bar{L}_j\right) + 2\gamma\sum_j\left(L_j\otimes\bar{L}_j\right)\right\}|\rho\rangle \qquad (2.64)$$

in the exactly equivalent vector form. The right side of (2.64) can be written as $\underline{\underline{L}} |\rho\rangle$. Therefore, this differential equation and its solution are

$$\frac{d}{dt} |\rho(t)\rangle = \underline{\underline{L}} |\rho(t)\rangle \qquad \qquad |\rho(t)\rangle = e^{t} \underline{\underline{L}} |\rho(0)\rangle$$

and the solution becomes when devectorized $\rho(t) = e^{t\mathcal{L}}(\rho(0))$ as shown above.

2.13 Dynamical Semigroups

The superoperator \mathcal{L} is linear, and it takes a $D \times D$ matrix (a density operator) and returns another $D \times D$ matrix. Thus, it is a linear map $\mathcal{L} : \mathsf{M}_D(\mathbb{C}) \to \mathsf{M}_D(\mathbb{C})$. (Operators take vectors to vectors, and superoperators take operators to operators.) It is interpreted as

$$e^{t\mathcal{L}} = \sum_{\ell=0}^{\infty} \frac{t^{\ell} \,\mathcal{L}^{\ell}}{\ell!}$$

by its Taylor series. Defined as $\mathcal{E}_t(\rho(0)) = e^{t\mathcal{L}}(\rho(0))$ the quantity \mathcal{E}_t is also a superoperator and has the three properties:

- (i) $\mathcal{E}_t(\rho(0)) = \rho(0)$ in all cases considered here
- (ii) \mathcal{E}_t is a completely positive trace-preserving map
- (iii) $\mathcal{E}_s(\mathcal{E}_t)) = \mathcal{E}_{s+t}$

It is not given that \mathcal{E}_t is for all the above examples a completely positive trace-preserving map. The equation of motion has been derived through several approximations. The starting point was a completely positive dynamics namely the Schrödinger equation such that the whole system evolved unitarily. Making approximations means eliminating terms which interact with the environment, and it is not clear why the equation of motion in the end should preserve complete positivity.

This is not obvious as the example of the pure quantum state $|\psi(t)\rangle = c(t) |0\rangle + d(t) |1\rangle$ that depends on a parameter t such as the quantum state of a single qubit shows. If one Taylor expands c(t) and d(t) and truncates then almost always the result such as $|\tilde{\psi}(t)\rangle = (1 + c_0 t) |0\rangle + |1\rangle$, for example, is not normalized. In other words, a state after an approximation may no longer be a state because Taylor expansion destroys normalization. The above state can only be normalized in a way depending on t because of the factor $1 + c_0 t$.

The fact that the equation of motion after several approximation in all the examples above did lead to a completely positive trace-preserving map \mathcal{E}_t has reasons. It will turn out that the only way to satisfy the three properties (i), (ii), (iii) is when \mathcal{L} has the above particular form. Dynamical semigroups are a mathematical topic which is independent of quantum mechanics. The topic are families of maps indexed by non-negative real numbers. Thus, the topic are maps $\mathcal{E}_s : \mathbb{C}^D \to \mathbb{C}^D$ which depend on a parameter $s \in \mathbb{R}^+$ and satisfy the properties:

(i)
$$\mathcal{E}_s \circ \mathcal{E}_t = \mathcal{E}_{s+s}$$

(ii) $\mathcal{E}_0 = \mathbb{I}$

where the property (i) is called the semigroup property.

Proposition 1 Let $\mathcal{E}_s \in M_D(\mathbb{C})$ be a dynamical semigroup which is continuous in $s \in \mathbb{R}+$. Then \mathcal{E}_s is differentiable and has the form

 $\mathcal{E}_s = e^{sL}$

for some $L \in \mathsf{M}(\mathbb{C})$.

Note that a continuous function does not need to be differentiable and that there are even continuous functions not differentiable almost everywhere. (The function f(x) = |x|, for example, is not differentiable at x = 0.) Here however to be continuous for a dynamical semigroup already ensures differentiability. There is also no reason why a differentiable function should be an exponential function but for dynamical semigroups this is the case.

The intuitive reason is that \mathcal{E}_s is continuous, \mathcal{E}_t is continuous and \mathcal{E}_{s+t} is continuous such that the semigroup property is a kind of convolution. A slightly more formal proof states that since $\mathcal{E}_0 = \mathbb{I}$ and \mathcal{E}_s is continuous there exists $\varepsilon > 0$ such that M_{ε} defined as

$$M_{\varepsilon} = \int_{0}^{\varepsilon} \mathcal{E}_{s} \, ds \qquad \qquad \frac{d}{d\varepsilon} M_{\varepsilon} \Big|_{\varepsilon=s} = \mathcal{E}_{s}$$

is invertible. (In the space of matrices $M_D(\mathbb{C})$ is \mathcal{E}_s a path starting from I.) The key property is that in this space of matrices the space of invertible matrices is a connected set and connected to the identity, and M_{ε} is an invertible matrix for a small enough ε as one can see from $\det(M_{\varepsilon}) \neq 0$ except for $\varepsilon = 0$. Inserting the identity gives

$$\mathcal{E}_s = M_{\varepsilon}^{-1} M_{\varepsilon} \, \mathcal{E}_s = M_{\varepsilon}^{-1} \int_0^{\varepsilon} \mathcal{E}_{s+t} \, dt = M_{\varepsilon}^{-1} \int_s^{s+\varepsilon} \mathcal{E}_t \, dt = M_{\varepsilon}^{-1} (M_{s+\varepsilon} - M_s)$$

and shows that \mathcal{E}_s is differentiable due to the fundamental theorem of calculus. One can therefore write $\frac{d}{ds}\mathcal{E}_s = L\mathcal{E}_s = \lim_{\varepsilon \to 0} M_{\varepsilon}^{-1}(M_{s+\varepsilon} - M_s).$

2.14 Quantum Dynamical Semigroups

In the case of quantum dynamical semigroups \mathcal{E}_s is a superoperator $\mathcal{E}_s : M_D \to M_D$, and one can vectorize it to get a dynamical semigroup. The main question is when \mathcal{E}_s is completely positive. In case it is then \mathcal{E}_s is called a completely positive semigroup or a quantum semigroup.

Proposition 2 Let $L : M_D(\mathbb{C}) \to M_D(\mathbb{C})$ be a linear map. The following statements are equivalent:

1. There exists a completely positive map $\phi : \mathsf{M}_D(\mathbb{C}) \to \mathsf{M}_D(\mathbb{C})$ and $K \in \mathsf{M}_D(\mathbb{C})$ such that

$$L(X) = \phi(X) - KX - XK^{\dagger}$$

for all $X \in \mathsf{M}_D(\mathbb{C})$.

2. L is hermiticity preserving and, if

$$\left|\Omega\right\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^{d} \left|j\right\rangle \left|j\right\rangle$$

then

$$P\Big[(L \otimes id)(|\Omega\rangle \langle \Omega|)\Big]P \ge 0$$

with $P = \mathbb{I} - |\Omega\rangle \langle \Omega|$.

Maps that satisfy the conditions in proposition 2 are called completely positive linear maps. Firstly it is proven that statement 1 implies statement 2 and that follows from

$$P\Big[\left(\phi\otimes id\right)\left(\left|\Omega\right\rangle\left\langle\Omega\right|\right)-\left(K\otimes\mathbb{I}\right)\left(\left|\Omega\right\rangle\left\langle\Omega\right|\right)-\left(\left|\Omega\right\rangle\left\langle\Omega\right|\right)\left(K^{\dagger}\otimes\mathbb{I}\right)\Big]P\geq0$$

because ϕ is a completely positive map and the last two terms vanish $(P | \Omega \rangle = 0)$. Secondly it is shown that statement 2 implies statement 1 using $\tau = (L \otimes id)(|\Omega \rangle \langle \Omega|)$ which is hermitian and satisfies $P[\tau]P \ge 0$. However, τ as a matrix has not only components $P\tau P$ but also components from $\mathbb{I} - P = |\Omega \rangle \langle \Omega|$. One can write $\tau = Q - |\psi\rangle \langle \Omega| - |\Omega\rangle \langle \psi|$ and $Q \ge 0$ to deal with these components where $|\psi\rangle$ contains all of entries of τ in columns and rows containing $|\Omega\rangle$ and $Q \ge 0$ such that it is only non-zero in the block orthogonal to $|\Omega\rangle$. A completely positive map ϕ is defined via $(\phi \otimes id)(|\Omega\rangle \langle \Omega|) = Q$ as well as K via $(K \otimes \mathbb{I}) |\Omega\rangle = |\psi\rangle$ using vectorization. Hence, one can take $L = \phi(1 - K(1 - C)K^{\dagger}$.

Proposition 3 The following statements are equivalent:

- 1. \mathcal{E}_s is a dynamical semigroup of completely positive maps continuous in s.
- 2. $\mathcal{E}_s = e^{sL}$ for some completely positive map L.

To show that statement 2 follows from statement 1 one already knows from proposition 1 that a generator $L: \mathsf{M}_D(\mathbb{C}) \to \mathsf{M}_D(\mathbb{C})$ exists such that $\mathcal{E}_s = e^{sL}$. Because \mathcal{E}_s is completely positive, $0 \leq (e^{sL} \otimes id)(|\Omega\rangle \langle \Omega|)$ and this imposes sever conditions on L. Taylor expansion gives

$$0 \le (e^{sL} \otimes id)(|\Omega\rangle \langle \Omega|) = |\Omega\rangle \langle \Omega| + s(L \otimes id)(|\Omega\rangle \langle \Omega|) + O(s^2)$$

and this is a projection and something of order s that is not a projection. Applying now the operator $P = \mathbb{I} - |\Omega\rangle \langle \Omega|$ defined in proposition 2 to get

$$\frac{1}{s}0 \leq \frac{1}{s}P\left(\left|\Omega\right\rangle\left\langle\Omega\right| + s(L\otimes id)(\left|\Omega\right\rangle\left\langle\Omega\right|) + O(s^2)P\right) = \frac{1}{s}P\left(s(L\otimes id)(\left|\Omega\right\rangle\left\langle\Omega\right|) + O(s^2)P\right)$$

because $P(|\Omega\rangle \langle \Omega|)P = 0$. With the limit $s \to 0$ it follows $P(L \otimes id)(|\Omega\rangle \langle \Omega|)P \ge 0$. Therefore, L has the form $L(X) = \phi(X) - KX - XK^{\dagger}$ of a completely positive map $\phi(X)$ minus two terms where K is non-hermitian.

In order to prove the other direction that statement 2 implies statement 1 one starts from $\mathcal{E}_s = e^{sL}$ and decomposes $L = \phi + \phi_K$ where $\phi_K = -KX - XK^{\dagger}$. Using the Lie-Trotter formula gives

$$e^{sL} = \lim_{n \to \infty} \left(e^{\frac{s\phi}{n}} e^{\frac{s\phi_{\mathbf{K}}}{n}} \right)$$

provable by Taylor expansion. The first term containing ϕ is completely positive as can also be shown by Taylor expansion and the second term can be written as

$$e^{\frac{s\phi_{\mathrm{K}}}{n}} = e^{\frac{-sK}{n}} X e^{\frac{-sK^{\dagger}}{n}}$$

and is also completely positive because it has the form MXM^{\dagger} for a matrix M. Thus, e^{sL} is completely positive.

To summarize, examples of systems embedded in environments have been studied above where $\hat{H}_{sys+env}$ is the generator of time evolution

$$U_{\rm sys+env}(t) = e^{-iH_{\rm sys+env}}$$

for the combination of the system and the environment. Restricting the attention just to the system and tracing out the environment allows to find equations of motions for the system alone to a very high degree of approximation although the dynamics of the system alone cannot be exactly described as a linear equation of motion. These approximated equations of motion looked like

$$\frac{d}{dt}\rho_{\rm sys} = -i\left[H_{\rm sys}, \rho_{\rm sys}\right] + \sum_{j} L_{j}\rho_{\rm sys}L_{j}^{\dagger} - \frac{1}{2}\left\{L_{j}^{\dagger}L_{j}, \rho_{\rm sys}\right\} = L[\rho_{\rm S}]$$

for an effective Hamiltonian \hat{H}_{sys} for the system. This is no longer unitary although the left term represents unitary evolution but the other two terms do not. The initially pure state $e^{sL}[\rho_{sys}(0)]$ can become not pure. This is necessary if there is an exchange of information between the system and the environment. It turned out that this kind of equation of motion occurs if and only if the dynamics generated by $e^{sL}[\rho_{sys}(0)]$ is completely positive. Calling $e^{sL} = \mathcal{E}_s$ with the two properties $\mathcal{E}_0 = \mathbb{I}$ and $\mathcal{E}_s \circ \mathcal{E}_t = \mathcal{E}_{s+t}$ one can ask whether these two properties already guarantee that the equation of motion satisfied by the channel \mathcal{E}_s is of the above form, and this is indeed the case. The corresponding results can be combined into a single theorem.

Theorem 1 (Lindblad) A linear map $L : M_D(\mathbb{C}) \to M_D(\mathbb{C})$ is the generator of a continuous dynamical semigroup of trace-preserving, completely positive, linear maps if and only if

$$L(\rho) = i\left[\rho, H\right] + \sum_{j} L_{j}\rho L_{j}^{\dagger} - \frac{1}{2} \left\{ L_{j}^{\dagger}L_{j}, \rho \right\}$$

$$(2.65)$$

with $H^{\dagger} = H$ and $L_j \in \mathsf{M}_D(\mathbb{C})$.

The proof is based on the propositions 1, 2, 3, and uses the fact that if \mathcal{E}_s is a completely positive and linear dynamical semigroup then $\mathcal{E}_s = e^{sL}$ with $L(X) = \phi(X) - KX - XK^{\dagger}$ where ϕ is a completely positive channel. The remaining property to be shown is the property trace-preserving and this means probability-preserving such that as s passes the density operator one gets by applying \mathcal{E}_s to some initial state is still a density operator. Because $\operatorname{tr}(\mathcal{E}_s(\rho))$ implies $\operatorname{tr}(L[\rho]) = 0$ for all possible ρ and $L(X) = \phi(X) - KX - XK^{\dagger}$ one ends up with $\operatorname{tr}(\phi(\rho) - K\rho - \rho K^{\dagger}) = 0$. It follows $\operatorname{tr}(\phi^*(\mathbb{I}) \cdot \rho) = \operatorname{tr}((K + K^{\dagger})\rho)$ if one defines $\phi^*(\mathbb{I})$ to be the matrix which satisfies $\operatorname{tr}(\phi^*(\mathbb{I}) \cdot \rho) = \operatorname{tr}(\mathbb{I} \cdot \phi(\rho))$ for all ρ . This means $\phi^*(\mathbb{I}) = K + K^{\dagger}$. According to a structure result called the Kraus representation any completely positive map ϕ may be written as

$$\phi(\rho) = \sum_{j} L_{j} \rho L_{j}^{\dagger}$$

for some $L_j \in \mathsf{M}_D(\mathbb{C})$. It follows that $\phi^*(\mathbb{I}) = \sum_j L_j^{\dagger} L_j$. The remaining task is to extract from $K\rho + \rho K^{\dagger}$ the first and last term in (2.65), and one can show that the definition

$$K = iH + \frac{1}{2}\sum_{j}L_{j}^{\dagger}L_{j}$$

exactly does this. Both matrices H and $L_j^{\dagger}L_j$ are hermitian, and an arbitrary matrix such as K can always be written as a hermitian part and i times a hermitian part. Thus, $L(\rho)$ can be written as

$$L(\rho) = \sum_{j} L_{j}\rho L_{j}^{\dagger} - \left(iH + \frac{1}{2}\sum_{j} L_{j}^{\dagger}L_{j}\right)\rho - \rho\left(-iH + \frac{1}{2}\sum_{j} L_{j}^{\dagger}L_{j}\right)$$

corresponding to (2.65).

This theorem of Lindblad confirms that the effective equation resulting from the master equation is a physical process. There is no reason why this equation should be a completely positive map after all these approximations and truncations, but luckily any time one has an effective equation of motion in the form (2.65) then one knows that it is an implementable operation in quantum mechanics.

2.15 Quantum Jumps

The path so far has started from a system embedded in an environment and one looks only at the system neglecting the environment. The result is an effective equation of motion for the system. However, one can as well go the other way. Given a Lindblad equation of the particular form (2.65) with some L_j and H the question arises whether there is a unitary process whose effective dynamics generate exactly this equation of motion.

Quantum jumps are theoretically an interesting way to realize non-unitary dynamics but they are actually also what one sees in the lab when looking at detectors. Thus, there are two reasons to study them. Note that there is a relation between quantum jumps and quantum trajectories. Above the path from the big unitary for a continuous measurement process to a Lindblad effective equation of motion has been explored. Now the reverse path from a Lindblad effective equation of motion to the continuous measurement process is studied. Given a Lindblad equation

$$\frac{d}{dt}\rho = -i[\hat{H},\rho] - \frac{1}{2}\{\hat{c}^{\dagger}\hat{c},\rho\} + \hat{c}\,\rho\,\hat{c}^{\dagger}$$

only this simple case is shown but the case with multiple \hat{c}_j can be generalized similarly. This equation will be derived as a result of a generalized continuous measurement process. The measurement is dichotomic and one gets either zero or one

$$M_0(dt) = \mathbb{I} - \left(\frac{\hat{R}}{2} + i\,\hat{H}\right)dt \qquad \qquad M_1(dt) = \sqrt{dt}\,\hat{c}$$

when using this measurement apparatus where $M_0(dt)$ with $\hat{R} = \hat{c}^{\dagger}\hat{c}$ means no click in a time window dtand $M_1(dt)$ means a click in the time window dt. The time window dt is not infinitesimal but arbitrarily small yet finite. One can check that these two measurement operators $M_0(dt)$ and $M_1(dt)$ satisfy

$$M_0^{\dagger}(dt) M_0(dt) + M_1^{\dagger}(dt) M_1(dt) = \mathbb{I}$$

and correspond therefore to a legal measurement process. To understand these two operators one has to know more about detectors but here they are just given. The operators \hat{c}^{\dagger} and \hat{c} are the creation and annihilation operators for a photon. (A click here means at least on click.)

The apparatus is always on and always interrogating the system where time is split into equal intervals of length dt, and every dt the apparatus makes a measurement with the result clicks or no clicks. As discussed above there are the two cases of non-selective and selective evolution, and here the non-selective evolution from $\rho(t)$ to $\rho(t + dt)$ with

$$\rho(t+dt) = M_0(dt)\,\rho(t)\,M_0^{\dagger}(dt) + M_1(dt)\,\rho(t)\,M_1^{\dagger}(dt)$$

is considered. Substituting the definitions for $M_0(dt)$ and $M_1(dt)$ gives

$$\rho(t+dt) = \frac{\left[\mathbb{I} - \left(\frac{\hat{R}}{2} + i\,\hat{H}\right)dt\right]\rho(t)\left[\mathbb{I} - \left(\frac{\hat{R}}{2} - i\,\hat{H}\right)dt\right]P_0(dt)}{P_0(dt)} + \frac{dt\,\hat{c}\,\rho(t)\,\hat{c}^{\dagger}\,P_1(dt)}{P_1(dt)}$$
$$= \left[\mathbb{I} - \left(\frac{\hat{R}}{2} + i\,\hat{H}\right)dt\right]\rho(t)\left[\mathbb{I} - \left(\frac{\hat{R}}{2} - i\,\hat{H}\right)dt\right] + dt\,\hat{c}\,\rho(t)\,\hat{c}^{\dagger}$$

where $P_0(dt) = \operatorname{tr}\left(M_0^{\dagger}(dt) M_0(dt) \rho(t)\right)$ and $P_1(dt) = \operatorname{tr}\left(M_1^{\dagger}(dt) M_1(dt) \rho(t)\right)$ are the probabilities added for the sake of the physical picture. This gives

$$\rho(t+dt) = \rho(t) - \left(\frac{\hat{R}}{2} + i\,\hat{H}\right)\rho(t)\,dt - \rho(t)\left(\frac{\hat{R}}{2} - i\,\hat{H}\right)dt + dt\,\hat{c}\,\rho(t)\,\hat{c}^{\dagger} + O(dt^2)$$
$$\approx \rho(t) - \frac{1}{2}\left\{\hat{c}^{\dagger}\hat{c},\rho(t)\right\}dt - i\left[\hat{H},\rho(t)\right]dt + \hat{c}\,\rho(t)\,\hat{c}^{\dagger}\,dt$$

expanded to order O(dt). It has the expected form of a Lindblad equation.

The selective evolution is interesting if one has an apparatus that counts clicks or no clicks and delivers a measurement record. To understand the selective evolution one has to know the probabilities of at least one click and of no click

$$P_1(dt) = \operatorname{tr}\left(\hat{c}^{\dagger}\hat{c}\,\rho\right) \cdot dt \qquad \qquad P_0(dt) = 1 - P_1(dt)$$

where $P_1(dt)$ is called here infinitesimal in the sense that it is arbitrarily small but finite. Therefore the probability $P_0(dt) = 1 - O(dt)$ is almost one. The probability $P_1(dt)$ is proportional to the size of the time slots dt. In probability theory this is called a Poisson process. The system changes as

$$\rho(t) \begin{cases} \xrightarrow{\text{no click}} & ?\\ \xrightarrow{\text{click}} & ? \end{cases} \qquad \qquad |\psi(t)\rangle \begin{cases} \xrightarrow{\text{no click}} & |\psi_0(t+dt)\rangle \\ \xrightarrow{\text{click}} & |\psi_1(t+dt)\rangle \end{cases}$$

restricted to pure states $|\psi(t)\rangle$ because if the system is in a pure state before the measurement it is also in a pure state afterwards. This gives

$$\begin{split} |\psi_{0}(t+dt)\rangle &= \frac{M_{0}(dt) |\psi(dt)\rangle}{\sqrt{\langle\psi | M_{0}^{\dagger}(dt)M_{0}(dt) | \psi\rangle}} = \left\{ \mathbb{I} - dt \left[i\hat{H} - \frac{1}{2}\hat{c}^{\dagger}\hat{c} - \frac{1}{2} \langle\hat{c}^{\dagger}\hat{c}\rangle \right] \right\} |\psi(t)\rangle + O(dt) \\ |\psi_{1}(t+dt)\rangle &= \frac{M_{1}(dt) |\psi(dt)\rangle}{\sqrt{\langle\psi | M_{1}^{\dagger}(dt)M_{1}(dt) | \psi\rangle}} = \frac{\hat{c} |\psi(t)\rangle}{\sqrt{\langle\hat{c}^{\dagger}\hat{c}\rangle}} \end{split}$$

where $|\psi_0(t+dt)\rangle$ is Taylor expanded. The state after the no-click event is the same as before such that $|\psi_0(t+dt)\rangle = \mathbb{I} |\psi(t)\rangle$ but one has gained information because one knows now that there was no photon, and this results in additional terms.

A click is called a quantum jump. One defines a random variable N(t) for the number of jumps in the time window [0, t]. The change dN(t) is either zero or one, and two clicks at the same time are impossible because the measurement is dichotomic and can only return yes or no for at least one click or no click. This gives

$$dN(t)^2 = dN(t) \qquad \qquad \mathbb{E}[dN(t)] = P_1(dt)$$

with the average $\mathbb{E}[dN(t)]$ being an value between 0 and 1. This average can also be written as

$$P_1(dt) = dt \operatorname{tr}(\hat{c}^{\dagger}\hat{c}\rho) = dt \langle \psi(t) | \hat{c}^{\dagger}\hat{c} | \psi(t) \rangle$$

since this is a selective evolution.

One can put all together and ask what is the change in the pure state and this is also a random variable

$$\begin{aligned} d \left| \psi(t) \right\rangle &= \left| \psi(t+dt) \right\rangle - \left| \psi(t) \right\rangle \\ &= \left[dN(t) \left(\frac{\hat{c}}{\sqrt{\langle \hat{c}^{\dagger} \hat{c} \rangle \left(t \right)}} - 1 \right) + \left[1 - dN(t) \right] dt \left(\frac{\langle \hat{c}^{\dagger} \hat{c} \rangle \left(t \right)}{2} - \frac{\hat{c}^{\dagger} \hat{c}}{2} - i \hat{H} \right) \right] \left| \psi(t) \right\rangle \end{aligned}$$

$$(2.66)$$

since it is not deterministic. It is $|\psi_0(t)\rangle$ with some probability and $|\psi_1(t)\rangle$ with some probability. (One can think of Brownian motion to get an idea of what this random variable is.) Each time one runs the experiment one gets a different trajectory. If dN(t) is not a random variable such that $dN(t)^2 = dN(t) = 0$ then the selective conditional evolution would be deterministic. One actually gets in this case unitary evolution because $\langle \hat{c}^{\dagger} \hat{c} \rangle(t)$ and $\hat{c}^{\dagger} \hat{c}$ would be zero.

Only the case that $dN(t) \cdot dt$ is an order smaller than dt is explored, and equation (2.66) becomes

$$d\left|\psi(t)\right\rangle = \left[dN(t)\left(\frac{\hat{c}}{\sqrt{\left\langle\hat{c}^{\dagger}\hat{c}\right\rangle(t)}} - 1\right) + dt\left(\frac{\left\langle\hat{c}^{\dagger}\hat{c}\right\rangle(t)}{2} - \frac{\hat{c}^{\dagger}\hat{c}}{2} - i\hat{H}\right)\right]\left|\psi(t)\right\rangle$$

by setting [1 - dN(t)]dt = dt. With the definitions $\pi(t) = |\psi\rangle \langle \psi|$ (a random projection depending on N(t)) and $\rho(t) = \mathbb{E}[\pi(t)]$ (expectation value ignoring the measurement record) one gets

$$d\pi(t) = |d\psi\rangle \langle \psi| + |\psi\rangle \langle d\psi| + |d\psi\rangle \langle d\psi| + \dots = \left\{ dN \,\mathcal{G}(\hat{c}) - dt \,\mathcal{H}\left[i\hat{H} + \frac{1}{2}\hat{c}^{\dagger}\hat{c}\right] \right\} \pi(t)$$

where $\mathcal{G}(\hat{c})X = \frac{\hat{c}X\hat{c}^{\dagger}}{\operatorname{tr}(X\hat{c}^{\dagger}\hat{c})}$ and $\mathcal{H}(\hat{c})X = \hat{c}X + X\hat{c}^{\dagger} - \operatorname{tr}(\hat{c}X + X\hat{c}^{\dagger})X$ are superoperators. The result becomes

$$d\rho = \mathbb{E}[dt] = i dt[\hat{H}, \rho] + \mathcal{D}(\hat{c})\rho$$

using dN dt is smaller than dt and $\mathbb{E}[dN f(\pi)] = dt \mathbb{E}[\operatorname{tr}(\pi \hat{c}^{\dagger} \hat{c}) f(\pi)]$. Thus, a typical solution of N(t) is a staircase that grows by 1 at times t_j where a click occurred. The evolution of $|\psi(t)\rangle$ is $|\psi(0)\rangle$ with

$$\mathcal{T}e^{\int_{t_{j-1}}^{t_j} \left(-i\hat{H} - \frac{1}{2}\hat{c}^{\dagger}\hat{c} - \frac{1}{2}\langle\hat{c}^{\dagger}\hat{c}\rangle\right)ds}$$

between the clicks and with quantum jumps $\frac{\hat{c}}{\sqrt{\langle \hat{c}^{\dagger}\hat{c} \rangle}}$ at the clicks.