Chapter 2

Open system dynamics

Idea

We discuss in this chapter basic tools for the dynamics of an "open quantum system" – where the Schrödinger equation alone is not sufficient because the system exchanges energy and information with its environment. Starting from a few physically well-motivated assumptions, we shall derive a surprisingly precise characterization of the possible dynamics. The time evolution of an open quantum system can be understood as a mapping $\hat{\rho}(0) \mapsto \hat{\rho}(t)$ between density matrices. This mapping must satisfy some constraints, for example, it must preserve the probability interpretation of quantum mechanics. In addition, it seems reasonable that initial density matrixes that are "mixtures" of pure states evolve in a linear way and remain mixtures.

2.1 Axiomatic foundations

We define a "dynamical map" $T : \rho(0) \mapsto \rho(t) = T[\rho(0)]$ as a linear map of density matrices to density matrices. Actually, we only need "convex linearity" because this is the canonical way to generate mixed states:

$$T(\sum_k p_k \hat{\rho}_k) = \sum_k T(\hat{\rho}_k), \qquad p_k \geq 0, \sum_k p_k = 1 \qquad (2.1)$$

but this construction is easily generalized to linear combinations with complex coefficients.

We start from the intuitive picture that T implements the time evolution of the density operator to state the following, apparently obvious properties for a "dynamical map" T.

Definition: dynamical map.

the map $T : \rho(0) \mapsto \rho(t) = T[\rho(0)]$ is linear (clearly motivated by convex sums as input states)

domain (*Definitionsbereich*) of the map T: all (initial) density operators $\rho(0)$

the image $\rho(t)$ is a density operator: hermitean, non-negative, and of trace unity. One calls the map itself therefore trace-preserving and "positive".

the map T is completely positive, as explained now.

"Complete positivity" means the following: imagine that we enlarge the space on which ρ operates and extend T in the following way to "larger" density matrices P. For factorized matrices, $P = \rho \otimes \rho_B$, we set

$$(T \otimes \mathbb{1})(P) = T(\rho) \otimes \rho_B \qquad (2.2)$$

and extend this to arbitrary ("entangled") operators P by linearity. We then require that the extended map $(T \otimes \mathbb{1})$ is positive for any dimension of the extended space.

> There are physical time evolutions that do not fit into this framework. For example, it is possible that the initial density operator $\hat{\rho}(0)$ for an open system does not contain enough information about the system–environment correlations to predict the system's future. See Pechukas (1994).

> At first sight, complete positivity looks as a quite natural condition, not a very strong constraint. It reveals its full power as soon as non-factorized states P on the larger Hilbert space ("entangled states") enter the game.

2.2 Characterization of completely positive maps

It may come as a surprising fact that these conditions already imply a very special form for the dynamical maps: this is the

Kraus-Stinespring representation theorem: All dynamical maps are of the form

$$T(\rho) = \sum_k \Omega_k \rho \Omega_k^\dagger \tag{2.3}$$

with $\sum_k \hat{\Omega}_k^\dagger \hat{\Omega}_k = \mathbb{1}$.

Note that this equation generalizes the unitary evolution that we recover when the sum over the "Kraus operators" Ω_k contains only a single term. Exercise: Eq.(2.3) defines a completely positive map and preserves the trace of ρ.

Sketch of a proof. Adapted from Chap. 4 in *Quantum Computing Devices: Principles, Designs and Analysis* by G. Chen & al, Taylor & Francis 2006, itself taken from Nielsen & Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press 2000).

You prove in the exercises that Eq.(2.3) defines a completely positive map. The only tricky point is the following extension to density operators P in a larger space

$$(T \otimes \mathbb{1})(P) = \sum_k (\Omega_k \otimes \mathbb{1})P(\Omega_k^\dagger \otimes \mathbb{1}) \tag{2.4}$$

where the factor $\otimes \mathbb{1}$ provides the necessary extension to larger dimensions.

We now want to prove the converse. Consider the extended Hilbert space $\mathcal{H} \otimes \mathcal{H}$. Take a vector $|\phi\rangle \in \mathcal{H} \otimes \mathcal{H}$ and construct the operator

$$P = (T \otimes \mathbb{1})(|\phi\rangle\langle\phi|) \tag{2.5}$$

Since T is completely positive, and $|\phi\rangle\langle\phi|$ is a density operator, P is a (positive) density operator. Since P is hermitean, its spectral representation exists and can be written in the form

$$P = \sum_k |\tilde{\varphi}_k\rangle\langle\tilde{\varphi}_k|. \tag{2.6}$$

We have lumped the non-negative eigenvalues into the non-normalized eigenvectors $|\tilde{\varphi}_k\rangle$.

We now construct linear maps Ω_k on the system Hilbert space. Let $|\psi\rangle, |\chi\rangle \in \mathcal{H}$. Define the ket $|\psi^\star\rangle$ with respect to a basis $\{|n\rangle\}$ of $\mathcal{H}$ by "taking the complex conjugate of the coefficients", i.e.:

$$|\psi^\star\rangle = \sum_n |n\rangle\langle n|\psi^\star\rangle, \qquad \langle n|\psi^\star\rangle \equiv (\langle n|\psi\rangle)^* = \langle\psi|n\rangle \tag{2.7}$$

The Kraus operators are now defined via their matrix elements as

$$\langle\chi|\Omega_k|\psi\rangle = \langle\chi \otimes \psi^\star|\tilde{\varphi}_k\rangle, \qquad \langle\psi|\Omega_k^\dagger|\chi\rangle = \langle\tilde{\varphi}_k|\chi \otimes \psi^\star\rangle, \tag{2.8}$$

where the adjoint operator is defined in the usual way. We use the notation $\langle\chi \otimes \psi^\star|$ for the tensor product between the bras (linear forms) $\langle\chi|$ and $\langle\psi^\star|$.

Let us now analyze the following matrix elements of the image density operator P, taking arbitary $|\chi\rangle, |\chi'\rangle, |\psi\rangle \in \mathcal{H}$

$$\begin{aligned}
&\langle\chi \otimes \psi^\star|P|\chi' \otimes \psi^\star\rangle \\
&= \sum_k \langle\chi \otimes \psi^\star|\tilde{\varphi}_k\rangle\langle\tilde{\varphi}_k|\chi' \otimes \psi^\star\rangle \qquad \text{from Eq.(2.6)} \\
&= \sum_k \langle\chi|\Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger|\chi'\rangle
\end{aligned} \tag{2.9}$$

We now specialize to the following form for the vector $|\phi\rangle \in \mathcal{H} \otimes \mathcal{H}$:

$$|\phi\rangle = \sum_n |n \otimes n\rangle \tag{2.10}$$

(this vector is a so-called maximally entangled state on the product Hilbert space). Its projector admits the following expansion

$$\begin{aligned}
|\phi\rangle\langle\phi| &= \sum_{n,m} |n \otimes n\rangle\langle m \otimes m| \\
&= \sum_{n,m} (|n\rangle\langle m|) \otimes (|n\rangle\langle m|)
\end{aligned} \tag{2.11}$$

in terms of skew operators $|n\rangle\langle m|$. It is quite astonishing that the full knowledge about T can be obtained by applying its extension (Eq.(2.5) to this single projector. We shall see in a moment that a dynamical map T (and its extensions) can be defined on skew operators as well, Eq.(2.16). Taking this for granted, we get

$$P = (T \otimes \mathbb{1})(|\phi\rangle\langle\phi|) = \sum_{n,m} T(|n\rangle\langle m|) \otimes (|n\rangle\langle m|) \tag{2.12}$$

Using the definition (2.7), we find that the matrix element of Eq.(2.9) becomes

$$\begin{aligned}
&\sum_{n,m} (\langle\chi| \otimes \langle\psi^\star|) [T(|n\rangle\langle m|) \otimes (|n\rangle\langle m|)] (|\chi' \otimes \psi^\star\rangle) \\
&= \sum_{n,m} \langle\chi|T(|n\rangle\langle m|)|\chi'\rangle\langle n|\psi\rangle\langle m|\psi\rangle^* \\
&= \langle\chi|T(|\psi\rangle\langle\psi|)|\chi'\rangle.
\end{aligned} \tag{2.13}$$

In the last step, we have used the expansion of $|\psi\rangle$ in the basis $\{|n\rangle\}$.

Combining with Eq.(2.9), we have shown that

$$\langle\chi|T(|\psi\rangle\langle\psi|)|\chi'\rangle = \sum_k \langle\chi|\Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger|\chi'\rangle \qquad (2.14)$$

Now, the vectors $|\chi\rangle$, $|\chi'\rangle$ are arbitrary and hence

$$T(|\psi\rangle\langle\psi|) = \sum_k \Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger \qquad (2.15)$$

Hence, we have proven the operator identity (2.3) for the special case of a pure state $\rho = |\psi\rangle\langle\psi|$. The proof is extended to a mixed state by decomposing ρ into projectors $|\psi_i\rangle\langle\psi_i|$ onto eigenvectors with non-negative weights (eigenvalues) p_i, and using the linearity of T.

To fill the gap, we need a prescription to apply a dynamical map to skew operators. We assume that $|\psi\rangle$ and $\chi\rangle$ are orthogonal and set

$$\begin{aligned}
T(|\psi\rangle\langle\chi|) &= \frac{1}{2}\left[T(\rho_{+1}) - T(\rho_{-1}) + iT(\rho_{+i}) - iT(\rho_{-i})\right] \qquad (2.16)\\
\rho_u &:= \frac{1}{2}\left[(|\psi\rangle + u|\chi\rangle)(\langle\psi| + u^*\langle\chi|)\right], \qquad |u| = 1
\end{aligned}$$

where T is applied to projectors onto superposition states of ψ and χ with suitably chosen phase factors u. For a complex linear map, Eq.(2.16) is actually trivially satisfied, as a direct calculation shows. (See exercises.)

Last gaps to fill. Check that the Kraus operators resolve the identity, $\sum_k \Omega_k^\dagger \Omega_k = \mathbb{1}$.

Remarks

- A map is completely positive if it is positive on the "doubled Hilbert space". This is actually all that we needed in the proof.

- If D is the dimension of the Hilbert space $\mathcal{H}$, then there are at most D^2 Kraus operators Ω_k. This is the maximum number of eigenvectors of P with nonzero eigenvalue (the maximum rank of P).

- The vector space of all linear maps is (at most) of dimension D^4: these "superoperators" can be written as $D^2 \times D^2$ matrices that act

on the D^2-dimensional space of density matrices. (All dimensional estimates are actually upper limits here.) This suggests that the completely positive maps only cover a small subspace of all linear maps, in particular if D is large.

- The Kraus theorem provides us a characterization of all completely positive maps. Current research is turned towards a similar result for "positive maps". These maps, extended to the double Hilbert space, may image density operators onto operators with negative eigenvalues. This is connected to the generation of entanglement between the system and its "copy".

- There are researchers who do not accept the requirement of complete positivity (Pechukas, *Phys Rev Lett* 1994): they maintain that factorized states actually never occur in Nature (there are always some correlations or entanglement with the "rest of the world"). From this viewpoint, the violation of complete positivity is related to the fact that the (forgotten) correlations between the system and its environment are needed to construct the proper time evolution. In this sense, time evolution need not be a (completely) positive map. A pragmatic solution (see Shaji and Sudarshan, *Phys Lett A* 2005) could be to restrict the application of a given (approximate) dynamical map to a subset of initial density operators where the map is completely positive.

- Current research is aimed at extending or exploiting the Kraus theorem to master equations "with memory" (non-Markov case). At the time of writing, there are a few generalizations attempted, but no general result has been proven.

2.2.1 Remarks and examples

Choi matrix. The density operator P defined in Eq.(2.12) is called the Choi matrix of the map T. The following re-formulation of the Kraus-Stinespring theorem is called the **Choi theorem**: the map T is completely positive if and only if its Choi matrix P is positive.

Random unitary. Imagine that you have a Hamiltonian $H(x)$ that depends on a "random parameter" x. It can take the values $x = x_k$ with probability p_k. This happens, for example, in your laboratory class when certain values of your apparatus are not well controlled. Then we can define the following "average density matrix" (denoted by the overbar) after time evolution under the unitary operator $U(x) = \exp[-iH(x)t]$:

$$\rho \mapsto \overline{U(x)\rho U^\dagger(x)} = \sum_k p_k U(x_k)\rho U^\dagger(x_k) \qquad (2.17)$$

Actually, from a quantum-mechanical perspective, this is the only way to describe the "preparation procedure" that you implement with the non-accurately known Hamiltonian. We observe that Eq.(2.17) is of the form of the Kraus theorem, with $\Omega_k = \sqrt{p_k}U(x_k)$.

Stinespring dilation theorem. Formulation for a physicist: every completely positive map can be represented by a unitary map on a larger Hilbert space, followed by a partial trace. The projection procedure in the 'system+bath' approach is therefore also the only way to construct a completely positive map.

The main idea is to collect the Kraus operators Ω_k ($k = 1 \ldots K$) into a block-diagonal matrix

$$U = \begin{pmatrix} \Omega_1 & & & \\ & \Omega_2 & & \\ & & \ddots & \\ & & & \Omega_n \end{pmatrix} \qquad (2.18)$$

where the basis $\{|n, k\rangle\}$ is chosen with an 'ancilla' system $\mathcal{K}$ of dimension K. It is easy to check that this gives a unitary matrix U on the enlarged Hilbert space and the representation

$$T(\rho) = \text{tr}_\mathcal{K}[U(\rho \otimes K^{-1}\mathbb{1})U^\dagger] \qquad (2.19)$$

where $K^{-1}\mathbb{1}$ is a completely mixed state on $\mathcal{K}$. The Kraus operators of the completely positive map thus encode a 'reversible' evolution if the quantum system ('ancilla') keeps track of which Kraus operator Ω_k has been applied. As long as the ancilla is not measured (no partial trace taken), the state remains pure on the enlarged Hilbert space.

GNS purification (after Gelfand and Naimark, and Segal). Generalize CP maps between different Hilbert spaces (i.e., the set of density operators). Read a state ρ as such a generalized CP map. The Stinespring dilation theorem allows to represent this as a pure state

$$\rho = \text{tr}_2|\Psi\rangle\langle\Psi| \qquad |\Psi\rangle = \sum_n \sqrt{p_n}|n \otimes n\rangle, \qquad \rho = \sum_n p_n|n\rangle\langle n| \qquad (2.20)$$

where the states $|n\rangle$ are the eigenvectors of ρ with eigenvalues p_n. The pure state $|\Psi\rangle$ is a superposition of eigenvectors tensorized with themselves: as long as the 'ancilla system' keeps a copy of the eigenvector, purity is not lost.

2.2.2 Nakajima–Zwanziger map

System+bath projector. The names Nakajima and Zwanziger are attached to the following natural prescription for the reduced density operator of a system coupled to a bath. This map a actually a completely positive map. We pick a fixed state ρ_B for the bath; this state is an equilibrium state of the bath, and specifies the bath parameter "temperature". Construct from this and the system density operator $\rho(0)$ an initial system+bath state as a tensor product $P(0) = \rho(0) \otimes \rho_B$ (this is a capital ρ). Then evolve this state with a Hamiltonian H_{SB} that contains everything: system and bath Hamiltonian and their mutual coupling. In terms of the corresponding unitary time evolution

$$P(0) \mapsto P(t) = U_{SB}(t)P(0)U_{SB}^\dagger(t) \qquad (2.21)$$

Finally, at time t, the system density operator is obtained in the usual way as a reduced density operator (tracing out the bath degrees of freedom), $\rho(t) = \text{tr}_B[P(t)]$. Putting everything together we have the Nakajima-Zwanziger formula

$$\rho(0) \mapsto \rho(t) = \text{tr}_B\left[U_{SB}(t)\rho(0) \otimes \rho_B U_{SB}^\dagger(t)\right] \qquad (2.22)$$

Exercise: show that this defines a completely positive map.

2.2.3 Partial transpose

Definition. For an operator ρ on a bipartite Hilbert space, consider a tensor product basis $\{|n, m\rangle\}$ and define the partially transposed operator ρ^Γ (the superscript is half a letter T) by its matrix elements

$$\langle n, m|\rho^\Gamma|n', m'\rangle = \langle n, m'|\rho|n', m\rangle \tag{2.23}$$

(No complex conjugation here; partially transpose does not mean "partially hermitean conjugate".)

The partial transpose is a linear map, but it does not preserve positivity. To see this, consider a two-qubit Hilbert space and the pure state

$$\rho = |\psi_+\rangle\langle\psi_+| \quad \text{with} \quad |\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \tag{2.24}$$

In the basis $\{|0, 0\rangle, |0, 1\rangle, |1, 0\rangle, |1, 1\rangle\}$, this projector and its partial transpose are represented by the matrix (please check it)

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \qquad \rho^\Gamma = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{2.25}$$

The determinant of ρ^Γ is -1, hence one eigenvalue must be negative, and ρ^Γ is not positive.

Note from Eq.(2.23) that the partial transpose is the natural extension of the transposition T to an enlarged Hilbert space: $\Gamma = \mathbb{1}\otimes T$. We therefore conclude that the transposition is not a completely positive map.

> The transposition is closely related to the complex conjugation of each matrix element of a density matrix, $\rho_{mn} \mapsto \rho_{mn}^*$: this is easy to see since ρ is hermitean and therefore invariant under hermitean conjugation = transpose and conjugate. It is interesting to realize that the "simple" conjugation is often related to time reversal. The statement above thus suggests the following conjecture: if we time-reverse the evolution of a subsystem, letting the "rest" evolve forward in time as usual, then this dynamics may lead to negative probabilities.

2.3 The Lindblad master equation

The Lindblad (Gorini-Kossakowski-Sudarshan) theorem provides an equation of motion for the density operator in terms of a differential equation.

In technical terms, the time evolution is supposed to be given by a family of completely positive (dynamical) maps that form a semigroup. The Lindblad theorem gives the (time-independent) generator of this semigroup. This result is sometimes called a Markovian master equation because it gives the time evolution of the density operator at time t in terms of $\rho(t)$ (the past is not important).

Semigroup. A family of dynamical maps $\{T_t|t \geq 0\}$ that can be concatenated (*hintereinander ausführen*). Indeed, it is plausible that the time evolutions $\rho(0) \mapsto \rho(t) = T_t(\rho(0))$ can be applied repeatedly,

$$T_{t_1+t_2} = T_{t_1}T_{t_2} \tag{2.26}$$

and the result is also a time evolution. What is missing from the usual group property: inverse element "T_{-t}". Evolution is always "forward in time only" (related to dissipation and loss of information).

Eq.(2.26) is a "functional equation" that is formally solved by an operator of exponential form

$$T_t = \exp(\mathcal{L}t) \tag{2.27}$$

where $\mathcal{L}$ is called the "generator" of the semigroup; it is itself time-independent. (The exponential map provides the homomorphism between concatenation of dynamical maps and addition of the time arguments.) Similar to the Kraus theorem, the constraints of linearity and complete positivity specify the structure of the generator. This is the so-called

2.3.1 Lindblad theorem

A completely positive semigroup $T_t = \exp(\mathcal{L}t)$ has a generator $\mathcal{L}$ that implements the time evolution of a density operator ρ in the form of the following differential equation. There is a hermitean operator H and a countable family of operators L_k (acting on the Hilbert space of the system) with

$$\begin{aligned} \frac{\partial\rho}{\partial t} &= -\mathrm{i}\,[H,\,\rho] + \sum_k \left(L_k\rho L_k^\dagger - \frac{1}{2}\left\{\rho,\, L_k^\dagger L_k\right\}\right) \\ &= -\mathrm{i}\,[H,\,\rho] + \frac{1}{2}\sum_k \left(\left[L_k\rho,\, L_k^\dagger\right] + \left[L_k,\, \rho L_k^\dagger\right]\right) \end{aligned} \tag{2.28}$$

The following sketch of a proof is adapted from Nielsen & Chuang and C. Henkel, *J Phys B* 2007. A slightly different version can be found in the book by Breuer & Petruccione (2002).

We evaluate the difference quotient

$$\frac{\rho(t + \Delta t) - \rho(t)}{\Delta t} \qquad (2.29)$$

with the help of the Kraus theorem and take the limit $\Delta t \to 0$. Write $\rho = \rho(t)$ for simplicity. In the Kraus representation (2.3) for the density matrix $\rho(t + \Delta t)$,

$$\rho(t + \Delta t) = \sum_k \Omega_k \rho \Omega_k^\dagger \qquad (2.30)$$

the operators Ω_k depend on Δt. They can be split into

$$\Omega_k = \omega_k \mathbb{1} + V_k \qquad (2.31)$$

where the first term contains the term proportional to the unit operator. This splitting can be made unique using the following scalar product on the space of operators:

$$(A|B) = \operatorname{tr}(A^\dagger B) \qquad (2.32)$$

Hence, the projection of Ω_k orthogonal to $\mathbb{1}$ which is V_k must satisfy

$$0 = (\mathbb{1}|V_k) = \operatorname{tr}(\mathbb{1}V_k) = \operatorname{tr} V_k \qquad (2.33)$$

in other words, it is traceless. Note that both ω_k and V_k depend on Δt.

In terms of these quantities, the change in the density matrix is computed to be

$$\rho(t + \Delta t) - \rho \qquad (2.34)$$
$$= (\sum_k |\omega_k|^2 - 1)\rho + \sum_k \left(\omega_k^* V_k \rho + \rho \, \omega_k V_k^\dagger \right) + \sum_k V_k^\dagger \rho V_k$$

where ω_k^* is complex conjugate to ω_k. We assume that the following continuity condition holds

$$\lim_{\Delta t \to 0} \left[\hat{A}\rho(t + \Delta t) - \hat{A}\rho(t) \right] = \mathcal{O}(\Delta t) \qquad (2.35)$$

for all operators $\hat{A}$ and initial density matrices $\rho(t)$. This permits us to extract all matrix elements in Eq.(2.34) and to conclude that the following terms must vanish separately

$$\lim_{\Delta t \to 0} \sum_k |\omega_k|^2 = 1 \qquad (2.36)$$

$$\lim_{\Delta t \to 0} \sum_k \omega_k^* \rho V_k = 0 \qquad (2.37)$$

$$\lim_{\Delta t \to 0} \sum_k V_k \rho V_k^\dagger = 0 \qquad (2.38)$$

where the last two lines apply to any density matrix ρ. We now assume that the following derivatives exist

$$\gamma \equiv \lim_{\Delta t \to 0} \frac{\sum_k |\omega_k|^2 - 1}{\Delta t} \qquad (2.39)$$

$$\Gamma - iH \equiv \lim_{\Delta t \to 0} \frac{\sum_k \omega_k^* V_k}{\Delta t} \qquad (2.40)$$

where Γ and H are both hermitean.

Differentiating the condition that the dynamical map preserves the trace of the density matrix, we find

$$0 = \lim_{\Delta t \to 0} \frac{\operatorname{tr}\left[\rho(t + \Delta t) - \rho\right]}{\Delta t}$$
$$= \operatorname{tr}\left[\gamma\rho + 2\Gamma\rho + \lim_{\Delta t \to 0} \frac{1}{\Delta t} \sum_k V_k^\dagger V_k \rho \right] \qquad (2.41)$$

Since this must hold for any density matrix ρ, we find another derivative (this argument uses that the scalar product (2.32) is non-degenerate)

$$\lim_{\Delta t \to 0} \frac{\sum_k V_k^\dagger V_k}{\Delta t} = -\gamma - 2\Gamma \qquad (2.42)$$

We can thus introduce the Lindblad operators L_k by the limiting procedure

$$L_k \equiv \lim_{\Delta t \to 0} \frac{V_k}{\sqrt{\Delta t}} \qquad (2.43)$$

where we used that the root of $\Delta t \geq 0$ can be taken. Using the derivatives defined in Eqs.(2.39, 2.40, 2.43), we can divide the difference $\rho(t + \Delta t) - \rho(t)$ in Eq.(2.34) by Δt, and take the limit $\Delta t \to 0$. This gives the differential equation (2.28).

Note that a Lindblad operator L proportional to the unit operator automatically gives a zero contribution in the Lindblad form. This is why the split in Eq.(2.31) makes sense.

2.3.2 Examples

Spontaneous emission

of a two-level atom is described by a single "Lindblad operator"

$$L = \sqrt{\gamma}\,\sigma \qquad (2.44)$$

where the strange unit arises because the "square of L" provides the actual time derivative of ρ. This result for spontaneous emission is derived in Sec.**??**.

We can best check that this is compatible with the Born-Markov master equation by switching to the Heisenberg picture. Taking the trace of the Lindblad master equation (2.28), multiplied with a system operator A, we find

$$\frac{\partial}{\partial t}\langle A\rangle = \mathrm{i}\langle[H,\,A]\rangle + \frac{1}{2}\sum_k\left\langle L_k^\dagger\,[A,\,L_k] + \left[L_k^\dagger,\,A\right]L_k\right\rangle \qquad (2.45)$$

where the first term is the familiar one. The second one involves commutators between A and the Lindblad operators. Simple calculations show that this leads indeed to the damping of the atomic dipole operators σ and $\sigma^\dagger$ (at the rate γ, Eq.(**??**)) and to the damping of the inversion σ_3, Eq.(**??**), as we found in the previous semester.

Lossy cavity

Let us consider a single-mode cavity with annihilation operator a and consider the non-Schrödinger processes if one mirror is partially transmitting. There are two Lindblad operators that describe the loss of photons from the cavity (bosonic operators a, $a^\dagger$) and the fact that thermal radiation can enter the cavity:

$$L_{\mathrm{loss}} = \sqrt{\kappa(\bar{n}+1)}\,a, \qquad L_{\mathrm{abs}} = \sqrt{\kappa\bar{n}}\,a^\dagger \qquad (2.46)$$

where κ is a loss rate (the inverse of the "photon lifetime") and $\bar{n} = (\mathrm{e}^{\hbar\omega_{\mathrm{A}}/k_{\mathrm{B}}T} - 1)^{-1}$ is the average thermal photon number at the cavity frequency. The temperature T corresponds to the radiation field outside the cavity. We recover for $T = 0$ a pure loss channel where the photon annihilation operator in L_{em} plays the role of the atomic ladder operator in Eq.(2.44).

The operator L_{loss} describes the emission of photons (spontaneous and stimulated) into the thermal field; the operator L_{abs} describes photon absorption. This can be easily checked by going back to a two-level model involving only the number states $|0\rangle$ and $|1\rangle$ and working out the equations of motion for the density matrix elements ρ_{00} and ρ_{10}. One gets the rate equations that have been used by Einstein in his proof of the Planck spectrum (*Physikal. Zeitschr.* 1917).

Both rates add up in the dynamics of off-diagonal elements of the density operator ρ_{10} (which plays the role of the atomic dipole, remember the matrix elements ρ_{eg}): their decay rate is $\kappa(2\bar{n}+1)$. This is a typical feature of master equations: the off-diagonal elements decay at least with the half-sum of the decay rates of the corresponding populations. In practice, their decay rate is even larger, due to additional dissipative processes ("dephasing").

Dephasing

is a process where only the off-diagonal elements of the density matrix decay, while the populations are left unchanged. The Lindblad operator is

$$L_{\mathrm{deph}} = \sqrt{\kappa}\,\sigma_3 \qquad (2.47)$$

with a rate κ. By solving the Lindblad master equation (exercise!), we find

$$\rho(t) = \begin{pmatrix} \rho_{\mathrm{ee}}(0) & \mathrm{e}^{-\kappa t}\rho_{\mathrm{eg}}(0) \\ \mathrm{e}^{-\kappa t}\rho_{\mathrm{ge}}(0) & \rho_{\mathrm{gg}}(0) \end{pmatrix} \qquad (2.48)$$

This process can be mimicked in a "classical way" by assuming that a superposition state vector

$$|\psi(t)\rangle = \alpha\,\mathrm{e}^{\mathrm{i}\varphi(t)}|\mathrm{e}\rangle + \beta\,\mathrm{e}^{-\mathrm{i}\varphi(t)}|\mathrm{g}\rangle \qquad (2.49)$$

acquires a relative phase $\varphi(t)$ that is "randomly fluctuating". Experimentally, this happens for a two-level system embedded in a solid: the motion of the immediate environment perturbs the form of the electronic orbitals and hence their energy, even if the electron stays in this orbital ("adiabatic perturbation"). Hence only the energy is randomized, but the population is kept constant.

In this context, we can define a quantum-mechanical "average ensemble" by building the density matrix $|\psi(t)\rangle\langle\psi(t)|$ and taking the average over the probability distribution of $\varphi(t)$ (denoted by an overbar):

$$\rho(t) = \overline{|\psi(t)\rangle\langle\psi(t)|} \tag{2.50}$$

With the identification

$$\overline{e^{i\varphi(t)}} = e^{-\kappa t} \tag{2.51}$$

we get the same result as with the Lindblad form. This is true if $\varphi(t)$ is a gaussian random variable with zero average and with variance $\langle\varphi(t)^2\rangle = \kappa t$. This behaviour is similar to Brownian motion (hence the name "phase diffusion"), in the mathematics literature, it is called a "Wiener process".

2.4 Exactly solvable open systems

Material based on the BSc thesis by Ch. Witzorky.

Two examples for a two-level system coupled to a bath. One is based on "dephasing", the other one (see exercises) on "spontaneous emission". No exact solutions are known when extra terms are added to the system Hamiltonian, for example, that break the simple form analyzed here.

2.4.1 Dephasing

References: N. G. van Kampen, *J Stat Phys* 1995 and G. Massimo Palma and Kalle-Antti Suominen and Artur K. Ekert, *Proc Roy Soc London A* 1996, in particular Section 4. The material of this Section can be used as a short student talk.

We consider a two-level system that couples to a quantized field (in the following: "bath") via

$$H_{\text{int}} = \sigma_3 \sum_k \left(g_k b_k^\dagger + g_k^* b_k \right) \tag{2.52}$$

with coupling constants g_k that are summarized by the spectral density (ω_k is the frequency of bath mode k)

$$S(\omega) = 2\pi \sum_k |g_k|^2 \delta(\omega - \omega_k) \tag{2.53}$$

From the master equation (2.45) in the Heisenberg picture, we see that the inversion σ_3 is conserved. Hence, only the "off-diagonal operator" σ is affected by the

bath. Going back to the Schrödinger picture, one can show that the off-diagonal elements of the density matrix behave like

$$\rho_{\text{eg}}(t) = e^{-\Gamma(t)}\rho_{\text{eg}}(0) \tag{2.54}$$

where the "decoherence factor" is given by

$$\Gamma(t) = \frac{1}{2}\sum_k |\xi_k(t)|^2 \coth(\beta\omega_k/2) \tag{2.55}$$

$$= 2\int_0^\infty \frac{d\omega}{2\pi} S(\omega)\frac{|1-e^{i\omega t}|^2}{\omega^2}\coth(\beta\omega/2) \tag{2.56}$$

where $\beta = \hbar/k_B T$ is the inverse temperature of the initial bath state (we assume factorized initial conditions) and

$$\xi_k(t) = 2g_k\frac{1-e^{i\omega_k t}}{\omega_k} \tag{2.57}$$

A proof of this result is sketched in Sec.2.4.1 below.

Discussion

For short times, we can expand the effective coupling constants $\xi_k(t)$ and get

$$t \to 0: \quad \Gamma(t) \approx 2t^2\sum_k |g_k|^2\coth(\beta\omega_k/2) = 2t^2\int_0^\infty \frac{d\omega}{2\pi} S(\omega)\coth(\beta\omega/2) \tag{2.58}$$

The quadratic dependence on time is characteristic for this initial regime. In fact, from perturbation theory, we see that the probability amplitude for states orthogonal to the initial one must increase linearly in t. The corresponding probability thus starts off proportional to t^2. The integral in Eq.(2.58) is often dominated by large frequencies, and can be made finite with a "UV cutoff frequency" $\omega_c = 1/\tau_c$. (Without this cutoff, the integral actually diverges and the short-time regime may even lead to mathematical inconsistencies.) The quadratic regime then applies only on time scales $t < \tau_c$ that are typically very short compared to the dissipative dynamics.

At larger times, we can make the approximation that $|\xi_k(t)|^2$ approaches a

δ-function:[1]

$$t \to \infty: \qquad \left|\frac{1 - e^{i\omega_k t}}{\omega_k}\right|^2 \to 2\pi t \, \delta^{(1/t)}(\omega_k) \tag{2.60}$$

where the width of the δ-function is of the order $1/t$. In this limit, only low-frequency modes contribute to the decoherence factor.

Let us first assume that $1/t$ is larger than $1/\beta$ (intermediate range $\tau_c \ll t \ll \hbar/k_B T$). Then we can make the zero-temperature approximation $\coth(\beta\omega/2) \approx 1$ for the relevant modes and get

$$\tau_c \ll t \ll \beta: \qquad \Gamma(t) \approx 2S(0)t \tag{2.61}$$

hence an exponential decay with a rate $\kappa = 2S(0)$ that involves the spectral strength at zero frequency (more precisely: at frequencies $k_B T/\hbar \ll \omega \ll \omega_c$). This behaviour is consistent with a Lindblad master equation because $e^{-\Gamma t}$ becomes exponential in t. We thus see that the Lindblad form is not valid on the short time scale τ_c that sets the correlation time of the bath fluctuations.

Finally, when $t \gg \beta$, we have to take into account the thermal occupation of the low-frequency modes. The integral cannot be performed any more without knowledge of the behaviour of the function $S(\omega)$, in particular the limit $\lim_{\omega \to 0} S(\omega) \coth(\beta\omega/2)$. One class of spectral densities gives power laws $e^{-\Gamma(t)} \propto t^\alpha$ with exponents α that depend on $S(\omega)$ and the temperature. An exponential decay at a T-dependent rate is possible as well, in particular in the so-called "Ohmic case" where the spectrum is linear for small frequencies, $S(\omega) \approx \alpha\omega$ with a dimensionless coefficient α. We then get at large t:

$$t \to \infty: \qquad \Gamma(t) \approx 4\pi t \int\limits_0^\infty \frac{d\omega}{2\pi} S(\omega) \delta^{(1/t)}(\omega) \coth(\beta\omega/2)$$

$$\approx 4\pi t \int\limits_0^\infty \frac{d\omega}{2\pi} \alpha\omega \, \delta^{(1/t)}(\omega) \frac{2}{\beta\omega} = 4\alpha t/\beta \tag{2.62}$$

The decoherence rate thus becomes $4\alpha k_B T/\hbar$.

---

[1]This is based on the integral

$$\int_{-\infty}^{\infty} dx \frac{\sin^2(x/2)}{x^2} = \frac{\pi}{2}. \tag{2.59}$$

Calculation of the decoherence factor

The material in this and the following section could be used for a BSc thesis. It collects calculations scattered in the literature on this exactly solvable model.

For the states $|g\rangle$ and $|e\rangle$ of the spin, the action of the full Hamiltonian is easy:

$$H|g\rangle = |g\rangle H_g, \qquad H_g = -\frac{\hbar\omega_A}{2} + H_B - \sum_k \hbar(g_k b_k^\dagger + g_k^* b_k) \tag{2.63}$$

where H_g acts on the bath variables only. A similar expression applies to H_e, with the opposite sign in the first and last term. We therefore get from the full time evolution operator $U(t)$:

$$\begin{aligned}
\langle\sigma\rangle_t &= \mathrm{tr}_{SB}[U^\dagger(t)|g\rangle\langle e|U(t)\rho(0) \otimes \rho_T(B)] \tag{2.64}\\
&= \mathrm{tr}_{SB}[|g\rangle\langle e|\rho(0) \otimes U_g^\dagger(t)U_e(t)\rho_T(B)] \tag{2.65}\\
&= \langle\sigma\rangle_0 \mathrm{tr}_B[U_g^\dagger(t)U_e(t)\rho_T(B)] \tag{2.66}
\end{aligned}$$

The bath trace can be taken for each mode separately since both $U_{g,e}(t)$ and $\rho_T(B)$ factorize into a product of single-mode operators. For a single mode b with parameters g, ω, we have (dropping the label k for the moment and assuming real g)

$$U_g^\dagger(t) = \exp[it(\omega b^\dagger b - gb - gb^\dagger)] = \exp[i\omega t(b^\dagger - \gamma)(b - \gamma)]\, e^{-itg^2/\omega} \tag{2.67}$$
$$U_e(t) = \exp[-it(\omega b^\dagger b - gb - gb^\dagger)] = \exp[-i\omega t(b^\dagger + \gamma)(b + \gamma)]\, e^{-itg^2/\omega}$$

with $\gamma = g/\omega$. We now recall the action of the displacement operator $D(\gamma)$ on a function of the operators b, $b^\dagger$:

$$D^\dagger(\gamma)f(b, b^\dagger)D(\gamma) = f(b + \gamma, b^\dagger + \gamma^*) \tag{2.68}$$

We can therefore write

$$\begin{aligned}
&U_g^\dagger(t)U_e(t)\rho_T(B) \\
&= D^\dagger(-\gamma)\exp(i\omega t b^\dagger b)D(-\gamma)D^\dagger(\gamma)\exp(-i\omega t b^\dagger b)D(\gamma) \tag{2.69}\\
&= D^\dagger(-\gamma)\exp(i\omega t b^\dagger b)D(-2\gamma)\exp(-i\omega t b^\dagger b)D(\gamma) \tag{2.70}
\end{aligned}$$

where in the last step, we have used $D^\dagger(\gamma) = D(-\gamma)$ and the composition law of the displacement operators. (The projective phase in QO I, Eq.(3.37) vanishes in this case.) We now use the identity, similar to Eq.(2.68)

$$U_0^\dagger(t)f(b, b^\dagger)U_0(t) = f(b\,e^{-i\omega t}, b^\dagger\,e^{i\omega t}) \tag{2.71}$$

where $U_0(t) = \exp(-\mathrm{i}\omega t b^\dagger b)$ is the 'free' time evolution operator. Applying this to the displacement operator $D(-2\gamma) = \exp(-2\gamma b^\dagger + 2\gamma^* b)$ that is 'sandwiched' in Eq.(2.70), we have

$$\exp(\mathrm{i}\omega t b^\dagger b) D(-2\gamma) \exp(-\mathrm{i}\omega t b^\dagger b) = D(-2\gamma\, \mathrm{e}^{\mathrm{i}\omega t}) =: D(-2\gamma(t)) \tag{2.72}$$

We end up with a product of three displacement operators

$$
\begin{aligned}
D(\gamma)D(-2\gamma(t))D(\gamma) &= \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\,\gamma^*\gamma(t)} D(\gamma - 2\gamma(t))D(\gamma) \tag{2.73}\\
&= \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\,\gamma^*\gamma(t)} \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\,\gamma^*(t)\gamma} D(\xi(t)) \tag{2.74}\\
\xi(t) &= 2g\frac{1 - \mathrm{e}^{\mathrm{i}\omega t}}{\omega} \tag{2.75}
\end{aligned}
$$

where the projective phases cancel and we recover the parameter $\xi_k(t)$ of Eq.(2.57).

We finally have to calculate the average of a displacement operator in a thermal state:

$$\langle D(\xi_t)\rangle_\mathrm{B} = \mathrm{tr}\,[D(\xi_t)\rho_T] \tag{2.76}$$

where Z is the partition function. The calculation of this trace is typically done in the number state basis, but this is quite involved. The fastest way is to remember the P-representation of the thermal state

$$\rho_T = \int \mathrm{d}^2\alpha |\alpha\rangle\langle\alpha| P_T(\alpha), \qquad P_T(\alpha) = \frac{\mathrm{e}^{-|\alpha|^2/\bar{n}}}{\pi\bar{n}} \tag{2.77}$$

and to calculate

$$
\begin{aligned}
\langle D(\xi_t)\rangle_\mathrm{B} &= \mathrm{tr}\int \mathrm{d}^2\alpha\, D(\xi_t)|\alpha\rangle\langle\alpha| P_T(\alpha)\\
&= \mathrm{tr}\int \mathrm{d}^2\alpha\, \mathrm{e}^{\mathrm{i}\,\mathrm{Im}\,\xi_t^*\alpha}|\alpha + \xi_t\rangle\langle\alpha| P_T(\alpha)\\
&= \int \mathrm{d}^2\alpha\, \mathrm{e}^{\mathrm{i}\,\mathrm{Im}\,\xi_t^*\alpha}\langle\alpha|\alpha + \xi_t\rangle P_T(\alpha)\\
&= \int \mathrm{d}^2\alpha\, \mathrm{e}^{2\mathrm{i}\,\mathrm{Im}\,\xi_t^*\alpha}\mathrm{e}^{-|\xi_t|^2/2} P_T(\alpha)
\end{aligned}
$$

At this point, we can take out the exponential factor $\mathrm{e}^{-|\xi_t|^2/2}$. Note that the projective phases now remain and determine the temperature dependence of the result. The gaussian integral can be performed and gives

$$\langle D(\xi_t)\rangle_\mathrm{B} = \mathrm{e}^{-|\xi_t|^2/2}\mathrm{e}^{-|\xi_t|^2\bar{n}} = \exp\left(-\tfrac{1}{2}|\xi_t|^2 \coth\beta\omega/2\right) \tag{2.78}$$

Going back to $\langle\sigma\rangle_t$, we restore the factor $\mathrm{e}^{-\mathrm{i}\omega_A t}$ that we forgot in Eqs.(2.67) and take the product over all modes. This gives a sum in the exponent and hence

$$
\begin{aligned}
\langle\sigma\rangle_t &= \mathrm{e}^{-\Gamma(t)}\langle\sigma\rangle_0 \tag{2.79}\\
\Gamma(t) &= \sum_k \tfrac{1}{2}|\xi_k(t)|^2 \coth(\beta\omega_k/2) \tag{2.80}
\end{aligned}
$$

which is Eq.(2.81).

Long-time limit

We evaluate here in more detail the decoherence factor $\mathrm{e}^{-\Gamma(t)}$ in the limit of long times. The spectral density is taken in Ohmic form with a dimensionless prefactor α and a cutoff frequency ω_c:

$$\Gamma(t) = 8\alpha \int_0^\infty \mathrm{d}\omega \frac{\omega\omega_c^2}{\omega^2 + \omega_c^2} \coth\frac{\omega}{2T} \frac{\sin^2(\omega t/2)}{\omega^2} \tag{2.81}$$

Observe that the integrand is even in ω, extend the integration from $-\infty$ to ∞ and write $\sin^2(\omega t/2) = \mathrm{Re}\tfrac{1}{2}(1 - \mathrm{e}^{\mathrm{i}\omega t})$. When we shift the integration path from the real axis to a large semi-circle at infinity, we encounter simple poles in the $\coth(\omega/2T)$ at $\omega = \mathrm{i}\xi_n = 2\pi nT$, the so-called Matsubara frequencies. Since

$$\coth\frac{\omega}{2T} = 2T\frac{\mathrm{d}}{\mathrm{d}\omega}\log\sinh\frac{\omega}{2T} \tag{2.82}$$

these poles arise from the zeros of $\sinh\frac{\omega}{2T}$ and have a residue $2T$. There is also a simple pole at $\omega = \mathrm{i}\omega_c$, from the cutoff of the mode density. Finally, we have to take into account half the residue of the singularity at $\omega = 0$. Because $\coth(\omega/2T) \approx 2T/\omega$ for small ω, we have a singularity $1/\omega^2$ (a double pole) at the origin. Hence, the residue is the first derivative of the rest of the integrand:

$$4\alpha T\,\mathrm{Re}\,\pi\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\omega}\frac{\omega_c^2}{\omega^2 + \omega_c^2}(1 - \mathrm{e}^{\mathrm{i}\omega t}) = 4\alpha T\,\mathrm{Re}\,\pi\mathrm{i}(-\mathrm{i}t) = 4\pi\alpha Tt \tag{2.83}$$

This coincides with the term linear in t that we found with the approximation $\delta^{(t)}(\omega)$ to the $\sin^2$ function, Eq.(2.62). The contributions from the other poles give the sum

$$\Gamma(t) = \gamma t + 4\alpha\,\mathrm{Re}\,2\pi\mathrm{i}\Big(\sum_{n=1}^\infty \frac{\omega_c^2}{\omega_c^2 - \xi_n^2}\frac{T(1 - \mathrm{e}^{-\xi_n t})}{\mathrm{i}\xi_n} + \frac{\omega_c^2}{2\mathrm{i}\omega_c}\coth\frac{\mathrm{i}\omega_c}{2T}\frac{1 - \mathrm{e}^{-\omega_c t}}{\mathrm{i}\omega_c}\Big) \tag{2.84}$$

For $t \gg \tau_c$, we can set $\mathrm{e}^{-\omega_c t} = 0$. If we further assume $\xi_1 t = 2\pi Tt \gg 1$, then also the sum becomes time-independent, and we have an expression for the offset

K (or "initial slip") between $\Gamma(t)$ and the linear approximation γt. Putting $N_c = \omega_c/2\pi T$,

$$K = 4\alpha\left(-\cot \pi N_c + \sum_{n=1}^{\infty} \frac{N_c^2}{n(N_c^2 - n^2)}\right) \tag{2.85}$$

Note that N_c is not an integer if ω_c does not coincide with any of the Matsubara frequencies ξ_n. A typical limiting case is a large cutoff, $N_c \gg 1$. The apparent divergence at $n \approx N_c$ is cancelled by the first term. We cannot take the limit $N_c \to \infty$ because the sum would not converge. Instead, we can take N_c to a half-integer so that the cotangent vanishes, split the sum into $n = 1 \ldots \lfloor N_c \rfloor$ and $n = \lceil N_c \rceil \ldots \infty$ and approximate the cutoff function of the mode density by simple limiting forms:

$$K \approx 4\alpha\left(\sum_{n=1}^{\lfloor N_c \rfloor} \frac{1}{n} - N_c^2 \sum_{n=\lceil N_c \rceil}^{\infty} \frac{1}{n^3}\right) \tag{2.86}$$

Replacing the summations by integrations, we get

$$K \approx 4\alpha\left(\log N_c - N_c^2 \frac{-3}{N_c^2}\right) = 4\alpha\left(\log \frac{\omega_c}{2\pi T} + 3\right) \tag{2.87}$$

up to corrections of order unity in the parenthesis.

2.4.2 Spontaneous decay

In this model, a two-level atom is coupled to a bosonic environment within the rotating-wave approximation,

$$H_{\text{int}} = \sum_k \left(g_k \sigma^\dagger a_k + g_k^* a_k^\dagger \sigma\right) \tag{2.88}$$

and the initial state is an excited atom and the field in the vacuum state. Since the quantum number "excitation" (see exercises: sum of photon number and number of excited states) is conserved, the subspace spanned by the states by $|e, \text{vac}\rangle$ and $|g, 1_k\rangle$ (atom in the ground state and one photon in mode k) is closed under time evolution. The following *Ansatz* for the full quantum state is thus exact:

$$|\Psi(t)\rangle = c_e(t)|e, \text{vac}\rangle + \sum_k c_k(t)|g, 1_k\rangle \tag{2.89}$$

One can find from the Schrödinger equation a closed integro-differential equation for the amplitude $c_e = \langle e, \text{vac}|\psi(t)\rangle$ of the state vector and solve it with the Laplace transform. The result is a non-exponential decay. An example is shown in Fig.2.1 where the decay happens only partially when the atomic frequency is in a spectral

Figure 2.1: Decay of an excited atom for a spectral strength that sharply grows above a cutoff frequency: $S(\omega) \sim \beta^{1/2}(\omega - \omega_c)^{1/2}$ for $\omega \geq \omega_c$. The detuning $\delta_c = \omega_c - \omega_A$ from the lower cutoff is given on the right. The ratio $|d(t)|^2/|d(0)|^2$ gives the probability $|c_e(t)|^2$. Taken from Boedecker & al. (2004).

region where the coupling strength $S(\omega_A) = 0$ (positive detuning δ_c).

If the spectral strength of the bath contains sharp peaks, the decay may even happen in an oscillating manner. Mathematically, this emerges from different poles in the Laplace transform of $c_e(t)$ that give interfering contributions in the back transformation. A simple exponential decay emerges at long times when one single pole is located close to the imaginary axis (in the Laplace variable). This corresponds to negative detuning in Fig.2.1.

Another generic feature are algebraic (non-exponential) "tails" that survive at long times whenever the spectral strength $S(\omega)$ can only be defined in a cut complex plane. This typically happens because at zero frequency, some derivative of $S(\omega)$ is discontinuous. As a consequence, at very long times, the decay is not exponential any more (Dittrich & al., 1998, chapter by G.-L. Ingold). This feature has not yet been measured in quantum optics, to our knowledge. It may actually be an artefact of the factorized initial conditions for this model. In fact, if similar techniques are applied for the Bloch equations in this context, one can easily generate solutions that "leave the Bloch sphere", i.e., with negative eigenvalues of the density matrix. This is manifestly non-physical, but it does not seem obvious how to repair this problem. See, e.g., Davidson & Kozak, *J Math Phys* 1971 and Barnett & Stenholm, *Phys Rev A* 2001.

2.5 Fluctuations and correlations

Introduction

We have so far analyzed so-called 'one-time averages' of an open quantum system, $\langle A(t)\rangle = \text{tr}\, A\rho(t)$, given by the density operator at time t, or via generalized Heisenberg equations. What can we say about time correlation functions like $\langle A(t)B(t')\rangle$ where two times enter? It is clear that we are dealing here with Heisenberg operators $A(t)$ and $B(t')$. We have

encountered these correlations when discussing vacuum fluctuations. Indeed, these correlation functions can be interpreted in analogy to classical stochastic processes where one deals with random variables (instead of operators) and where $\langle A(t)B(t') \rangle$ is a measure of the correlations between the variables A and B at different times.

In practise, one often studies stationary cases in the wide sense where the correlations depend only on the time difference,

$$\langle A(t)B(t') \rangle = \langle A(t - t')B(0) \rangle \qquad (2.90)$$

One can easily show by cyclic permutations under the trace that this property is true if $A(t)$ and $B(t')$ evolve in time by a Hamiltonian H that commutes with the (initial) state ρ. This is a model that is not general enough to account for dissipation and coupling to an unobserved environment, of course. In the stationary case, we define a "correlation spectrum" by taking the Fourier transform

$$S_{AB}(\omega) = \int d\tau \, \langle A(t + \tau)B(t) \rangle \, e^{-i\omega\tau} \qquad (2.91)$$

(the sign in the exponential is conventional). There are also different conventions regarding the operator order: a symmetrized operator product is useful to make the mapping to classical physics easy. In that case, the correlation function $\frac{1}{2}\langle A(t + \tau)B(t) + B(t)A(t + \tau) \rangle$ is real and depends only on τ (provided the average is taken in a stationary state). This implies that the real part of the spectrum is even in ω. We keep the operator order here because we want to deal also with normally ordered averages, for example $\langle a^\dagger(t)a(t') \rangle$.

2.5.1 Power spectrum and signal analysis

The Eq.(2.91) we used to define the spectrum is actually a theorem, named after Wiener and Khintchine. In many physics textbooks, it does not become clear what is the *theorem* behind this formula. In brief, Wiener showed that the following integral exists for a certain class of autocorrelation functions:

$$\mu_A(\omega) = \int d\tau \frac{e^{-i\omega\tau} - 1}{-i\tau} \langle A(t + \tau)A(t) \rangle \qquad (2.92)$$

57

...and Khintchine showed that the autocorrelation function has a spectral representation

$$\langle A(t + \tau)A(t) \rangle = \int \frac{d\mu_A(\omega)}{2\pi} e^{i\omega\tau} \qquad (2.93)$$

where $d\mu_A(\omega)$ is a certain positive integration measure. It is clear that $\mu_A(\omega)$ is the integrated spectrum – a quantity that is less singular than the spectral density (which may contain δ functions).

E. Wolf in his books (Born & Wolf, 1959; Mandel & Wolf, 1995) introduces the spectrum via a time-limited Fourier transform:

$$S_A(\omega, t) = \lim_{T \to \infty} \frac{1}{T} \left\langle \left| \int_{t-T/2}^{t+T/2} dt' \, e^{i\omega t'} A(t') \right|^2 \right\rangle \qquad (2.94)$$

which is a formula well-suited for actual data processing. The time integrals cover only a finite window T and the average can be calculated by shifting this window across a time series (time averaging). In practice, Eq.(2.94) can be used if T is larger than the correlation time τ_c of the process. It is a simple exercise to show that it coincides with the Wiener-Khinchine formula.

A third definition of the power spectrum appears in the mathematical theory of (linear) filters. This can be physically motivated by remembering that we never actually observe the value $A(t)$ of an observable, but some time average. This can be formalized by considering a "detector function" $\varphi(t)$ and forming the integral

$$A_\varphi = \int dt \, \varphi^*(t)A(t) \qquad (2.95)$$

The spectrum then appears as the link between the Fourier transform of the detector and the variance of the filtered signal (we assume that $\langle A_\varphi \rangle = 0$)

$$\langle A_\varphi^\dagger A_\varphi \rangle = \int \frac{d\omega}{2\pi} S_A(\omega) \, |\tilde{\varphi}(\omega)|^2 \qquad (2.96)$$

where $\tilde{\varphi}(\omega)$ is the Fourier transform of the detector function (it exists by assumption because the detector function is smooth and integrable). The advantage of this formulation is that the integrals always exists because $\tilde{\varphi}(\omega)$ has built-in cutoffs at small and large frequencies if it is integrable. And that in actual experiments, we only have access to the spectral density

58

in a certain range of frequencies (defined by the resolution of the detectors). By taking for $\varphi(t)$ an exponential $\mathrm{e}^{\mathrm{i}\omega t}$ restricted to a finite interval, one recovers the definition (2.94) of Wolf and the prefactor $1/T$ that appears there.

Question. The previous equation was formulated for a stationary process (autocorrelation function depends on the time difference only). How can it be generalized to non-stationary processes?

2.5.2 An interpretation via a sequence of measurements

To conclude, let us formulate a "standard interpretation" of correlation functions that appears in the literature and that may be taken with care in the quantum context. For the general correlation

$$\langle A(t+\tau)B(t)\rangle \qquad (2.97)$$

one makes the reasoning: with some probability distribution $P(B(t) = b)$ one measures the value b for the observable B at time t. Then, given this measurement and evolving the system forward over a time step τ, one gets a value a for the observable A with some conditional probability $P(A(t+\tau) = a|\text{"}B(t)$ has been measured"). This gives the following recipe for the correlation function as a multi-average

$$\langle A(t+\tau)B(t)\rangle = \int \mathrm{d}a\,\mathrm{d}b\,aP(A(t+\tau) = a|\ldots)bP(B(t) = b) \qquad (2.98)$$

Note however, that in quantum mechanics, the measurement at time t in general perturbs the system. This can only be avoided if we write the stationary state (at time t) in a diagonal expansion over eigenstates of the operator B. The conditional probability then involves the time evolution of one of these eigenstates over a time step τ. If this trick is not applied, it may happen that the state after the first "measurement" is not a physical state (it is not a hermitean density operator, but something skew). In addition, at intermediate times, it may not be appropriate to talk about the observable B having a value b with a positive probability: this line of thought has somewhat the flavour of a "hidden variable" which we know is problematic from the EPR paradox.

2.5.3 Examples

Single-mode laser

The frequency spectrum of a **single-mode laser** is given by the Fourier transform of the autocorrelation function

$$C_a(\tau) = \lim_{t\to\infty}\langle \hat{a}^\dagger(t+\tau)\hat{a}(t)\rangle \qquad (2.99)$$

where the limit $t \to \infty$ ensures that the system has reached a steady state.[2]

Exercise. Introduce the (formal) Fourier transform of the mode operator

$$\tilde{a}(\omega) = \int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\hat{a}(t) \qquad (2.100)$$

and show that for a stationary correlation function, the Fourier transform has the covariance

$$\langle \tilde{a}^\dagger(\omega)\tilde{a}(\omega)\rangle = S_a(\omega)2\pi\delta(\omega - \omega') \qquad (2.101)$$

where $S_a(\omega)$ is the Fourier transform of $C_a(\tau)$ [Eq.(2.99)].

The simplest case corresponds to a "freely evolving mode" (frequency ω_L where

$$\langle \hat{a}^\dagger(t+\tau)\hat{a}(t)\rangle = \langle \hat{a}^\dagger\hat{a}\rangle\,\mathrm{e}^{\mathrm{i}\omega_L\tau} \qquad (2.102)$$

and the spectrum is monochromatic

$$S_a(\omega) = \langle \hat{a}^\dagger\hat{a}\rangle\delta(\omega - \omega_L) \qquad (2.103)$$

Its amplitude is given by the stationary average photon number $\langle \hat{n}\rangle = \langle \hat{a}^\dagger\hat{a}\rangle$.

In a physical system, there are several reasons why the spectrum is not monochromatic:

---

[2]The time difference τ cannot be too large, of course, otherwise one would again get sensitive to initial transients. This can be made more precise with the mathematical tools of "filter theory" and wavelet analysis. The physicist helps himself by introducing a measurement interval of length T which overlaps with the stationary regime, and by reducing the Fourier transform to this interval. The spectrum is then defined in the limit $T \to \infty$ after suitable normalization.

— the measurement time T is finite. The δ-function in Eq.(2.103) has a width $\mathcal{O}(1/T)$. This is a "trivial" limitation, and one takes in practice the limit $T \to \infty$.

— losses from the laser cavity at a rate κ. This gives a width $\mathcal{O}(\kappa)$ which can be interpreted in terms of time-frequency uncertainty, now for the "lifetime of a photon" in the cavity.

— spontaneous (not stimulated) emission of the active laser medium. This gives a fundamental limit to the frequency width of the laser, named after Schawlow & Townes. The broadening is of the order $\mathcal{O}(\kappa/\langle \hat{n} \rangle)$ and decreases as the laser intensity is raised. It fundamentally arises due to the discrete nature of the photons.

2.6 Quantum regression hypothesis

The approach discussed so far illustrates that correlation functions like $\langle A(t+\tau)B(t) \rangle$, in their dependence on the *time difference* τ have a dynamics that is very similar to the one-time averages that we calculated with the master equation. Indeed, for the phase diffusion, we assumed that between t and $t + \tau$, the phase (and even the full laser amplitude) evolves according to the same diffusion (or Fokker-Planck) equation as if nothing special happened at $t = 0$. The problem here is that one sometimes *interprets* the correlation function by saying "at time t, we have measured the operator A and at the later time $t + \tau$, we measure B". This is not exactly true as the operators do not coincide with their expectation values.

To elaborate this further, let us write down the meaning of the correlation function $\langle a^\dagger(t+\tau)a(t) \rangle$ (any other choice of operators would give the same physics) in the language of "system + bath" dynamics. At the time t, we identify the Heisenberg and Schrödinger picture and use the stationary density operator $\rho(t) = \rho_{\mathrm{st}}$. We need to know also the density operator $P(t) = P_{\mathrm{st}}$ for system + bath. Then, without any further approximation

$$
\begin{aligned}
\langle a^\dagger(t+\tau)a(t) \rangle &= \mathrm{tr}_{\mathrm{SB}} \left\{ \mathrm{e}^{iH\tau} a \mathrm{e}^{-iH\tau} a P_{\mathrm{st}} \right\} \\
&= \mathrm{tr}_{\mathrm{S}} \Big\{ a \underbrace{\mathrm{tr}_{\mathrm{B}} \left(\mathrm{e}^{-iH\tau} a P_{\mathrm{st}} \mathrm{e}^{iH\tau} \right)}_{=: \varrho(\tau|a\rho_{\mathrm{st}})} \Big\}
\end{aligned} \tag{2.104}
$$

Here, we identify a reduced "density matrix" of the system, $\varrho(\tau|a\rho_{\mathrm{st}})$ that is derived by the same system+bath procedure that we discussed in the first part of this Chapter: "blow up" the system density operator to a system+bath state, evolve this state under the (total) Hamiltonian and trace out the bath. The difference to the usual picture is that the initial density operator $a\rho_{\mathrm{st}}$ (for the system) or aP_{st} is not a proper one, since it is not hermitean. This difference is not really a problem if we remember that by linearity, we could extend a positive map to "skew states" as well, like $\rho = |\psi\rangle\langle\chi|$. So we get the following

Quantum regression hypothesis. If the stationary state of system + bath can be described by the factorized form $P_{\mathrm{st}} = \rho_{\mathrm{st}} \otimes \rho_{\mathrm{B}}$, then the correlation function evolves in the time difference τ according to the same master equation as the one-time average:

$$
\langle a^\dagger(t+\tau)a(t) \rangle = \mathrm{tr} \left(a^\dagger \varrho(\tau|a\rho_{\mathrm{st}}) \right) = \mathrm{tr} \left(a^\dagger \mathrm{e}^{\mathcal{L}\tau} a \rho_{\mathrm{st}} \right) \tag{2.105}
$$

$$
\frac{\mathrm{d}}{\mathrm{d}\tau} \varrho = \mathcal{L}\varrho, \qquad \varrho(0|a\rho_{\mathrm{st}}) = a\rho_{\mathrm{st}} \tag{2.106}
$$

The only difference is that one has to evolve a skew operator to find the "conditional state" $\varrho(\tau|a\rho_{\mathrm{st}})$. The "Liouville (super)operator" $\mathcal{L}$ used here contains both the commutator with the Hamiltonian and the dissipative Lindblad terms.

The word "regression" is due to Onsager who formulated a "regression hypothesis" in classical physics: "fluctuations of a system in equilibrium (correlations) show the same dynamics as deviations from equilibrium (one-time averages)". This hypothesis is sometimes called "theorem" because the assumptions beyond the validity of the master equation seem minimal. One thing to check is that the system+bath approach gives exactly the same reduced dynamics even for skew states (the bath average of the coupling vanishes in first order, for example). An exception occurs when "memory terms" play a role, but then even the Lindblad master equation does not apply: the generator $\mathcal{L}$ cannot be constant in time. So within the second-order perturbation theory and in the Markov (no memory) limit, we have good reasons to use the quantum regression "theorem". Combined with the stationarity of the correlations [see Eq.(1.39)], one thus gets the required spectra from the usual dissipative "forward-in-time" evolution.

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