

Chapter 1

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.

1.1 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:

$$T\left(\sum_k p_k \hat{\rho}_k\right) = \sum_k T(\hat{\rho}_k), \quad p_k \geq 0, \sum_k p_k = 1 \quad (1.1)$$

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

$$(T \otimes \mathbb{1})(P) = T(\rho) \otimes \rho_B \tag{1.2}$$

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.

1.2 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

$$T(\rho) = \sum_k \Omega_k \rho \Omega_k^\dagger \quad (1.3)$$

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.(1.3) 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.(1.3) defines a completely positive map. The only tricky point is the following extension to density operators P in a larger space

$$(T \otimes \mathbb{1})(P) = \sum_k (\Omega_k \otimes \mathbb{1}) P (\Omega_k^\dagger \otimes \mathbb{1}) \quad (1.4)$$

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

$$P = (T \otimes \mathbb{1})(|\phi\rangle\langle\phi|) \quad (1.5)$$

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

$$P = \sum_k |\tilde{\varphi}_k\rangle\langle\tilde{\varphi}_k|. \quad (1.6)$$

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 $|\psi^*\rangle$ with respect to a basis $\{|n\rangle\}$ of \mathcal{H} by “taking the complex conjugate of the coefficients”, i.e.:

$$|\psi^*\rangle = \sum_n |n\rangle\langle n|\psi^*\rangle, \quad \langle n|\psi^*\rangle \equiv (\langle n|\psi\rangle)^* = \langle\psi|n\rangle \quad (1.7)$$

The Kraus operators are now defined via their matrix elements as

$$\langle \chi | \Omega_k | \psi \rangle = \langle \chi \otimes \psi^* | \tilde{\varphi}_k \rangle, \quad \langle \psi | \Omega_k^\dagger | \chi \rangle = \langle \tilde{\varphi}_k | \chi \otimes \psi^* \rangle, \quad (1.8)$$

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

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

$$\begin{aligned} & \langle \chi \otimes \psi^* | P | \chi' \otimes \psi^* \rangle \\ &= \sum_k \langle \chi \otimes \psi^* | \tilde{\varphi}_k \rangle \langle \tilde{\varphi}_k | \chi' \otimes \psi^* \rangle \quad \text{from Eq.(1.6)} \\ &= \sum_k \langle \chi | \Omega_k | \psi \rangle \langle \psi | \Omega_k^\dagger | \chi' \rangle \end{aligned} \quad (1.9)$$

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

$$|\phi\rangle = \sum_n |n \otimes n\rangle \quad (1.10)$$

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

$$\begin{aligned} |\phi\rangle\langle\phi| &= \sum_{n,m} |n \otimes n\rangle\langle m \otimes m| \\ &= \sum_{n,m} (|n\rangle\langle m|) \otimes (|n\rangle\langle m|) \end{aligned} \quad (1.11)$$

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.(1.5) 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.(1.16). Taking this for granted, we get

$$P = (T \otimes \mathbb{1})(|\phi\rangle\langle\phi|) = \sum_{n,m} T(|n\rangle\langle m|) \otimes (|n\rangle\langle m|) \quad (1.12)$$

Using the definition (1.7), we find that the matrix element of Eq.(1.9) becomes

$$\begin{aligned} & \sum_{n,m} (\langle \chi | \otimes \langle \psi^* |) [T(|n\rangle\langle m|) \otimes (|n\rangle\langle m|)] (|\chi' \otimes \psi^*\rangle) \\ &= \sum_{n,m} \langle \chi | T(|n\rangle\langle m|) | \chi' \rangle \langle n | \psi \rangle \langle m | \psi \rangle^* \\ &= \langle \chi | T(|\psi\rangle\langle\psi|) | \chi' \rangle. \end{aligned} \quad (1.13)$$

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

Combining with Eq.(1.9), we have shown that

$$\langle\chi|T(|\psi\rangle\langle\psi|)|\chi'\rangle = \sum_k \langle\chi|\Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger|\chi'\rangle \quad (1.14)$$

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

$$T(|\psi\rangle\langle\psi|) = \sum_k \Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger \quad (1.15)$$

Hence, we have proven the operator identity (1.3) 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

$$\begin{aligned} T(|\psi\rangle\langle\chi|) &= \frac{1}{2} [T(\rho_{+1}) - T(\rho_{-1}) + iT(\rho_{+i}) - iT(\rho_{-i})] \quad (1.16) \\ \rho_u &:= \frac{1}{2} [(|\psi\rangle + u|\chi\rangle)(\langle\psi| + u^*\langle\chi|)], \quad |u| = 1 \end{aligned}$$

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.(1.16) 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.

1.2.1 Remarks and examples

Choi matrix. The density operator P defined in Eq.(1.12) 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 $U(x) = \exp[-iH(x)t]$:

$$\rho \mapsto \overline{U(x)\rho U^\dagger(x)} = \sum_k p_k U(x_k)\rho U^\dagger(x_k) \quad (1.17)$$

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.(1.17) is of the form of the Kraus theorem, with $\Omega_k = \sqrt{p_k}U(x_k)$.

System+bath projector. The names Nakajima and Zwanzig are attached to the following natural prescription for the reduced density operator of a system coupled to a bath. This map is 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

$$P(0) \mapsto P(t) = U_{SB}(t)P(0)U_{SB}^\dagger(t) \quad (1.18)$$

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-Zwanzig formula

$$\rho(0) \mapsto \rho(t) = \text{tr}_B \left[U_{SB}(t)\rho(0) \otimes \rho_B U_{SB}^\dagger(t) \right] \quad (1.19)$$

Exercise: show that this defines a completely positive map.

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

$$\langle n, m | \rho^\Gamma | n', m' \rangle = \langle n, m' | \rho | n', m \rangle \quad (1.20)$$

(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

$$\rho = |\psi_+\rangle\langle\psi_+| \quad \text{with} \quad |\psi_+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \quad (1.21)$$

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)

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad \rho^\Gamma = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (1.22)$$

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

Note from Eq.(1.20) 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.

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 ($k = 1 \dots K$) into a block-diagonal matrix

$$U = \begin{pmatrix} \Omega_1 & & & \\ & \Omega_2 & & \\ & & \ddots & \\ & & & \Omega_n \end{pmatrix} \quad (1.23)$$

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

$$T(\rho) = \text{tr}_{\mathcal{K}}[U(\rho \otimes K^{-1}\mathbb{1})U^\dagger] \quad (1.24)$$

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

$$\rho = \text{tr}_2 |\Psi\rangle\langle\Psi| \quad |\Psi\rangle = \sum_n \sqrt{p_n} |n \otimes n\rangle, \quad \rho = \sum_n p_n |n\rangle\langle n| \quad (1.25)$$

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.

1.3 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,

$$T_{t_1+t_2} = T_{t_1}T_{t_2} \quad (1.26)$$

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.(1.26) is a “functional equation” that is formally solved by an operator of exponential form

$$T_t = \exp(\mathcal{L}t) \quad (1.27)$$

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

1.3.1 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

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -i[H, \rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \{ \rho, L_k^\dagger L_k \} \right) \\ &= -i[H, \rho] + \frac{1}{2} \sum_k \left([L_k \rho, L_k^\dagger] + [L_k, \rho L_k^\dagger] \right) \end{aligned} \quad (1.28)$$

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

$$\frac{\rho(t + \Delta t) - \rho(t)}{\Delta t} \quad (1.29)$$

with the help of the Kraus theorem and take the limit $\Delta t \rightarrow 0$. Write $\rho = \rho(t)$ for simplicity. In the Kraus representation (1.3) for the density matrix $\rho(t + \Delta t)$,

$$\rho(t + \Delta t) = \sum_k \Omega_k \rho \Omega_k^\dagger \quad (1.30)$$

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

$$\Omega_k = \omega_k \mathbb{1} + V_k \quad (1.31)$$

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:

$$(A|B) = \text{tr}(A^\dagger B) \quad (1.32)$$

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

$$0 = (\mathbb{1}|V_k) = \text{tr}(\mathbb{1}V_k) = \text{tr} V_k \quad (1.33)$$

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

$$\begin{aligned} & \rho(t + \Delta t) - \rho \quad (1.34) \\ &= \left(\sum_k |\omega_k|^2 - 1 \right) \rho + \sum_k \left(\omega_k^* V_k \rho + \rho \omega_k V_k^\dagger \right) + \sum_k V_k^\dagger \rho V_k \end{aligned}$$

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

$$\lim_{\Delta t \rightarrow 0} \left[\hat{A} \rho(t + \Delta t) - \hat{A} \rho(t) \right] = \mathcal{O}(\Delta t) \quad (1.35)$$

for all operators \hat{A} and initial density matrices $\rho(t)$. This permits us to extract all matrix elements in Eq.(1.34) and to conclude that the following terms must vanish separately

$$\lim_{\Delta t \rightarrow 0} \sum_k |\omega_k|^2 = 1 \quad (1.36)$$

$$\lim_{\Delta t \rightarrow 0} \sum_k \omega_k^* \rho V_k = 0 \quad (1.37)$$

$$\lim_{\Delta t \rightarrow 0} \sum_k V_k \rho V_k^\dagger = 0 \quad (1.38)$$

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

$$\gamma \equiv \lim_{\Delta t \rightarrow 0} \frac{\sum_k |\omega_k|^2 - 1}{\Delta t} \quad (1.39)$$

$$\Gamma - iH \equiv \lim_{\Delta t \rightarrow 0} \frac{\sum_k \omega_k^* V_k}{\Delta t} \quad (1.40)$$

where Γ and H are both hermitean.

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

$$\begin{aligned} 0 &= \lim_{\Delta t \rightarrow 0} \frac{\text{tr}[\rho(t + \Delta t) - \rho]}{\Delta t} \\ &= \text{tr}[\gamma \rho + 2\Gamma \rho + \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \sum_k V_k^\dagger V_k \rho] \end{aligned} \quad (1.41)$$

Since this must hold for any density matrix ρ , we find another derivative (this argument uses that the scalar product (1.32) is non-degenerate)

$$\lim_{\Delta t \rightarrow 0} \frac{\sum_k V_k^\dagger V_k}{\Delta t} = -\gamma - 2\Gamma \quad (1.42)$$

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

$$L_k \equiv \lim_{\Delta t \rightarrow 0} \frac{V_k}{\sqrt{\Delta t}} \quad (1.43)$$

where we used that the root of $\Delta t \geq 0$ can be taken. Using the derivatives defined in Eqs.(1.39, 1.40, 1.43), we can divide the difference $\rho(t + \Delta t) - \rho(t)$ in Eq.(1.34) by Δt , and take the limit $\Delta t \rightarrow 0$. This gives the differential equation (1.28).

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.(1.31) makes sense.

1.3.2 Examples

Spontaneous emission

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

$$L = \sqrt{\gamma} \sigma \quad (1.44)$$

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.1.5.1.

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 (1.28), multiplied with a system operator A , we find

$$\frac{\partial}{\partial t} \langle A \rangle = i \langle [H, A] \rangle + \frac{1}{2} \sum_k \langle L_k^\dagger [A, L_k] + [L_k^\dagger, A] L_k \rangle \quad (1.45)$$

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 σ^\dagger (at the rate γ , Eq.(1.150)) and to the damping of the inversion σ_3 , Eq.(1.149), 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:

$$L_{\text{loss}} = \sqrt{\kappa(\bar{n} + 1)} a, \quad L_{\text{abs}} = \sqrt{\kappa\bar{n}} a^\dagger \quad (1.46)$$

where κ is a loss rate (the inverse of the “photon lifetime”) and $\bar{n} = (e^{\hbar\omega_\Delta/k_B T} - 1)^{-1}$ 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.(1.44).

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

$$L_{\text{deph}} = \sqrt{\kappa} \sigma_3 \quad (1.47)$$

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

$$\rho(t) = \begin{pmatrix} \rho_{\text{ee}}(0) & e^{-\kappa t} \rho_{\text{eg}}(0) \\ e^{-\kappa t} \rho_{\text{ge}}(0) & \rho_{\text{gg}}(0) \end{pmatrix} \quad (1.48)$$

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

$$|\psi(t)\rangle = \alpha e^{i\varphi(t)} |e\rangle + \beta e^{-i\varphi(t)} |g\rangle \quad (1.49)$$

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):

$$\rho(t) = \overline{|\psi(t)\rangle\langle\psi(t)|} \quad (1.50)$$

With the identification

$$\overline{e^{i\varphi(t)}} = e^{-\kappa t} \quad (1.51)$$

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”.

1.4 Exactly solvable open systems

Material not covered in SS 2012.

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.

1.4.1 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

$$H_{\text{int}} = \sigma_3 \sum_k (g_k b_k^\dagger + g_k^* b_k) \quad (1.52)$$

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

$$S(\omega) = 2\pi \sum_k |g_k|^2 \delta(\omega - \omega_k) \quad (1.53)$$

From the master equation (1.45) 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

$$\rho_{\text{eg}}(t) = e^{-\Gamma(t)} \rho_{\text{eg}}(0) \quad (1.54)$$

where the “decoherence factor” is given by

$$\Gamma(t) = \frac{1}{2} \sum_k |\xi_k(t)|^2 \coth(\beta\omega_k/2) \quad (1.55)$$

$$= 2 \int_0^\infty \frac{d\omega}{2\pi} S(\omega) \frac{|1 - e^{i\omega t}|^2}{\omega^2} \coth(\beta\omega/2) \quad (1.56)$$

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

$$\xi_k(t) = 2g_k \frac{1 - e^{i\omega_k t}}{\omega_k} \quad (1.57)$$

A proof of this result is sketched in Sec.1.4.1 below.

Discussion

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

$$t \rightarrow 0 : \quad \Gamma(t) \approx 2t^2 \sum_k |g_k|^2 \coth(\beta\omega_k/2) = 2t^2 \int_0^\infty \frac{d\omega}{2\pi} S(\omega) \coth(\beta\omega/2) \quad (1.58)$$

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.(1.58) 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

$$t \rightarrow \infty : \quad \left| \frac{1 - e^{i\omega_k t}}{\omega_k} \right|^2 \rightarrow 2\pi t \delta^{(1/t)}(\omega_k) \quad (1.60)$$

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

$$\tau_c \ll t \ll \beta : \quad \Gamma(t) \approx 2S(0)t \quad (1.61)$$

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 $\lim_{\omega \rightarrow 0} S(\omega) \coth(\beta\omega/2)$. 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 :

$$\begin{aligned} t \rightarrow \infty : \quad \Gamma(t) &\approx 4\pi t \int_0^\infty \frac{d\omega}{2\pi} S(\omega) \delta^{(1/t)}(\omega) \coth(\beta\omega/2) \\ &\approx 4\pi t \int_0^\infty \frac{d\omega}{2\pi} \alpha\omega \delta^{(1/t)}(\omega) \frac{2}{\beta\omega} = 4\alpha t/\beta \end{aligned} \quad (1.62)$$

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

¹This is based on the integral

$$\int_{-\infty}^{\infty} dx \frac{\sin^2(x/2)}{x^2} = \frac{\pi}{2}. \quad (1.59)$$

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:

$$H|g\rangle = |g\rangle H_g, \quad H_g = -\frac{\hbar\omega_A}{2} + H_B - \sum_k \hbar(g_k b_k^\dagger + g_k^* b_k) \quad (1.63)$$

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 $U(t)$:

$$\langle\sigma\rangle_t = \text{tr}_{\text{SB}}[U^\dagger(t)|g\rangle\langle e|U(t)\rho(0) \otimes \rho_T(B)] \quad (1.64)$$

$$= \text{tr}_{\text{SB}}[|g\rangle\langle e|\rho(0) \otimes U_g^\dagger(t)U_e(t)\rho_T(B)] \quad (1.65)$$

$$= \langle\sigma\rangle_0 \text{tr}_B[U_g^\dagger(t)U_e(t)\rho_T(B)] \quad (1.66)$$

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)

$$U_g^\dagger(t) = \exp[it(\omega b^\dagger b - gb - gb^\dagger)] = \exp[i\omega t(b^\dagger - \gamma)(b - \gamma)] e^{-itg^2/\omega} \quad (1.67)$$

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

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

$$D^\dagger(\gamma)f(b, b^\dagger)D(\gamma) = f(b + \gamma, b^\dagger + \gamma^*) \quad (1.68)$$

We can therefore write

$$\begin{aligned} & U_g^\dagger(t)U_e(t)\rho_T(B) \\ &= D^\dagger(-\gamma) \exp(i\omega t b^\dagger b) D(-\gamma) D^\dagger(\gamma) \exp(-i\omega t b^\dagger b) D(\gamma) \end{aligned} \quad (1.69)$$

$$= D^\dagger(-\gamma) \exp(i\omega t b^\dagger b) D(-2\gamma) \exp(-i\omega t b^\dagger b) D(\gamma) \quad (1.70)$$

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.(1.68)

$$U_0^\dagger(t)f(b, b^\dagger)U_0(t) = f(b e^{-i\omega t}, b^\dagger e^{i\omega t}) \quad (1.71)$$

where $U_0(t) = \exp(-i\omega t b^\dagger b)$ 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.(1.70), we have

$$\exp(i\omega t b^\dagger b) D(-2\gamma) \exp(-i\omega t b^\dagger b) = D(-2\gamma e^{i\omega t}) =: D(-2\gamma(t)) \quad (1.72)$$

We end up with a product of three displacement operators

$$D(\gamma) D(-2\gamma(t)) D(\gamma) = e^{-2i \operatorname{Im} \gamma^* \gamma(t)} D(\gamma - 2\gamma(t)) D(\gamma) \quad (1.73)$$

$$= e^{-2i \operatorname{Im} \gamma^* \gamma(t)} e^{-2i \operatorname{Im} \gamma^*(t) \gamma} D(\xi(t)) \quad (1.74)$$

$$\xi(t) = 2g \frac{1 - e^{i\omega t}}{\omega} \quad (1.75)$$

where the projective phases cancel and we recover the parameter $\xi_k(t)$ of Eq.(1.57).

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

$$\langle D(\xi_t) \rangle_B = \operatorname{tr} [D(\xi_t) \rho_T] \quad (1.76)$$

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

$$\rho_T = \int d^2\alpha |\alpha\rangle \langle \alpha| P_T(\alpha), \quad P_T(\alpha) = \frac{e^{-|\alpha|^2/\bar{n}}}{\pi \bar{n}} \quad (1.77)$$

and to calculate

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

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

$$\langle D(\xi_t) \rangle_B = e^{-|\xi_t|^2/2} e^{-|\xi_t|^2 \bar{n}} = \exp\left(-\frac{1}{2} |\xi_t|^2 \coth \beta\omega/2\right) \quad (1.78)$$

Going back to $\langle \sigma \rangle_t$, we restore the factor $e^{-i\omega_A t}$ that we forgot in Eqs.(1.67) and take the product over all modes. This gives a sum in the exponent and hence

$$\langle \sigma \rangle_t = e^{-\Gamma(t)} \langle \sigma \rangle_0 \quad (1.79)$$

$$\Gamma(t) = \sum_k \frac{1}{2} |\xi_k(t)|^2 \coth(\beta\omega_k/2) \quad (1.80)$$

which is Eq.(1.81).

Long-time limit

We evaluate here in more detail the decoherence factor $e^{-\Gamma(t)}$ 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 :

$$\Gamma(t) = 8\alpha \int_0^\infty d\omega \frac{\omega\omega_c^2}{\omega^2 + \omega_c^2} \coth \frac{\omega}{2T} \frac{\sin^2(\omega t/2)}{\omega^2} \quad (1.81)$$

Observe that the integrand is even in ω , extend the integration from $-\infty$ to ∞ and write $\sin^2(\omega t/2) = \text{Re} \frac{1}{2}(1 - e^{i\omega t})$. 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 $\omega = i\xi_n = 2\pi nT$, the so-called Matsubara frequencies. Since

$$\coth \frac{\omega}{2T} = 2T \frac{d}{d\omega} \log \sinh \frac{\omega}{2T} \quad (1.82)$$

these poles arise from the zeros of $\sinh \frac{\omega}{2T}$ and have a residue $2T$. There is also a simple pole at $\omega = i\omega_c$, 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:

$$4\alpha T \text{Re} \pi i \frac{d}{d\omega} \frac{\omega_c^2}{\omega^2 + \omega_c^2} (1 - e^{i\omega t}) = 4\alpha T \text{Re} \pi i (-it) = 4\pi\alpha T t \quad (1.83)$$

This coincides with the term linear in t that we found with the approximation $\delta^{(t)}(\omega)$ to the \sin^2 function, Eq.(1.62). The contributions from the other poles give the sum

$$\Gamma(t) = \gamma t + 4\alpha \text{Re} 2\pi i \left(\sum_{n=1}^{\infty} \frac{\omega_c^2}{\omega_c^2 - \xi_n^2} \frac{T(1 - e^{-\xi_n t})}{i\xi_n} + \frac{\omega_c^2}{2i\omega_c} \coth \frac{i\omega_c}{2T} \frac{1 - e^{-\omega_c t}}{i\omega_c} \right) \quad (1.84)$$

For $t \gg \tau_c$, we can set $e^{-\omega_c t} = 0$. If we further assume $\xi_1 t = 2\pi T t \gg 1$, 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 $N_c = \omega_c/2\pi T$,

$$K = 4\alpha \left(-\cot \pi N_c + \sum_{n=1}^{\infty} \frac{N_c^2}{n(N_c^2 - n^2)} \right) \quad (1.85)$$

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 $N_c \rightarrow \infty$ 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 $n = 1 \dots \lfloor N_c \rfloor$ and $n = \lceil N_c \rceil \dots \infty$ and approximate the cutoff function of the mode density by simple limiting forms:

$$K \approx 4\alpha \left(\sum_{n=1}^{\lfloor N_c \rfloor} \frac{1}{n} - N_c^2 \sum_{n=\lceil N_c \rceil}^{\infty} \frac{1}{n^3} \right) \quad (1.86)$$

Replacing the summations by integrations, we get

$$K \approx 4\alpha \left(\log N_c - N_c^2 \frac{-3}{N_c^2} \right) = 4\alpha \left(\log \frac{\omega_c}{2\pi T} + 3 \right) \quad (1.87)$$

up to corrections of order unity in the parenthesis.

1.4.2 Spontaneous decay

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

$$H_{\text{int}} = \sum_k \left(g_k \sigma^\dagger a_k + g_k^* a_k^\dagger \sigma \right) \quad (1.88)$$

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:

$$|\Psi(t)\rangle = c_e(t)|e, \text{vac}\rangle + \sum_k c_k(t)|g, 1_k\rangle \quad (1.89)$$

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.1.1 where the decay happens only partially when the atomic frequency is in a spectral

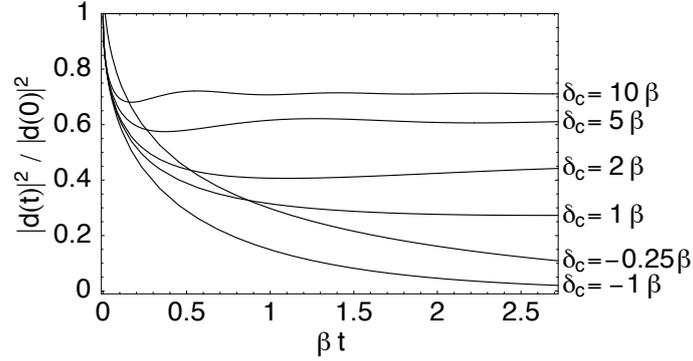


Figure 1.1: Decay of an excited atom for a spectral strength that sharply grows above a cutoff frequency: $S(\omega) \sim \beta^{1/2}(\omega - \omega_c)^{1/2}$ for $\omega \geq \omega_c$. The detuning $\delta_c = \omega_c - \omega_A$ from the lower cutoff is given on the right. The ratio $|d(t)|^2/|d(0)|^2$ gives the probability $|c_e(t)|^2$. Taken from Boedeker & 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.1.1.

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.

1.5 System+bath models

Introduction

The concept of a system in a bath is a typical setting in quantum optics, but applies also to other areas of physics (condensed matter, statistical physics). The main idea is that we want to make a simple model where a system (Hamiltonian H_S) is in contact with an “environment” whose detailed behaviour is not accessible. By definition, we cannot make measurements on the “bath”. It is therefore characterized by only a few parameters.

A simple case is the one of a “bosonic bath” where the total Hamiltonian takes the form

$$H = H_S + H_B + V \quad (1.90)$$

where the bath is described by a collection of bosons, i.e., harmonic oscillators

$$H_B = \sum_k \hbar\omega_k a_k^\dagger a_k = \sum_k \left(\frac{p_k^2}{2m_k} + \frac{m_k}{2} \omega_k^2 q_k^2 \right) + \text{const.} \quad (1.91)$$

with annihilation and creation operators a_k, a_k^\dagger or conjugate “position” and “momentum” coordinates q_k, p_k . The system-bath interaction V is a product of system and bath observables and can be written in the form

$$V = S^\dagger B + \text{h.c.} \quad (1.92)$$

Sometimes a coupling constant is introduced here, this can be useful to count orders in perturbation theory. For the moment, we have incorporated the coupling constant in the definition of the bath observable B . Example of a system “atom” coupled to the bath “electromagnetic field”: S is the electric dipole operator and B the electric field operator. The observables S and B could also be hermitean. In quantum optics, one frequently uses a non-hermitean operator B , expanded as a sum of single-mode operators a_k . (See exercise 1.2 for details.)

Bath spectral density

Since not much information is available about the bath, it is characterized in a simple way, using a few numbers. Its temperature, some characteristic

rate of energy exchange with the system (e.g., the rate of spontaneous emission, or a friction coefficient), some characteristic frequency for its spectral features. The bath is described by a continuous distribution of frequencies, i.e., eventually one goes from a summation over k into a frequency integral. This is encoded in the bath spectral density defined by (the factor 2π is a convention not used by everybody)

$$J(\omega) = 2\pi \sum_k |g_k|^2 \delta(\omega - \omega_k) \quad (1.93)$$

$$(1.94)$$

$$B = \hbar \sum_k g_k a_k \quad (1.95)$$

which is meaning when the bath operator B is given. Roughly speaking, $J(\omega)$ encodes how many bath degrees of freedom have a frequency near ω , weighted with the coupling strength (parameter g_k) to the system.

In the exercises, you learn more about the physical meaning of $J(\omega)$ and the role of temperature.

Reduced density operator

The information about the system is encoded in its so-called *reduced density operator* ρ . This is defined by

$$\rho = \begin{cases} \text{tr}_B |\Psi_{SB}\rangle \langle \Psi_{SB}| \\ \text{tr}_B \rho_{SB} \end{cases} \quad (1.96)$$

where the definition depends on how the total system is described. If its wave function (quantum state) $|\Psi_{SB}\rangle$ is known, the first line applies. If its density operator ρ_{SB} is given, the second line. The operation “ tr_B ” means “take the partial trace over the bath variables” or “trace out the bath”. It is defined in Eq.(1.99) below. In both cases, the system itself is *not* described by a pure state (a wave function), but a mixed one, and we have to use a density operator.

Definition of the partial trace

Take a basis $\{|n\rangle, n = \dots\}$ for the system Hilbert space and a basis $\{|b\rangle, b = \dots\}$ for the bath Hilbert space. (At least the second basis is likely

to be infinite-dimensional.) Calculate the elements of the density matrix by summing over the bath states

$$\rho_{mn} = \sum_b \langle m, b | \rho_{SB} | n, b \rangle \quad (1.97)$$

where the same bath state appears on both sides. This is why one speaks of a “partial trace”. Then construct the density operator, acting on the Hilbert space of the system

$$\rho = \sum_{mn} |m\rangle \langle n| \rho_{mn} \quad (1.98)$$

The operation “partial trace” or “tracing out the bath” is therefore given by the map

$$P \mapsto \rho = \text{tr}_B P = \sum_{mn,b} |m\rangle \langle m, b| P |n, b\rangle \langle n| \quad (1.99)$$

System observables

An important statement is the following: *The reduced density operator encodes the expectation values for all system observables.* This is the “luxury” one typically has in quantum optics: all system observables can potentially be measured and have to be dealt with in the theory. In other fields of physics, one is happy with a reduced set of “relevant observables” (current and charge distribution, etc). In this context, it is often not necessary to calculate the full (system) density operator, a smaller set of “observables of interest” is sufficient.

The usual rule for expectation values

$$\langle S \rangle = \text{tr}(S\rho) = \text{tr}(\rho S) \quad (1.100)$$

where the trace is now over the system Hilbert space. This rule generalizes the expectation value for a pure state (full knowledge about the wave function) where $\langle S \rangle = \langle \psi | S | \psi \rangle$. Under the trace, one can permute cyclically, since the trace of ρ exists (“ ρ is trace class”).

Now, be S any system observable. According to orthodox quantum mechanics, it is a linear operator acting on the system’s Hilbert space. Hence, we can write for the action on the basis state $|n\rangle$:

$$S|n\rangle = \sum_m |m\rangle S_{mn}, \quad S_{mn} = \langle m | S | n \rangle \quad (1.101)$$

(Note the position of the indices.) There is thus a one-to-one correspondence, in a given basis, between the matrix (S_{mn}) and the operator S . The expectation value becomes, using (1.98) and (1.101):

$$\begin{aligned}
\langle S \rangle &= \text{tr} \sum_{mn} (S|n\rangle\langle m|\rho_{nm}) \\
&= \text{tr} \sum_{mm'n} (|m'\rangle S_{m'n}\langle m|\rho_{nm}) \\
&= \sum_{kn} S_{kn}\rho_{nk}
\end{aligned} \tag{1.102}$$

which is just the trace of the matrix product between the matrix representing S and the density matrix ρ . We have simply checked that the basis-free definition (1.100) is consistent with the rules for matrix algebra.

So, how does “any” system operator look like? It is given by any matrix S_{mn} that is compatible with a few basic requirements. Sometimes one restricts to self-adjoint operators S , hence hermitean matrices (S_{mn}) , but this can be relaxed. We could also choose a matrix S_{mn} that has a single element one somewhere (at the indices mn , say) the others being zero. Then the corresponding expectation value gives simply the matrix element ρ_{nm} – the *elements of the density matrix are observable*.

Programme for open quantum systems

We can formulate a few basic questions:

- the stationary state of the system ρ_{ss} , given the coupling to the bath at temperature T and some “control fields” (like a laser that illuminates an atom)
- the state of thermal equilibrium ρ_{eq} , given the coupling to the bath at temperature T
- the dynamics (time evolution) $\rho(t)$ of the system

To the second question, a formal answer can be given (P. Hänggi, Augsburg):

$$\rho_{eq}(T) = \text{tr}_B \left(\frac{1}{Z_{SB}} e^{-\beta \hat{H}} \right) \neq \frac{1}{Z_S} e^{-\beta \hat{H}_S} \tag{1.103}$$

where the partial trace of the canonical equilibrium density operator for the total system is taken. Note that the two expressions differ because the system-bath coupling V enters the Hamiltonian H in the first one, while only the system Hamiltonian H_S appears in the second one. The two coincide only for a sufficiently weak system-bath coupling. You analyze in Problem ?? a simple toy model where Eq.(1.103) can be worked out for a classical system.

In general, the stationary density operator ρ_{ss} is equal to the equilibrium one only if the control fields are sufficiently weak. This means that we have to develop tools to handle *non-equilibrium systems*.

The answer to the third question, the time evolution of the density operator, is given by different methods (and approximations)

- master equations
- quantum Langevin equations
- path integrals with influence functionals
- quantum Monte Carlo techniques

a number of which are going to discuss in this lecture.

1.5.1 Derivation of the quantum optical master equation

Material not covered in SS 2012.

Motivation

Experimentally observed: excited states decay at some rate γ to the ground state.

Evolution of population: *rate equation*

$$\begin{aligned}\dot{p}_e &= -\gamma p_e \\ \dot{p}_g &= \gamma p_e\end{aligned}\tag{1.104}$$

Total population conserved. Stationary state: $p_e = 0$.

Problem: not possible to obtain with a Hamiltonian. Standard interaction $V = \frac{1}{2}\hbar\Omega(|g\rangle\langle e| + |e\rangle\langle g|)$ couples population $p_e = \langle e|\rho|e\rangle = \rho_{ee}$ to an off-diagonal matrix element (a “coherence”)

$$\dot{p}_e = -\frac{i}{\hbar}\langle e|[V, \rho]|e\rangle = i\frac{\Omega}{2}(\langle e|\rho|g\rangle - \langle g|\rho|e\rangle) = \Omega \operatorname{Im}\langle g|\rho|e\rangle$$

Challenge: find quantum description for decay processes and combine with coherent dynamics (like Rabi oscillations).

Idea: density matrix ρ for atom+field system. Take the trace over the field and get the *reduced density matrix* ρ_A for the atom:

$$\rho_A = \text{tr}_F \rho.$$

Use second order perturbation theory (“weak interaction”) combined with a separation of “slow” and “fast” timescales: “fast” = fluctuations of the field (short correlation time τ_c); “slow” = dissipative dynamics (decay) of the atom. Recall that $\tau_c \approx \hbar/k_B T \approx 10^{-12}$ s for a thermal field (“fast”) and $1/\gamma \approx 10^{-9}$ s (“slow”) for typical lifetimes. And also $1/\omega_A \approx 10^{-14}$ s for a typical optical period (“very fast”). The resulting equation is “better” than simple time-dependent perturbation theory — it allows to describe the atomic dynamics on long timescales, even longer than a decay time.

The calculation we present is due to Wigner and Weis(s?)kopf. Our presentation is inspired by the chapter IV.B of the book “Atom-photon interactions” by Cohen-Tannoudji, Dupont-Roc, and Grynberg.

Density matrix, interaction picture

Schrödinger equation for the atom+field density matrix

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [H, \rho]$$

with the Hamiltonian

$$H = H_A + H_F + H_{\text{int}}$$

Atom plus laser mode: describe both by H_A .

Interaction picture: unitary transformation

$$\rho(t) = e^{-i(H_A+H_F)t/\hbar} \tilde{\rho}(t) e^{i(H_A+H_F)t/\hbar}$$

gives Schrödinger equation

$$\frac{d\tilde{\rho}}{dt} = \frac{1}{i\hbar} [H_{\text{int}}(t), \tilde{\rho}] \quad (1.105)$$

where the time-dependence of the interaction is that of the free evolution

$$H_{\text{int}}(t) = e^{i(H_A+H_F)t/\hbar} H_{\text{int}} e^{-i(H_A+H_F)t/\hbar},$$

as we saw before. In the following, we drop the tilde to simplify the writing.

Formal solution to (1.105):

$$\rho(t + \Delta t) = \rho(t) + \frac{1}{i\hbar} \int_t^{t+\Delta t} dt_1 [H_{\text{int}}(t_1), \rho(t_1)]$$

Iteration to second order:

$$\begin{aligned} \rho(t + \Delta t) = & \rho(t) + \frac{1}{i\hbar} \int_t^{t+\Delta t} dt_1 [H_{\text{int}}(t_1), \rho(t)] \\ & - \frac{1}{\hbar^2} \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 [H_{\text{int}}(t_1), [H_{\text{int}}(t_2), \rho(t_2)]] \end{aligned} \quad (1.106)$$

Reduced atom dynamics

Now take the trace over the field to find $\rho_A(t + \Delta t)$. Specify the initial conditions and the interaction.

- Initial conditions: atom+field state factorizes

$$\rho(t) = \rho_A(t) \otimes \rho_F \quad (1.107)$$

Take arbitrary state $\rho_A(t)$ for the atom and a thermal state for the field. Idea: field is a “big” system and its state changes a little when coupled to the atom.

- Interaction: as usual, electric dipole interaction

$$H_{\text{int}}(t) = -\mathbf{d}(t) \cdot \mathbf{E}(t)$$

The time-dependence is that of the free evolution.

Immediate consequence: the trace over the field of the first order term in (1.106) vanishes:

$$\text{tr}_F (H_{\text{int}}(t)\rho(t)) = -\rho_A \mathbf{d}(t) \cdot \text{tr}(\mathbf{E}(t)\rho_F) = 0$$

because the average electric field vanishes in a thermal state.

Hence, the dynamics will be given by the second order term. Note that the unknown density matrix $\rho(t_2)$ appears under the integral in (1.106). In the spirit of perturbation theory, we replace it by the initial $\rho(t)$. If we took into account corrections, they would be due to the interaction, and the double integral is already of second order in H_{int} . This approximation makes the evolution of the reduced density matrix only dependent on its value at time t , it is called the “Markov approximation” and one says that the field has an “infinitely short memory time”.

We note that the assumption (1.107), that at time t , the atom+field density matrix factorizes, cannot be true at all times. The atom-field interaction creates correlations, and these are precisely responsible for getting a nonzero result at second order. Thus, we can only approximate the full density matrix by a factorized one. The idea is that the atom-field correlations decay on the fast timescale given by the field correlation time τ_c , and that after a time step Δt , they have died out. The Markov approximation precisely assumes that this decay happens quasi-instantaneously. Note also that when we work at zero temperature, we assume that the photons the atom possibly emits “disappear” in the field reservoir (since its state remains the vacuum state). This means that the master equation cannot describe the re-absorption of spontaneously emitted radiation, as it may happen in front of a mirror or in a cavity. For this, either one must use the correct mode functions for the geometry (the van der Waals shift then appears as a second-order level shift), or one must single out the cavity mode from the field and combine it with the atom into the “system” Hamiltonian.

Field correlations

Now we have to deal with the average of two electric field operators (a first-order coherence function). For example, the first term of the double commutator involves

$$1 : \quad \text{tr}_F (E_i(t_1)E_j(t_2)\rho_F) =: C_{ij}(\tau)$$

This coherence function only depends on the time difference $\tau = t_1 - t_2$ because the field is in a stationary (in particular, thermal) state and its density matrix commutes with the field Hamiltonian. *Proof:* Under the trace, we permute cyclically and find

$$\begin{aligned} & \text{tr}_F \left(e^{iH_F t_1/\hbar} E_i e^{iH_F(t_2-t_1)/\hbar} E_j e^{-iH_F t_2/\hbar} \rho_F \right) \\ &= \text{tr}_F \left(e^{iH_F(t_1-t_2)/\hbar} E_i e^{iH_F(t_2-t_1)/\hbar} E_j \rho_F \right). \end{aligned}$$

This is a general property of the coherence function of stationary states. A field in a stationary state is thus “stationary” in the sense mentioned in the exercises (sounds consistent): its coherence function only depends on time differences. (Note, however, that we deal here with the full field operators and not a normally ordered coherence function.)

In the second term in the double commutator, the fields $\mathbf{E}(t_1)$ and $\mathbf{E}(t_2)$ appear in reverse order, leading to the coherence function $C_{ji}(t_2 - t_1) = C_{ji}(-\tau)$.

The coherence function $C_{ij}(\tau)$ of the electromagnetic field is related to the blackbody spectrum, as discussed in the exercises. In particular, in free space, it

is proportional to the Kronecker δ_{ij} , and we can write $C_{ij}(\tau) = \delta_{ij}C(\tau)$. We also note that $C(-\tau) = [C(\tau)]^*$.

The four terms in the expansion of the double commutator thus give (the numbers on the left hand side simply enumerate these terms)

$$\begin{aligned} 1 : & \quad \mathbf{d}(t_1) \cdot \mathbf{d}(t_2) \rho_A C(\tau) \\ 2 : & \quad -d_i(t_1) \rho_A d_i(t_2) C(-\tau) \\ 3 : & \quad -d_i(t_2) \rho_A d_i(t_1) C(\tau) \\ 4 : & \quad \rho_A \mathbf{d}(t_2) \cdot \mathbf{d}(t_1) C(-\tau) \end{aligned}$$

Summation over the index i is understood. The terms 1, 4 are hermitean conjugates of each other. Same for the pair 2, 3.

Dipole operator

To proceed, we specify the time-dependence of the dipole operator

$$\mathbf{d}(t) = \mathbf{d}\sigma_+(t) + \mathbf{d}^*\sigma_-(t) = \mathbf{d}\sigma_+e^{i\omega_A t} + \mathbf{d}^*\sigma_-e^{-i\omega_A t}$$

where $\mathbf{d} = \langle e|\hat{\mathbf{d}}|g\rangle$ is the (complex) vector of matrix elements for the dipole operator. Noting that $\sigma_+^2 = \sigma_-^2 = 0$, we find for the product of dipole operators

$$\mathbf{d}(t_1) \cdot \mathbf{d}(t_2) = |\mathbf{d}|^2 \sigma_+\sigma_-e^{i\omega_A \tau} + |\mathbf{d}|^2 \sigma_-\sigma_+e^{-i\omega_A \tau}$$

The term 1 is thus equal to

$$1 : \quad C(\tau) |\mathbf{d}|^2 \left(\sigma_+\sigma_-e^{i\omega_A \tau} + \sigma_-\sigma_+e^{-i\omega_A \tau} \right) \rho_A \quad (1.108)$$

Note that it only depends on the time difference τ .

Short and long timescales

This suggests that the other time integral can be done, giving Δt . More precisely, using the new variables t_1 and τ , we can write

$$\int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 = \int_t^{t+\Delta t} dt_1 \int_0^{t_1-t} d\tau = \int_0^{\Delta t} d\tau \int_{t+\tau}^{t+\Delta t} dt_1$$

In the t_1, t_2 -plane, the integration domain is a triangle below the diagonal. In the last step, we have parametrized this triangle by lines of fixed τ , i.e. parallel to the diagonal, starting at $t_1 = t + \tau$ and ending at $t_1 = t + \Delta t$, as shown in figure 1.2.

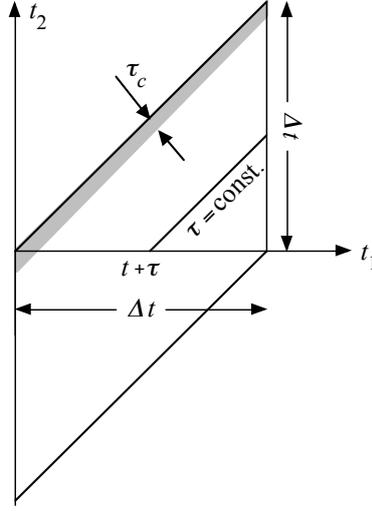


Figure 1.2: Domain of integration in the t_1, t_2 -plane. Due to the short coherence time τ_c of the field, only the gray area just below the diagonal does contribute to the integral.

We now take advantage of the short correlation time of the field: as a function of τ , the coherence function $C(\tau)$ decreases on a scale given by the coherence time τ_c . Since we are interested in the “slow” dynamics of the atom, the time interval Δt can be chosen large compared to τ_c . In this limit, we can also replace the integration domain by the parallelogram shown in fig. 1.2. This means that the integration limits for the t_1 integral change to

$$\int_0^{\Delta t} d\tau \int_{t+\tau}^{t+\Delta t} dt_1 \approx \int_0^{\Delta t} d\tau \int_t^{t+\Delta t} dt_1.$$

Since the term 1 (1.108) does not depend on t_1 , the integral over t_1 yields Δt . Term 4 (its hermitean conjugate) behaves in the same way. Such a simplification does not hold for the terms 2 and 3. Here, we have to invoke a different argument. Spelling out the dependence on τ and t_1 , we have

$$2 : \quad -C(\tau) \left(d_i \sigma_+ e^{i\omega_A(t_1 - \tau)} + d_i^* \sigma_- e^{-i\omega_A(t_1 - \tau)} \right) \\ \times \rho_A \left(d_i \sigma_+ e^{i\omega_A t_1} + d_i^* \sigma_- e^{-i\omega_A t_1} \right)$$

The product gives either terms independent of t_1 or involving $e^{\pm 2i\omega_A t_1}$. If $\omega_A \Delta t \gg 1$, these oscillating terms average out when integrating over t_1 . Note that if the optical period is shorter than the correlation time τ_c of the field, this approximation is even less severe than the condition $\Delta t \gg \tau_c$ we already used. It is thus consistent

to make this “secular approximation” as it is called; note its similarities to the rotating wave approximation.

Doing so, the term 2 reduces to something independent of t_1 and proportional to the squared dipole matrix element:

$$2 : \quad -C(\tau)|\mathbf{d}|^2 \left(e^{i\omega_A\tau} \sigma_- \rho_A \sigma_+ + e^{-i\omega_A\tau} \sigma_+ \rho_A \sigma_- \right). \quad (1.109)$$

The t_1 integral again gives Δt .

Field spectrum

We now have to treat the integral over τ that is still left. It contains the following two integrals

$$\int_0^{\Delta t} d\tau C(\tau) e^{\pm i\omega_A\tau}.$$

(The terms with $C(-\tau)$ can be expressed in terms of the complex conjugate.) Since we work on “long timescales” $\Delta t \gg \tau_c$, the correlation function is already zero at the upper limit, and we can replace this limit by $+\infty$ without much error. We thus get a “one-sided” Fourier integral. We write the correlation function in terms of its (normal) Fourier expansion,

$$C(\tau) = \int \frac{d\omega}{2\pi} S(\omega) e^{-i\omega\tau}$$

where $S(\omega)$ is essentially the blackbody spectrum. The relation $C(-\tau) = [C(\tau)]^*$ entails that $S(\omega)$ is real. With the following formula for the τ integral

$$\int_0^{\infty} d\tau e^{i(\omega_A - \omega)\tau} = \pi\delta(\omega_A - \omega) - i\mathcal{P} \frac{1}{\omega - \omega_A}$$

(\mathcal{P} means the principal value), we find

$$\Delta t \gg \tau_c : \quad \int_0^{\Delta t} d\tau C(\tau) e^{\pm i\omega_A\tau} = \frac{1}{2} S(\pm\omega_A) - i\mathcal{P} \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega \mp \omega_A}. \quad (1.110)$$

To simplify the notation, we shall write the second term as $-iR(\pm\omega_A)$.

The first and second terms are thus given by

$$1 : \quad \frac{1}{2} |\mathbf{d}|^2 (S(\omega_A) \sigma_+ \sigma_- + S(-\omega_A) \sigma_- \sigma_+) \rho_A \\ - i |\mathbf{d}|^2 (R(\omega_A) \sigma_+ \sigma_- + R(-\omega_A) \sigma_- \sigma_+) \rho_A \quad (1.111)$$

$$2 : \quad -|\mathbf{d}|^2 \left[\left(\frac{1}{2} S(\omega_A) - iR(\omega_A) \right) \sigma_- \rho_A \sigma_+ \right. \\ \left. + \left(\frac{1}{2} S(-\omega_A) - iR(-\omega_A) \right) \sigma_+ \rho_A \sigma_- \right] \quad (1.112)$$

When adding term 3 (the complex conjugate of term 2), the imaginary parts involving $R(\pm\omega_A)$ drop out because the operators $\sigma_- \rho_A \sigma_+$ and $\sigma_+ \rho_A \sigma_-$ are hermitean. But $R(\pm\omega_A)$ survives in terms 1 and 4.

The master equation

Coarse grained derivative We now collect our results. Recalling that the double integral reduces to something proportional to Δt , we can make a difference quotient appear on the left hand side. This gives the following “master equation”

$$\frac{\Delta \rho_A}{\Delta t} = \frac{1}{i\hbar} [H^{(2)}, \rho_A] + \mathcal{L}[\rho_A] \quad (1.113)$$

The terms on the right hand side are discussed in a minute. This difference quotient can be written as a derivative averaged over the “slow” timescale

$$\frac{\Delta \rho_A}{\Delta t} = \frac{1}{\Delta t} \int_t^{t+\Delta t} dt_1 \frac{d\rho_A(t_1)}{dt}$$

Such an average is sometimes called “coarse grained” (*grobkörnig*) because one is not interested in the rapid fluctuations that occur on timescales faster than Δt .

In the following, we focus on long timescales and use the notation $\Delta\rho/\Delta t \mapsto d\rho/dt$, not making the difference between the ordinary derivative and its coarse grained average.

Level shifts On the right hand side of the master equation (1.113), we have a “Hamiltonian-like” term that is given by

$$\begin{aligned} H^{(2)} &= -\frac{|\mathbf{d}|^2}{\hbar} (R(\omega_A)\sigma_+\sigma_- + R(-\omega_A)\sigma_-\sigma_+) \\ &= -\frac{|\mathbf{d}|^2}{\hbar} (R(\omega_A)|e\rangle\langle e| + R(-\omega_A)|g\rangle\langle g|) \end{aligned} \quad (1.114)$$

This Hamiltonian describes the energy shifts due to the coupling with the field. It is very similar to the Lamb shift we saw in chapter 3. Indeed, for the ground state, we get

$$\langle g|H^{(2)}|g\rangle = -\frac{|\mathbf{d}|^2}{\hbar} R(-\omega_A) = -\frac{|\mathbf{d}|^2}{\hbar} \mathcal{P} \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega + \omega_A}.$$

Let us focus on the field at zero temperature, as in chapter 3. The spectrum is then given by

$$S_{ij}(\omega) = \int d\tau e^{i\omega\tau} \langle E_i(\tau) E_j(0) \rangle$$

$$\begin{aligned}
&= \sum_{\mathbf{k}\mu} E_k^2 \varepsilon_{\mathbf{k}\mu}^i \varepsilon_{\mathbf{k}\mu}^{j*} \underbrace{\langle a_{\mathbf{k}\mu} a_{\mathbf{k}\mu}^\dagger \rangle}_{=1} \int d\tau e^{i(\omega - \omega_k)\tau} \\
&= 2\pi \sum_{\mathbf{k}\mu} \delta(\omega - \omega_k) E_k^2 \varepsilon_{\mathbf{k}\mu}^i \varepsilon_{\mathbf{k}\mu}^{j*}
\end{aligned} \tag{1.115}$$

Putting this into the ground level shift, we recover the formula (??) for the Lamb shift:

$$\langle g|H^{(2)}|g\rangle = - \sum_{\mathbf{k}\mu} \frac{E_k^2 |\mathbf{d} \cdot \boldsymbol{\varepsilon}|^2}{\hbar(\omega_k + \omega_A)}. \tag{1.116}$$

As an exercise, you can work out the corresponding expression for the excited state shift. These shifts are usually ignored by incorporating them into the atomic Hamiltonian, $H_A \mapsto H_A + H^{(2)}$. In fact, the coupling to the electromagnetic field is always there and shifts the energy levels. The observed atomic transition frequency thus already contains them, and the “bare” (not shifted) frequency ω_A that we put at the beginning is not observable as such. This procedure is called “renormalization” and is the second trick to handle the infinities that occur in quantum electrodynamics.

There are quantum optics applications where the level shift is not “hidden” in a renormalized frequency and must be taken into account. For example when the atom is placed close to a mirror or other macroscopic objects. One gets a position-dependent modification of the Lamb shift, better known as van der Waals potential that enters the master equation as an additional potential: it shifts the atomic transition frequency and, more generally, the energy levels. One also finds that the atomic decay rate, discussed below, is changed in front of a mirror.

Decay rates The last term, $\mathcal{L}[\rho_A]$, of the master equation (1.113) contains the “superoperator” \mathcal{L} or “Liouvillian” that is a linear mapping of the density matrix. It cannot be written in terms of a commutator. Collecting the terms of our derivation, it has the following form

$$\begin{aligned}
\mathcal{L}[\rho_A] &= -\frac{\gamma_e}{2} \{\sigma_+ \sigma_-, \rho_A\} + \gamma_e \sigma_- \rho_A \sigma_+ \\
&\quad - \frac{\gamma_g}{2} \{\sigma_- \sigma_+, \rho_A\} + \gamma_g \sigma_+ \rho_A \sigma_-
\end{aligned} \tag{1.117}$$

where $\{A, B\} = AB + BA$ is the anti-commutator and where the rates $\gamma_{e,g}$ are given by

$$\gamma_g^e = \frac{|\mathbf{d}|^2}{\hbar^2} S(\pm\omega_A) \tag{1.118}$$

Note that the Liouvillian (1.117) also conserves the trace of the density matrix (as it must).

Rate equations

The Liouvillian superoperator \mathcal{L} describes decay processes. To see this, let us work out the equations of motion for the populations $p_{e,g}$, i.e., the diagonal elements of the density matrix. Using again $\sigma_+\sigma_- = |e\rangle\langle e|$ and $\sigma_-\sigma_+ = |g\rangle\langle g|$, we get

$$\begin{aligned}\dot{p}_e &= -\gamma_e p_e + \gamma_g p_g \\ \dot{p}_g &= -\gamma_g p_g + \gamma_e p_e\end{aligned}\tag{1.119}$$

We see here explicitly that the total population is conserved. We recover the rate equations (1.104) when $\gamma = \gamma_e$ and $\gamma_g = 0$, as is the case for a field at zero temperature. In this case, the rate γ_e is the spontaneous decay rate of the excited state. This can be seen using the field spectrum (1.115):

$$\gamma_e = \frac{2\pi}{\hbar^2} \sum_{\mathbf{k}\mu} \delta(\omega_A - \omega_k) E_k^2 |\mathbf{d} \cdot \boldsymbol{\varepsilon}|^2 = \frac{2\pi}{\hbar} \sum_{\mathbf{k}\mu} \delta(E_{e0} - E_{g1}) |\langle g; 1_{\mathbf{k}\mu} | \mathbf{d} \cdot \mathbf{E} | e; 0 \rangle|^2$$

The last expression is Fermi's Golden Rule for the transition rate between the state $|e; 0\rangle$ into the continuum of states $|g; 1_{\mathbf{k}\mu}\rangle$ due to the electric dipole coupling. At nonzero temperature, also the ground state can “decay” via the absorption of thermally excited photons.

The stationary state of the rate equations (1.119) is attained at large times and reads

$$\begin{aligned}p_e(t \rightarrow \infty) &= \frac{\gamma_g}{\gamma_g + \gamma_e} \\ p_g(t \rightarrow \infty) &= \frac{\gamma_e}{\gamma_g + \gamma_e}\end{aligned}\tag{1.120}$$

For zero temperature, we find $p_g(t \rightarrow \infty) = 1$. For finite temperature, we can expect that we recover the Boltzmann factor:

$$\frac{p_e(t \rightarrow \infty)}{p_g(t \rightarrow \infty)} = \frac{\gamma_g}{\gamma_e} = e^{-\hbar\omega_A/k_B T}$$

It is a simple exercise to show that the ground state excitation rate is proportional to the mean photon number at the transition frequency (stimulated absorption), $\gamma_g \propto \bar{n}(\omega_A)$, while for the excited state decay, stimulated emission gives $\gamma_e \propto 1 + \bar{n}(\omega_A)$. Using the mean photon number $\bar{n}(\omega_A) = (e^{\hbar\omega_A/k_B T} - 1)^{-1}$, we indeed get the Boltzmann factor:

$$\frac{\bar{n}(\omega_A)}{1 + \bar{n}(\omega_A)} = \frac{1}{e^{\hbar\omega_A/k_B T} - 1} \frac{e^{\hbar\omega_A/k_B T} - 1}{e^{\hbar\omega_A/k_B T} - 1 + 1} = e^{-\hbar\omega_A/k_B T}.$$

Decoherence

Finally, the real benefit of our master equation is the equation of motion for the off-diagonal elements (the coherences) of the density matrix. From (1.113), we get for example

$$\frac{d\rho_{eg}}{dt} = -\frac{\gamma_e + \gamma_g}{2}\rho_{eg} \quad (1.121)$$

and its complex conjugate. We observe that the coherences decay due to the coupling to the field. This process is often called “decoherence” — quantum superpositions (with nonzero off-diagonal density matrix elements) turn into classical probabilistic alternatives (described by diagonal density matrices) due to the interaction with some “environment”. The decoherence rate is sometimes written $1/T_2$ in distinction to the rate $\gamma_e = 1/T_1$ for the populations. Note that there exist couplings where one gets a decoherence rate that is larger than the value $(\gamma_e + \gamma_g)/2$ obtained here. This value is a lower limit, except special cases (a “squeezed reservoir”, for example). In the important case of zero temperature (more precisely, $\hbar\omega_A \gg k_B T$), the “optical coherence” ρ_{eg} decays with $\gamma_e/2$, hence at half the rate of the excited state population.

1.6 Quantum Langevin formulation

1.6.1 Idea

Many systems in quantum optics are “open” and follow equations of motion that go beyond the Schrödinger equation. This applies to systems for which the Hamiltonian is not completely known or systems in contact with an “environment”. The equations of motion can be formulated as so-called master equations (similar to the Schrödinger picture, dynamics for the system density operator) or as so-called Langevin equations (similar to the Heisenberg picture, dynamics of the system operators). These equations are the quantum analogue of kinetic theories that describe the dynamics of a system including different dissipative effects. They provide, among others, the approach of the system towards thermal equilibrium, but also non-equilibrium states that are driven by external forces, the typical example being a laser field.

In quantum optics, the “system” can be an atom, a collection of atoms, or a field mode in a cavity. The system is “open” because it interacts with the “environment” (rest of the world), that is modelled as a continuum of quantized field modes. An atom decays irreversibly by emitting a photon into previously empty vacuum modes. This phenomenon of “spontaneous emission” does not allow for a description in terms of a Hamiltonian. In fact, the state of the atom does not remain pure, and entropy increases because the photon can be emitted into any direction of space. A cavity mode decays because photons escape through the cavity mirrors, effectively becoming excitations of the “modes outside the cavity”. Alternatively, the field energy can be absorbed by the material making up the mirrors.

We focus first on the derivation of a master equation for a two-level atom. We shall find from the general theory two results: (1) the rate of spontaneous emission of an electronically excited state and (2) Glauber’s formula for the signal of a photodetectors in terms of normally ordered correlation functions of the electric field operator.

Time scales

The derivation builds on the following hierarchy of time scales:

$$\frac{2\pi}{\omega_A} \leq \tau_c \ll \frac{2\pi}{\Omega} \sim \frac{1}{\gamma} \quad (1.122)$$

where the shortest time scale is the optical period of the light field that is near-resonant with the atomic transition frequency ω_A . This is typically smaller than a few fs (femtoseconds) (in the visible range).

The “correlation time” τ_c of the electromagnetic field describes qualitatively the time interval over which the quantum fluctuations of the electromagnetic field (that couple significantly to the atom) are “smooth”. Two electric field measurements are not significantly “similar” if they are taken at intervals larger than τ_c . We give an estimate below, it turns out to be a few times larger than the optical period.

The third time scale is the Rabi period that scales with the inverse of the Rabi frequency of a laser. This depends of course on the laser power (and the atomic transition dipole), but typical values are in the 1–10 ns (nanoseconds) range. Note that this is much longer than the optical period and the field correlation time.

The last time scale is the lifetime of the excited state of the atom, inversely proportional to the spontaneous decay rate γ . This is typically in the 1–10 ns range as well, depending on the atom.

We thus have a situation similar to “Brownian motion”: the atom is “shaken around” by the vacuum field fluctuations that vary much faster than the typical dynamics for the atomic state (Rabi oscillations, spontaneous decay). The master equation takes advantage of this separation of time scales to find an equation of motion that can be applied on “slow time scales”. As a result, one gets a single equation that describes both, the “Hamiltonian” effects of a laser (Rabi oscillations) and the “dissipative / friction” effects due to vacuum fluctuations.

Hamiltonian

Two-level atom, field, and electric dipole interaction:

$$H = \frac{\hbar\omega_A}{2}\sigma_3 + \sum_k \hbar\omega_k a_k^\dagger a_k + \sum_k \hbar \left(g_k^* a_k^\dagger \sigma + g_k \sigma^\dagger a_k \right) \quad (1.123)$$

neglect the zero-point energy of the field. Coupling constant $\hbar g_k = -\mathbf{d}_{\text{eg}} \cdot \mathbf{f}_k(x_A)(\hbar\omega_k/2\varepsilon_0)^{1/2}$ with the mode function $\mathbf{f}_k(x)$ evaluated at the position of the atom. Sometimes called ‘vacuum Rabi frequency’.

In the following, we also use the (re-scaled) electric field operator

$$E(t) = \sum_k g_k a_k(t) + \text{h.c.} \quad (1.124)$$

Field correlation time

To get an estimate of the field correlation time, we compute the two-time correlation (or coherence) function

$$C(\tau) = \langle E(t + \tau)E(t) \rangle \quad (1.125)$$

If we use the coupling constants g_k to write the mode expansion of the quantized field (this is equivalent to re-scaling the electric field so that it has units of frequency), we get

$$\begin{aligned} \langle E(t + \tau)E(t) \rangle &= \sum_k |g_k|^2 \langle a_k(t + \tau)a_k^\dagger(t) \rangle \\ &= \sum_k |g_k|^2 e^{-i\omega_k\tau} \end{aligned} \quad (1.126)$$

An explicit calculation using the mode amplitudes in free space leads to an integral of the form

$$C(\tau) \sim \int_0^\infty d\omega \omega^3 e^{-i\omega\tau} \quad (1.127)$$

which looks like a third derivative of a δ -function in τ . Well, not exactly since the integrations starts at $\omega = 0$. Generalizing to finite temperature, the Fourier transform of the correlation function (1.127) becomes

$$C(\omega) \sim \omega^3 \bar{n}(\omega) = \frac{\omega^3}{\exp(\hbar\omega/k_B T) - 1} \quad (1.128)$$

The sign convention of the Fourier transform is chosen here such that $\omega > 0$ corresponds to photon numbers $a^\dagger a$ (‘normal order’), while at $\omega < 0$, the anti-normal order aa^\dagger is picked. See Fig.1.3: the spectrum is proportional to $-\omega^3$ for negative frequencies, $-\omega \gg k_B T/\hbar$. Near zero frequency, it has a

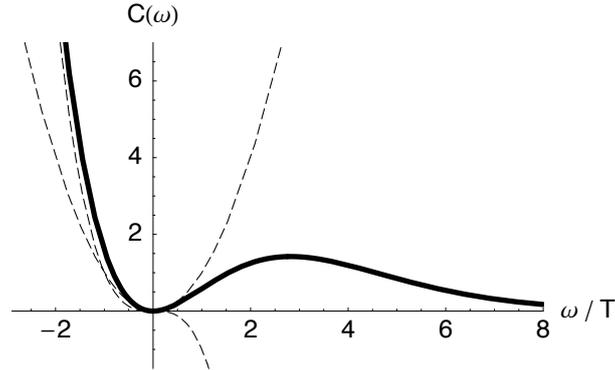


Figure 1.3: Spectrum $C(\omega)$, Eq.(1.128), of the radiation field (normal order) at finite temperature. The frequency is plotted in units of $k_B T/\hbar$. The dashed lines are ω^2 and $-\omega^3$.

quadratic behaviour, at positive frequencies, a maximum near $\omega = 2k_B T/\hbar$ (Wien displacement law) and an exponential decay for $\omega \gg k_B T/\hbar$.

Actually, we forgot one thing in this estimate: the Hamiltonian we start with is only valid for field modes k near-resonant with the atomic transition, $\omega_k \sim \omega_A$. It thus seems reasonable to restrict the frequency integral in Eq.(1.127) to an interval around ω_A , with a width $\Delta\omega$ that is typically smaller than ω_A .

Now, from the properties of the Fourier transformation, we know that the correlation function $C(\tau)$ given by the integral (1.127) has a “width in time” given by $\Delta\tau \Delta\omega \sim 1$. Since this width is precisely the definition of the correlation time, we have

$$\frac{1}{\omega_A} \leq \frac{1}{\Delta\omega} \sim \tau_c. \quad (1.129)$$

Typical value: a few 10 fs.

1.6.2 Evolution of the atomic operators

We shall work in the Heisenberg picture. Note that operators describing different degrees of freedom (field, atom) commute at equal times.

Atomic dipole

“eliminate” the field operators by solving their equation of motion:

$$\frac{da_k}{dt} = \frac{i}{\hbar} [H, a_k] = -i\omega_k a_k - ig_k^* \sigma \quad (1.130)$$

$$a_k(t) = a_k(0) e^{-i\omega_k t} - ig_k^* \int_0^t dt' \sigma(t') e^{-i\omega_k(t-t')} \quad (1.131)$$

the “particular solution” contains the “past” of the atomic dipole operator $\sigma(t')$. Insert this into the equation for σ . Let’s look at this equation first:

$$\begin{aligned} \frac{d\sigma}{dt} &= \frac{i}{\hbar} [H, \sigma] = -i\omega_A \sigma + i \sum_k g_k [\sigma^\dagger, \sigma] a_k \\ &= -i\omega_A \sigma + i \sum_k g_k \sigma_3 a_k \end{aligned} \quad (1.132)$$

We see here that the two-level atom leads to nonlinear equations of motion: the operator product $\sigma_3 a_k$ appears. For the moment, these operators commute (at equal times). But we now want to insert the solution (1.131) for $a_k(t)$, and the two terms that appear here do not commute separately with σ_3 . For this reason, we take now a specific operator order (so-called “normal order”) where the annihilation operators (a_k or σ) act first. This is the order already used in Eq.(1.132), and we thus get

$$\frac{d\sigma}{dt} = -i\omega_A \sigma + i\sigma_3 \mathcal{E}_0(t) + \int_0^t dt' \sum_k |g_k|^2 e^{-i\omega_k(t-t')} \sigma_3(t) \sigma(t') \quad (1.133)$$

where we used the abbreviation

$$\mathcal{E}_0(t) = \sum_k g_k a_k(0) e^{-i\omega_k t} \quad (1.134)$$

for the freely evolving electric field operator (positive frequency component only, and re-scaled by the atomic transition dipole). In the integral over t' , we see that the correlation function $C(t-t')$ appears, and using $\tau = t-t'$ as integration variable, we have

$$\frac{d\sigma}{dt} = -i\omega_A \sigma + i\sigma_3 \mathcal{E}_0(t) + \int_0^t d\tau C(\tau) \sigma_3(t) \sigma(t-\tau) \quad (1.135)$$

Now comes the *key observation*: under the time integral occur two very different functions. The correlation function $C(\tau)$ is very narrow in τ . The atomic operator $\sigma(t - \tau)$ contains a “fast free evolution” (generated by the first term in its equation of motion), but once this is factored out, we anticipate that its evolution is “slow”:

$$\sigma(t - \tau) = e^{-i\omega_A(t-\tau)} \tilde{\sigma}(t - \tau) \approx e^{-i\omega_A(t-\tau)} \tilde{\sigma}(t) = e^{+i\omega_A\tau} \sigma(t) \quad (1.136)$$

Here, we introduced temporarily the dipole operator $\tilde{\sigma}(t')$ (in an interaction picture).

The main benefit of this approximation is that only atomic operators at time t appear in the equation of motion. The two-level commutation rules² give $\sigma_3(t)\sigma(t) = -\sigma(t)$, and we end up with

$$\frac{d\sigma}{dt} = -i\omega_A\sigma + i\sigma_3\mathcal{E}_0(t) - \sigma(t) \int_0^t d\tau C(\tau) e^{i\omega_A\tau} \quad (1.137)$$

The upper integration limit t is actually the difference between our initial time and the actual time where the equation of motion is computed. We now let this time difference be much larger than the correlation time τ_c . This is consistent with the assumption that the atomic dynamics is slow on the scale of the field’s correlation time. Then the integrand is effectively zero at the upper limit, and we get a constant complex number

$$\gamma + i\delta\omega_A = \int_0^{t \gg \tau_c} d\tau C(\tau) e^{i\omega_A\tau} = \frac{S(\omega_A)}{2} + i\mathcal{P} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega - \omega_A} \quad (1.138)$$

where $S(\omega)$ is the Fourier transform of the correlation function $C(\tau)$ and \mathcal{P} means the principal part of the integral. Putting this complex number into the equation of motion (1.137):

$$\frac{d\sigma}{dt} = -i(\omega_A + \delta\omega_A)\sigma(t) - \gamma\sigma(t) + i\sigma_3\mathcal{E}_0(t), \quad (1.139)$$

we see that the real part γ leads to an exponential decay of the dipole operator $\langle\sigma\rangle$: this is called spontaneous decay (or natural linewidth). While $\delta\omega_A$ gives a shift of the atomic frequency, called the Lamb shift.

²A pedantic remark: operator products evolve as products under the Heisenberg equations of motion. This is because taking the commutator with a product is compatible with the product rule of (time) derivatives.

Spontaneous decay rate and Lamb shift

Explicit calculation: spectrum of vacuum fluctuations

$$S(\omega) = 2\pi \sum_k |g_k|^2 \delta(\omega_k - \omega) \quad (1.140)$$

Take a plane wave expansion and sum over the polarization vectors $\mathbf{u}_{\mathbf{k}\lambda}$ in the coupling constants g_k

$$\sum_\lambda |\mathbf{d}_{\text{eg}} \cdot \mathbf{u}_{\mathbf{k}\lambda}|^2 = |\mathbf{d}_{\text{eg}}|^2 - |\mathbf{d}_{\text{eg}} \cdot \hat{\mathbf{k}}|^2 \quad (1.141)$$

where $\hat{\mathbf{k}}$ is the unit vector along \mathbf{k} . This formula arises because the $\mathbf{u}_{\mathbf{k}\lambda}$ are perpendicular to \mathbf{k} . Integration over the angles of \mathbf{k} gives

$$\int d\Omega(\hat{\mathbf{k}}) (|\mathbf{d}_{\text{eg}}|^2 - |\mathbf{d}_{\text{eg}} \cdot \hat{\mathbf{k}}|^2) = 4\pi |\mathbf{d}_{\text{eg}}|^2 - \frac{4\pi}{3} |\mathbf{d}_{\text{eg}}|^2 = \frac{8\pi}{3} |\mathbf{d}_{\text{eg}}|^2 \quad (1.142)$$

The integral over the length of \mathbf{k} is trivial because of the δ -function in Eq.(1.140), its length is fixed to $|\mathbf{k}| = \omega/c$. Putting everything together, we get

$$S(\omega) = \frac{2\pi}{3\hbar^2} |\mathbf{d}_{\text{ge}}|^2 \frac{\hbar\omega}{2\varepsilon_0} \frac{8\pi\omega^2}{(2\pi c)^3} \quad (1.143)$$

where the last factor is the density of field modes per $d\omega$ and volume. We can thus say that the spontaneously decaying atom is a “detector” for vacuum field fluctuations. The decay rate γ

$$\gamma = \frac{1}{2} S(\omega_A) = \frac{|\mathbf{d}_{\text{ge}}|^2 (\omega_A/c)^3}{6\pi\hbar\varepsilon_0} \quad (1.144)$$

is also called the “natural linewidth” of the atomic transition $|g\rangle \leftrightarrow |e\rangle$ because it gives the width in frequency of the spontaneous emission spectrum. In order of magnitude, with $|\mathbf{d}_{\text{ge}}| \sim ea_0$ (electron charge \times atom size)

$$\frac{\gamma}{\omega_A} \sim \alpha_{\text{fs}} (a_0/\lambda_A)^2 \sim \alpha_{\text{fs}}^3 \quad (1.145)$$

with fine structure constant $\alpha_{\text{fs}} = e^2/4\pi\varepsilon_0\hbar c \approx 1/137.04$ and wavelength λ_A of resonant transition. Hence, indeed decay is “slow” on the scale of the optical period.

Frequency shift $\delta\omega_A$ is related to asymmetry of vacuum spectrum around the transition frequency. Interpretation from second order perturbation

theory: modes slightly below the atomic resonance, $\omega_k \leq \omega_A$ tend to push the level $|e\rangle$ upwards. Modes above resonance: push downwards. Null effect if spectrum is flat.

Actual calculation requires UV cutoff ω_{uv} and interaction Hamiltonian beyond the resonance (rotating wave) approximation (Hans Bethe \sim 1948, calculation of the Lamb shift). Order of magnitude:

$$\delta\omega_A \approx \gamma \log(\omega_{uv}/\omega_A) \quad (1.146)$$

and a consistent cutoff is the electron rest mass, $\omega_{uv} \sim m_e c^2/\hbar$. Hence comparable to the natural linewidth. Note: relativistic theory required, where wavelengths up to electron Compton wavelength $\hbar/m_e c$ are involved. This goes beyond the “long wavelength approximation” because $\hbar/m_e c \sim \alpha_{fs} a_0 \ll a_0$.

Atomic populations

Actually, we did not yet show that γ is the rate of decay for the excited state. For this, we need the equation of motion for the occupations of the two energy levels. This is described by the atomic operator σ_3 , also called the “inversion” because $\langle \sigma_3 \rangle > 0$ when the excited state is more occupied than the ground state.

Heisenberg equation of motion

$$\begin{aligned} \frac{d\sigma_3}{dt} &= +2i \sum_k \left[g_k^* a_k^\dagger \sigma - g_k \sigma^\dagger a_k \right] \\ &= 2i \left[\mathcal{E}_0^\dagger(t) \sigma - \sigma^\dagger \mathcal{E}_0(t) \right] \\ &\quad - 2 \int_0^t dt' \left[C^*(t-t') \sigma^\dagger(t') \sigma(t) + C(t-t') \sigma^\dagger(t) \sigma(t') \right] \end{aligned} \quad (1.147)$$

where we brought the operator products in normal order (first line) and inserted the formal solution for $a_k(t)$ (second line). We apply to the t' -integral the same prescription as before and get

$$\begin{aligned} &\int_0^t dt' \left[C^*(t-t') e^{i\omega_A(t'-t)} \sigma^\dagger(t) \sigma(t) + C(t-t') e^{-i\omega_A(t'-t)} \sigma^\dagger(t) \sigma(t) \right] \\ &\approx (\gamma - i\delta\omega_A) \sigma^\dagger(t) \sigma(t) + (\gamma + i\delta\omega_A) \sigma^\dagger(t) \sigma(t) = \gamma(\sigma_3(t) + \mathbb{1}) \end{aligned} \quad (1.148)$$

where the frequency shift drops out. By construction, the operator $\sigma_3(t) + \mathbb{1}$ gives the occupation of the excited state. From Eqs.(1.147, 1.148), we can thus read off the decay rate 2γ for the excited state population, while the ground state remains stable.

Finally, the equation for the inversion operator becomes

$$\frac{d\sigma_3}{dt} = -2\gamma(\sigma_3(t) + \mathbb{1}) + 2i [\mathcal{E}_0^\dagger(t)\sigma - \sigma^\dagger\mathcal{E}_0(t)] \quad (1.149)$$

Combined with the equation of motion for the atomic dipole operator

$$\frac{d\sigma}{dt} = -(\gamma + i\omega_A)\sigma + i\sigma_3\mathcal{E}_0(t) \quad (1.150)$$

we have thus found the “optical Bloch equations”.

In Eq.(1.150), we have made the replacement $\omega_A + \delta\omega_A \mapsto \omega_A$ for the atomic frequency. This is called “renormalization”: we combine the shift induced by the coupling to the vacuum field with the “naked” transition frequency into the frequency that can be physically observed. Recall that in reality, we can never “switch off” the coupling to the vacuum. Hence the “naked” two-level atom that we started with is actually a theoretical artefact.

Approximations

Let us collect the approximations that we had to make.

1. weak coupling between atom and field. We used second order perturbation theory.
2. effective evolution of the atom occurs at long timescales. We found $1/\gamma_e \approx 10^{-9} \text{ s} \gg \tau_c \approx 10^{-12} \text{ s}$. This allows to choose $\tau_c \ll \Delta t \ll 1/\gamma_e$. Note that the field correlation time τ_c is only “short” when the field has a “broad” frequency spectrum $S(\omega)$ (width much larger than γ_e).
3. the period of the emitted radiation is much shorter than $1/\gamma_e$. O.k. for atoms where $\omega_A \gg \gamma_e$.
4. the field state is unaffected by the presence of the atom. Radiated photons escape from the atom and do not interact a second time. The field is a large “reservoir”.

1.6.3 Application 1: Bloch equations

Note that we did not specify yet the state of the light field: it is in fact encoded in the operator $\mathcal{E}_0(t)$ that depends on the initial field operators $a_k(0)$. Two examples will be studied now, the first one being an atom driven by a laser field. We have argued that to a good approximation, we can assume that the light field is in a coherent state $|\alpha_L\rangle$. We assume that at $t = 0$, the total system is in the product state $|\psi(0), \alpha_L\rangle$ and take the expectation value of the Bloch equation. This gives the dynamics of the Bloch vector as follows (optical Bloch equations in the proper sense)

$$\frac{ds}{dt} = -(\gamma + i\omega_A)s + (i/2)s_3\Omega e^{-i\omega_L t} \quad (1.151)$$

$$\frac{ds_3}{dt} = -2\gamma(s_3(t) + 1) + i \left[\Omega^*(t)e^{i\omega_L t} s - s^* \Omega e^{-i\omega_L t} \right] \quad (1.152)$$

where $\Omega/2 = \langle \alpha_L | \mathcal{E}_0(0) | \alpha_L \rangle$ is the (complex) Rabi frequency and ω_L the frequency of the laser mode.

These equations have time-dependent coefficients, but this can be removed by making a transformation into a “rotating frame”. We make the replacement

$$s(t) \mapsto s(t)e^{-i\omega_L t} \quad (1.153)$$

where the “new” $s(t)$ satisfies Bloch equations with time-independent coefficients

$$\begin{aligned} \frac{ds}{dt} &= -(\gamma - i\delta)s + (i/2)s_3\Omega \\ \frac{ds_3}{dt} &= -2\gamma(s_3(t) + 1) + i[\Omega^*s - s^*\Omega] \end{aligned} \quad (1.154)$$

where $\delta = \omega_L - \omega_A$ is the “laser detuning”. Note that the symbols are not the same throughout the books: the Rabi frequency Ω or the decay rate γ can differ by a factor of 2 (or -2), the detuning can have the opposite sign.

The Bloch equations are a “workhorse” of atomic physics and quantum optics. They are used to compute light absorption, excitation spectra, population transfer, radiation forces on atoms etc. In the exercises, you compute the stationary state of the Bloch equations (attention with the different sign for δ : this one should be correct)

$$s_{ss} = \frac{-i(\Omega/2)(\gamma + i\delta)}{\gamma^2 + \delta^2 + \Omega^2/2} \quad (1.155)$$

$$s_{3,ss} = \frac{-(\gamma^2 + \delta^2)}{\gamma^2 + \delta^2 + \Omega^2/2} \quad (1.156)$$

Discussion: average atomic dipole operator (induced by laser field), average inversion. Line broadening.

Exercise: total excitation N , does not commute when laser included. Expectation value of \dot{N} in stationary state, interpretation as total scattered intensity.

Exercise: spectrum of spontaneous emission, from formal solution. Need formal solution of atomic dipole operator, Eq.(1.161).

1.6.4 Application 2: the Glauber photodetector

Roy Glauber (Nobel prize 2005) developed in the 1960s the theory of photodetection. His main result is that the signal of a photodetector is proportional to

$$I(t) \propto \langle E^{(-)}(t)E^{(+)}(t) \rangle \quad (1.157)$$

where $E^{(+)}(t)$ is the positive frequency part of the electric field operator at the detector position. This signal is constructed in such a way that if the field is in the vacuum state, a detector gives no signal: perfectly reasonable. But due to the presence of vacuum fluctuations (also nonzero expectation values of a product of field operators!), not easy to implement in the theory.

We can recover the relevant features of Glauber's theory with our two-level atom. We shall actually show that under suitable approximations,

$$I(t) \propto \langle \mathcal{E}_0^\dagger(t)\mathcal{E}_0(t) \rangle \quad (1.158)$$

where $\mathcal{E}_0(t)$ is the re-scaled electric field operator we introduced in Eq.(1.134). Note that it contains positive frequency components only, and also only those modes that are near-resonant with the atomic transition frequency ω_A . Indeed, Glauber's model for a photodetector is a two-state system that is prepared in the ground state. Incident light can be absorbed, leading to some population in the excited state. This population is then "rapidly removed" from the system. A physical example: the excited atom is ionized and the free electron moves away (it cannot come back to recombine into the ground state). This is actually the process that happens in a photomultiplier ("avalanche photodiode").

So let us see what our Heisenberg equations (1.149, 1.150) give when the atom is in the ground state and the field is in an arbitrary state. We are interested in the rate of change of the excited state population:

$$I := \frac{dp_e}{dt} = \frac{d}{dt} \left\langle \frac{\sigma_3 + \mathbb{1}}{2} \right\rangle = \frac{1}{2} \frac{d\langle \sigma_3 \rangle}{dt} \quad (1.159)$$

Since the atom is in the ground state, the operator $\sigma_3 + \mathbb{1}$ that appears in Eq.(1.149) averages to zero. We are left with

$$I = i \langle \mathcal{E}_0^\dagger(t) \sigma(t) - \sigma^\dagger(t) \mathcal{E}_0(t) \rangle \quad (1.160)$$

and insert the formal solution for the atomic dipole operator [similar to Eq.(1.131)]:

$$\sigma(t) = \sigma(0) e^{-(\gamma+i\omega_A)t} + i \int_0^t dt' \sigma_3(t') \mathcal{E}_0(t') e^{-(\gamma+i\omega_A)(t-t')} \quad (1.161)$$

This gives

$$\begin{aligned} I &= - \int_0^t dt' \left[\langle \mathcal{E}_0^\dagger(t) \sigma_3(t') \mathcal{E}_0(t') \rangle e^{-(\gamma+i\omega_A)(t-t')} + \text{h.c.} \right] \\ &= \int_0^t d\tau \left[\langle \mathcal{E}_0^\dagger(t) \mathcal{E}_0(t-\tau) \rangle e^{-(\gamma+i\omega_A)\tau} + \text{h.c.} \right] \end{aligned} \quad (1.162)$$

where in the second line, we used the approximation that the inversion $\sigma_3(t')$ is evolving slowly and took its expectation value in the initial state (atom in the ground state, not correlated with the field). If we also assume that the expectation value evolves slowly with time t , $\langle \mathcal{E}_0^\dagger(t) \mathcal{E}_0(t-\tau) \rangle \approx \langle \mathcal{E}_0^\dagger(t+\tau) \mathcal{E}_0(t) \rangle$ [this is strictly true for a stationary field, but stationary fields do not give not very interesting signals on a photodetector], we can combine the '+h.c.' term into the single integral

$$I = \int_{-t}^t dt' \langle \mathcal{E}_0^\dagger(t) \mathcal{E}_0(t+\tau) \rangle e^{-\gamma|\tau|+i\omega_A\tau} \quad (1.163)$$

We observe that the photodetector signal is similar to the Fourier transform of the two-time field correlation function. We can already confirm that the signal is given by a normally ordered expectation value of field operator. Let us consider two limits.

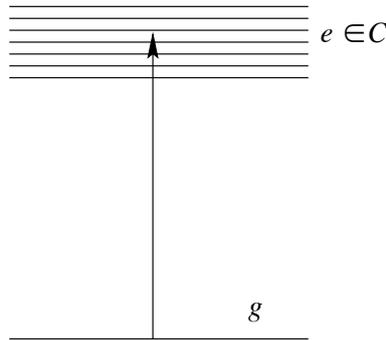


Figure 1.4: Two-level model for a fast photodetector. The signal corresponds to a sum of transition rates into all components of the upper state (quasi)continuum.

Narrow-band detector

If the decay time $1/\gamma$ is “very long” (compared to the correlation time of the field), the photodetector signal is essentially given by the field spectrum, taken at the transition frequency ω_A . Indeed, the τ -integral in Eq.(1.163) picks from the positive frequency operator $\mathcal{E}_0(t + \tau)$ those components that evolve like $e^{-i\omega_A\tau}$. A narrow band photodetector is thus simply a ‘spectrometer’, and the quantity it measures is the Fourier transform of the temporal correlation (or coherence) function. Experimentally, this situation can be achieved by placing a narrow-band frequency filter in front of a photodetector.

Fast detector

In some photodetectors, the excited state has a very short lifetime $1/\gamma$. This happens for example when the excited state actually ionizes and gives away its electron. The excitation rate I is then actually an integral over all components of the excited state ‘continuum’, as sketched in Fig.1.4. Under the integral, the exponential $e^{-\gamma|\tau|}$ becomes very short-ranged in τ , and we can make the replacement

$$e^{-\gamma|\tau|} \mapsto \frac{2}{\gamma} \delta(\tau) \quad (1.164)$$

This leads to Glauber's formula

$$I(t) = \eta \langle \mathcal{E}_0^\dagger(t) \mathcal{E}_0(t) \rangle \quad (1.165)$$

where the expectation value of the instantaneous intensity operator $\mathcal{E}_0^\dagger(t) \mathcal{E}_0(t)$ appears, in normal order, of course. The prefactor η actually is a number characteristic for the detector and is called "quantum efficiency". It must be determined experimentally. If the intensity is scaled to "photons per second", then η gives the detection probability per photon, and I the "rate of detected photons per second".

Intensity (photon) correlations

Generalization to multiple detection events: $I(t)$ interpreted as probability per unit time to detect one photon at time t . Probability to detect one photon at time t_1 and another one at t_2 :

$$I(t_1, t_2) = \eta^2 \langle \mathcal{E}_0^\dagger(t_1) \mathcal{E}_0^\dagger(t_2) \mathcal{E}_0(t_2) \mathcal{E}_0(t_1) \rangle, \quad t_2 > t_1 \quad (1.166)$$

time- and normal-ordered operator product. Interpretation.

Temporal coherence

Definition in terms of factorization of $\langle \mathcal{E}_0^\dagger(t) \mathcal{E}_0(t') \rangle$ (first-order temporal coherence). And for second-order.

Examples: monochromatic field always first-order coherent. Black-body radiation not. Two-photon state is second-order coherent, but not in first-order.

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