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The preliminary programme for this lecture:

0. Reminder: Atom-field interaction, density matrices

1. Positive maps $\hat{\rho}(t)$

   — Kraus-Stinespring theorem, Lindblad theorem

   — solvable models: dephasing, spontaneous emission

   — [entanglement, "PPT" criterion] [discrete and continuous variables]

   — examples: two-level atom, Bloch vector dynamics, quantum theory of the micromaser and the laser

2. Correlations and fluctuations $\langle \hat{A}(t)\hat{B}(t)\rangle$

   — quantum regression formula ("theorem")

   — quantum Langevin equations

   — examples: resonance fluorescence, Schawlow-Townes linewidth of the laser, broad-band squeezing

   — quantum fluctuation–dissipation theorem

3. Applications $\nabla\langle \mathbf{d}(t)\cdot\mathbf{E}(t)\rangle$

   — [optomechanics]

   — Casimir(–Polder) interactions

   — miscellaneous (on request)

Chapter 0

Reminder: atom-field interactions

0.1 Hamiltonian and relevant approximations

Hamiltonian $H_{\rm A} + H_{\rm F} + H_{\rm AF}$

$$H_{\rm A} = E_e|e\rangle\langle e| + E_g|g\rangle\langle g| = \frac{\hbar\omega_{\rm A}}{2}\sigma_3, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1}$$

two relevant atomic states $|{\rm g}\rangle$ and $|{\rm e}\rangle$, transition matrix element of the electric dipole operator $\mathbf{d}_{\rm ge} = \langle {\rm g}|\hat{\mathbf{d}}|{\rm e}\rangle$, two-level annihilation operator $\sigma = |{\rm g}\rangle\langle {\rm e}|$

Coupling to the electromagnetic field via the electric dipole moment, in resonance ("rotating wave") approximation

$$H_{\rm AF} = -\hat{\mathbf{d}}\cdot\mathbf{E}(\mathbf{x}_{\rm A}, t) \approx -\left(\mathbf{d}_{\rm eg}\sigma^\dagger \cdot \hat{\mathcal{E}}(\mathbf{x}_{\rm A}, t) + {\rm h.c.}\right), \qquad \sigma = |g\rangle\langle e| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{2}$$

Split of the electric field into positive and negative frequency components

$$\hat{\mathbf{E}}(\mathbf{x}_{\rm A}, t) = \underbrace{\hat{\mathcal{E}}(\mathbf{x}_{\rm A}, t)}_{a_k\, {\rm e}^{-{\rm i}\omega_k t}} + \underbrace{\hat{\mathcal{E}}^\dagger(\mathbf{x}_{\rm A}, t)}_{a_k^\dagger\, {\rm e}^{{\rm i}\omega_k t}} \tag{3}$$

Expansion in modes with quantum number k, (classical) mode functions $\mathbf{f}_k(\mathbf{x})$, annihilation operator $a_k(t)$, one-photon field amplitude $\mathcal{E}_k = (\hbar\omega_k/2\varepsilon_0)^{1/2}$.

Classical approximation (laser field): $\hat{\mathcal{E}} \mapsto \mathcal{E}_L(t)$ complex amplitude. In the quantum theory: field (mode) in coherent state $a_k|\alpha_k\rangle = \alpha_k|\alpha_k\rangle$. Time dependence of the field in quantum theory: via field Hamiltonian

$$H_{\mathrm{F}} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \tfrac{1}{2}\right) \tag{4}$$

one-photon coupling frequency

$$\hbar g_k = -\mathcal{E}_k \mathbf{d}_{\mathrm{ge}} \cdot \mathbf{f}_k(\mathbf{x}_{\mathrm{A}}) \tag{5}$$

Approximations

Electric dipole approximation: atom size small compared to "relevant wavelengths".

Resonance approximation: field modes (incl. laser mode) near the resonance frequency ω_{A}, hence only a narrow spectral band needed, with wavelength $\lambda_{\mathrm{A}} = 2\pi c/\omega_{\mathrm{A}} \gg a_0$ (Bohr radius: size of atom)

"Rotating-wave approximation": only resonant (energy-conserving) terms in the interaction Hamiltonian, $a_k\sigma^\dagger$ and $a_k^\dagger\sigma$: one photon disappears and atom becomes excited (absorption) or the inverse (photon emission).

0.2 Density operators

Generalize "pure states" of ordinary quantum mechanics and combines them with "statistical mixtures" known from statistical physics.

A state vector $|\psi\rangle$ corresponds to a density operator in the form of a projector $\rho = |\psi\rangle\langle\psi|$, this is what we are calling a "pure state". In mathematical physics, this is the consistent definition of a quantum state since the unobservable phase of the vector $|\psi\rangle$ disappears. ("States are rays in Hilbert space.")

Properties

Definition: Density operator.

linear operator on the Hilbert space $\hat{\rho} : \mathcal{H} \mapsto \mathcal{H}$

$\hat{\rho}$ is hermitean (could be called an "observable")[1]

$\hat{\rho}$ is positive: $\langle\phi|\hat{\rho}|\phi\rangle \geq 0$. This provides the probability interpretation; for a pure state, $\langle\phi|\hat{\rho}|\phi\rangle = |\langle\phi|\psi\rangle|^2 \geq 0$.

normalized (trace-class operator) $\mathrm{tr}\,\hat{\rho} = 1$

This definition also allows for "non-pure" or "mixed" states, for example

$$\hat{\rho} = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|, \qquad |\langle\psi_1|\psi_2\rangle| < 1 \tag{6}$$

with two pure states. The inequality ensures that the two states are not identical. But they are not necessarily orthogonal. If they are normalized, the sum of the two prefactors is $p_1 + p_2 = 1$. For this reason, one calls the mixed state (6) a "convex sum" which is a special linear superposition. Quite generally, the properties of density operators are preserved under convex sums (we could talk of a "convex vector space")

$$\hat{\rho} = p_1\hat{\rho}_1 + p_2\hat{\rho}_2 \tag{7}$$

The degree of being pure can be quantified with two numbers,

the purity $\mathrm{Pu}(\hat{\rho}) = \mathrm{tr}(\hat{\rho}^2 - \hat{\rho}) \begin{cases} = 0 & \text{if } \hat{\rho} \text{ is pure} \\ < 0 & \text{mixed state} \end{cases}$

the von Neumann entropy $S = -\mathrm{tr}(\hat{\rho}\log\hat{\rho})$ which is the Shannon information of the set of eigenvalues $\{p_1, \ldots p_N\}$ of $\hat{\rho}$. Indeed, these eigenvalues can be interpreted as a probability distribution.

Quantum states of a two-level system ("qbit")

Stationary states with respect to H_A ("free atom Hamiltonian") are $|e\rangle$ and $|g\rangle$. A general pure state is

$$|\psi(t)\rangle = \alpha(t)|\mathrm{e}\rangle + \beta(t)|\mathrm{g}\rangle \tag{8}$$

normalization $|\alpha(t)|^2 + |\beta(t)|^2 = 1$ consistent with probability interpretation.

[1] Indeed, if we are allowed for an infinite number of copies of the system prepared in $\hat{\rho}$, then the probabilities of finding the system in any of its states can be determined with arbitrary precision.

time evolution under H_A in the Schrödinger picture

$$\alpha(t) = \alpha(0)\,\mathrm{e}^{-\mathrm{i}\omega_\mathrm{A}t/2} \quad (9)$$

$$\beta(t) = \beta(0)\,\mathrm{e}^{\mathrm{i}\omega_\mathrm{A}t/2} \quad (10)$$

with our choice of zero energy. (Other choices: common, time-dependent phase factor.)

density matrix for a pure state $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ (projector), a hermitean 2×2-matrix

quantum average of atom observable $\mathcal{A} = \sigma, \sigma_3, \ldots$:

$$\langle\mathcal{A}\rangle = \langle\psi|\mathcal{A}|\psi\rangle = \mathrm{tr}\,[\mathcal{A}\rho] = \mathrm{tr}\,[\rho\mathcal{A}] \quad (11)$$

mixed state: density matrix ρ, cannot be written as projector.

example: thermal state at temperature T,

$$\rho = Z^{-1}\left(|\mathrm{g}\rangle\langle\mathrm{g}| + \mathrm{e}^{-\hbar\omega_\mathrm{A}/k_\mathrm{B}T}|\mathrm{e}\rangle\langle\mathrm{e}|\right), \qquad Z = 1 + \mathrm{e}^{-\hbar\omega_\mathrm{A}/k_\mathrm{B}T} \quad (12)$$

Boltzmann factor for weighting the stationary states: combination of quantum and classical (ensemble) average.

geometric significance: Bloch vector and Bloch sphere

three components $\mathbf{s} = (s_1, s_2, s_3)$, expectation value of the spin operator

$$s_1 = \langle\sigma_1\rangle = \langle\sigma + \sigma^\dagger\rangle = 2\,\mathrm{Re}(\alpha^*\beta) \quad (13)$$

$$s_2 = \langle\sigma_2\rangle = (\cdot)\,\mathrm{Im}(\alpha^*\beta) \quad (14)$$

$$s_3 = \langle\sigma_3\rangle = |\alpha|^2 - |\beta|^2 \quad (15)$$

sometimes complex notation used, $s = \langle\sigma\rangle = (s_1 - \mathrm{i}s_2)/2 = \alpha^*\beta$

pure state: $1 = \mathbf{s}^2 = s_1^2 + s_2^2 + s_3^2 = 4|s|^2 + s_3^2$, on the surface of the Bloch sphere.

"north pole": excited state $|\mathrm{e}\rangle$ (consistent with "spin up")

"south pole": ground state $|\mathrm{e}\rangle$ ("spin down")

on the equator: superposition states with equal weight, e.g. $(|\mathrm{g}\rangle + \mathrm{e}^{\mathrm{i}\phi}|\mathrm{e}\rangle)/\sqrt{2}$. Relative phase ϕ determines position on the equator:

$$s = \pm\frac{1}{2} \qquad \frac{|\mathrm{g}\rangle \pm |\mathrm{e}\rangle}{\sqrt{2}}$$

$$s = \pm\frac{\mathrm{i}}{2} \qquad \frac{|\mathrm{g}\rangle \pm \mathrm{i}\,|\mathrm{e}\rangle}{\sqrt{2}} \quad (16)$$

(free) time evolution: rotation of the Bloch vector around the 3-axis with angular frequency ω_{A}.

spin precession in the Heisenberg picture:

$$\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{A}}, \boldsymbol{\sigma}\right] = (\cdot)\omega_{\mathrm{A}}\mathrm{e}_3 \times \boldsymbol{\sigma} \tag{17}$$

take expectation value: gives equation of motion for the Bloch vector.

rotation of the Bloch vector: pure states remain pure

mixed states: are located inside the Bloch sphere. For the thermal state (12), for example:

$$\mathbf{s} = -\mathbf{e}_3 \tanh(\hbar\omega_{\mathrm{A}}/2k_{\mathrm{B}}T) \tag{18}$$

in the "infinite temperature limit", $\mathbf{s} \to \mathbf{0}$, the "completely mixed state".

Quantitative measures of "being pure": purity and entropy, see exercises.

0.3 Coherent + dissipative dynamics: Bloch equations

In this lecture, we are going to analyze the dynamics of a two-level system whose excited state $|e\rangle$ can decay spontaneously with a rate γ. The equation of motion of the density operator $\hat{\rho}(t)$ is then no longer given by the von Neumann equation, but contains an extra term

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = -\frac{\mathrm{i}}{\hbar}\left[\hat{H}_{\mathrm{A}} + \hat{H}_{\mathrm{AL}}, \hat{\rho}\right] + \mathcal{L}(\hat{\rho}) \tag{19}$$

with the dissipative "superoperator"

$$\mathcal{L}(\hat{\rho}) = \gamma\sigma\hat{\rho}\sigma^\dagger - \frac{\gamma}{2}\underbrace{\left\{\sigma^\dagger\sigma, \hat{\rho}\right\}}_{\sigma^\dagger\sigma\hat{\rho} + \hat{\rho}\sigma^\dagger\sigma} \tag{20}$$

where the first term is related to a quantum jump $|\psi\rangle \mapsto |g\rangle$ to the ground state. This can be interpreted as the result of detecting an emitted photon.

We observer that the trace of the density operator is conserved under Eq.(19):

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tr}\,\hat{\rho}(t) = 0; \tag{21}$$

this is consistent with the probability interpretation where the trace of $\hat{\rho}$ is the probability of finding the system in "any state". Note that sometimes, one deals with"lossy systems" where this property does not hold – the system can then "disappear" from a set of "detectable states".

Here is the master equation for a two-level atom driven by a monochromatic laser field with Rabi frequency Ω and coupled to the electromagnetic vacuum field: we use of course the frame rotating at the laser frequency ω. It is simple to show that the corresponding unitary transformation leaves the master equation unchanged: only products $\sigma_+\sigma_-$ appear, and the phase factors $\sigma_\pm \mapsto \sigma_\pm \, \mathrm{e}^{\pm \mathrm{i}\omega t}$ cancel. The atomic Hamiltonian is thus given by the expression (1.31) of chapter 1 (lecture QO I)

$$H_A = -\frac{\hbar\Delta}{2} + \frac{\hbar\Omega}{2}\left(\sigma_+ + \sigma_-\right) \tag{22}$$

The detuning $\Delta = \omega - \omega_A$ contains, of course, the renormalized transition frequency. The Rabi frequency Ω can be chosen real.

The full master equation, written in terms of the standard representation (not the interaction representation), contains also a commutator

$$\frac{\mathrm{d}\rho_A}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\left[H_A,\, \rho_A\right] + \mathcal{L}[\rho_A] \tag{23}$$

The elements of the density matrix thus evolve according to

$$\frac{\mathrm{d}\rho_{ee}}{\mathrm{d}t} = \mathrm{i}\frac{\Omega}{2}\left(\rho_{ge} - \rho_{eg}\right) - \gamma_e\rho_{ee} \tag{24}$$

$$\frac{\mathrm{d}\rho_{eg}}{\mathrm{d}t} = \mathrm{i}\Delta\,\rho_{eg} + \mathrm{i}\frac{\Omega}{2}\left(\rho_{gg} - \rho_{ee}\right) - \frac{\gamma_e}{2}\rho_{eg} \tag{25}$$

$$\frac{\mathrm{d}\rho_{gg}}{\mathrm{d}t} = -\mathrm{i}\frac{\Omega}{2}\left(\rho_{ge} - \rho_{eg}\right) + \gamma_e\rho_{ee} \tag{26}$$

We thus learn that, starting from the ground state, the laser field first creates the coherence ρ_{eg} between the ground and excited states — and this only if there is a population difference. The coherence is then turned into an excited state population — if it contains a nonzero imaginary part. These equations give the basic description for many physical phenomena: absorption and emission of light, lasing, resonance fluorescence etc.

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:

$$T(\sum_k p_k \hat{\rho}_k) = \sum_k T(\hat{\rho}_k), \qquad p_k \geq 0, \sum_k p_k = 1 \tag{1.1}$$

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, $\mathrm{P} = \rho \otimes \rho_{\mathrm{B}}$, we set

$$(T \otimes \mathbb{1})(\mathrm{P}) = T(\rho) \otimes \rho_{\mathrm{B}} \tag{1.2}$$

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

$$T(\rho) = \sum_k \Omega_k \rho \Omega_k^\dagger \tag{1.3}$$

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

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

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

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

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

$$P = \sum_k |\tilde{\varphi}_k\rangle\langle\tilde{\varphi}_k|. \tag{1.6}$$

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

$$|\psi^\star\rangle = \sum_n |n\rangle\langle n|\psi^\star\rangle, \qquad \langle n|\psi^\star\rangle \equiv (\langle n|\psi\rangle)^* = \langle\psi|n\rangle \tag{1.7}$$

The Kraus operators are now defined via their matrix elements as

$$\langle\chi|\Omega_k|\psi\rangle = \langle\chi\otimes\psi^\star|\tilde{\varphi}_k\rangle, \qquad \langle\psi|\Omega_k^\dagger|\chi\rangle = \langle\tilde{\varphi}_k|\chi\otimes\psi^\star\rangle, \tag{1.8}$$

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

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

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

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

$$|\phi\rangle = \sum_n |n\otimes n\rangle \tag{1.10}$$

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

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

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

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

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

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

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

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

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

$$T(|\psi\rangle\langle\psi|) = \sum_k \Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger \tag{1.15}$$

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

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

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.

Examples

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 $U(x) = \exp[-\mathrm{i}H(x)t]$:

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

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. Is 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

$$\langle n,m|\rho^\Gamma|n',m'\rangle = \langle n,m'|\rho|n',m\rangle \tag{1.18}$$

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

$$\rho = |\psi_+\rangle\langle\psi_+| \quad \text{with} \quad |\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \tag{1.19}$$

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

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \qquad \rho^\Gamma = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{1.20}$$

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

Note from Eq.(1.18) that the partial transpose is the natural extension of the transposition T to an enlarged Hilbert space: $\Gamma = \mathbb{1}\otimes\mathrm{T}$. We therefore conclude that the transposition is not a completely positive map.

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,

$$T_{t_1+t_2} = T_{t_1} T_{t_2} \tag{1.21}$$

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

$$W(t) = \exp(\mathcal{L}t) \tag{1.22}$$

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 (acting on the Hilbert space of the system) with

$$\frac{\partial \rho}{\partial t} \;=\; -\mathrm{i}\,[H,\,\rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \left\{ \rho, L_k^\dagger L_k \right\} \right)$$

$$= \quad -\mathrm{i}\,[H,\,\rho] + \frac{1}{2}\sum_k \left(\left[L_k\rho,\,L_k^\dagger\right] + \left[L_k,\,\rho L_k^\dagger\right]\right) \tag{1.23}$$

The following sketch of a proof is adapted from Nielsen & Chuang and C. Henkel, *J Phys B* 2007.

We evaluate the difference quotient

$$\frac{\rho(t+\Delta t)-\rho(t)}{\Delta t} \tag{1.24}$$

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

$$\rho(t+\Delta t) = \sum_k \Omega_k \rho \Omega_k^\dagger \tag{1.25}$$

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

$$\Omega_k = \omega_k \mathbb{1} + V_k \tag{1.26}$$

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:

$$(A|B) = \mathrm{tr}(A^\dagger B) \tag{1.27}$$

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

$$0 = (\mathbb{1}|V_k) = \mathrm{tr}(\mathbb{1}V_k) = \mathrm{tr}\,V_k \tag{1.28}$$

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

$$\begin{aligned}\rho(t+\Delta t)-\rho \quad &= \quad \left(\sum_k |\omega_k|^2 - 1\right)\rho + \sum_k \left(\omega_k^* V_k\,\rho + \rho\,\omega_k V_k^\dagger\right) \\ &\quad + \sum_k V_k^\dagger \rho V_k\end{aligned} \tag{1.29}$$

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

$$\lim_{\Delta t\to 0}\left[\hat{A}\rho(t+\Delta t) - \hat{A}\rho(t)\right] = \mathcal{O}(\Delta t) \tag{1.30}$$

for all operators $\hat{A}$ and initial density matrices $\rho(t)$. This permits us to extract all matrix elements in Eq.(1.29) and to conclude that the following terms must vanish separately

$$\lim_{\Delta t\to 0}\sum_k |\omega_k|^2 = 1 \tag{1.31}$$

$$\lim_{\Delta t\to 0}\sum_k \omega_k^* \rho V_k \; = 0 \tag{1.32}$$

$$\lim_{\Delta t\to 0}\sum_k V_k\, \rho V_k^\dagger = 0 \tag{1.33}$$

where the last two lines apply to any density matrix ρ. We can thus hope that the following derivatives exist

$$\gamma \;\equiv\; \lim_{\Delta t\to 0}\frac{\sum_k |\omega_k|^2 - 1}{\Delta t} \tag{1.34}$$

$$\Gamma - iH \;\equiv\; \lim_{\Delta t\to 0}\frac{\sum_k \omega_k^* V_k}{\Delta t} \tag{1.35}$$

where Γ and H are both hermitean.

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

$$\begin{aligned} 0 \;&=\; \lim_{\Delta t\to 0}\frac{\mathrm{tr}\,[\rho(t+\Delta t)-\rho]}{\Delta t} \\ &=\; \mathrm{tr}\Big[\gamma\rho + 2\Gamma\rho + \lim_{\Delta t\to 0}\frac{1}{\Delta t}\sum_k V_k^\dagger V_k\,\rho\Big] \end{aligned} \tag{1.36}$$

Since this must hold for any density matrix ρ, we find another derivative

$$\lim_{\Delta t\to 0}\frac{\sum_k V_k^\dagger V_k}{\Delta t} = -\gamma - 2\Gamma \tag{1.37}$$

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

$$L_k \equiv \lim_{\Delta t\to 0}\frac{V_k}{\sqrt{\Delta t}} \tag{1.38}$$

Using the derivatives defined in Eqs.(1.34, 1.35, 1.38), we can divide the difference $\rho(t+\Delta t)-\rho(t)$ in Eq.(1.29) by Δt, and take the limit $\Delta t \to 0$. This gives the differential equation (1.23).

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.(1.26) makes sense.

1.3.2 Remarks

Effect. A family of positive operators F_i on the Hilbert space with the property $\sum_i F_i = \mathbb{1}$. Appears typically as family of projectors onto eigenvalues of observables. After measuring the i'th value, the von-Neumann projection postulate tells us that the density operator is mapped to

$$\rho \mapsto M_i \rho M_i^\dagger \tag{1.39}$$

with probability $p_i = \mathrm{tr}(F_i \rho)$. which still needs to be normalized. Here, the positive operator has been factorized into $F_i = M_i^\dagger M_i$. The Kraus operators Ω_k can thus be understood as effects due to the outcome k of some measurement, with subsequent projection and classical mixing:

$$\rho \mapsto \sum_i p_i \frac{M_i \rho M_i^\dagger}{\mathrm{tr}(M_i \rho M_i^\dagger)} \tag{1.40}$$

Choi matrix.

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

$$U = \begin{pmatrix} \Omega_1 & & & \\ & \Omega_2 & & \\ & & \ddots & \\ & & & \Omega_n \end{pmatrix} \tag{1.41}$$

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

$$T(\rho) = \mathrm{tr}_{\mathcal{K}}[U(\rho \otimes K^{-1}\mathbb{1})U^\dagger] \tag{1.42}$$

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

$$\rho = \mathrm{tr}_2|\Psi\rangle\langle\Psi \qquad |\Psi\rangle = \sum_n \sqrt{p_n}|n \otimes n\rangle, \qquad \rho = \sum_n p_n|n\rangle\langle n| \tag{1.43}$$

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.

1.4 Examples

Spontaneous emission

is described by a single "Lindblad operator"

$$L = \sqrt{\gamma}\sigma \tag{1.44}$$

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.1.6.

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

$$\frac{\partial}{\partial t}\langle A\rangle = \mathrm{i}\langle[H,\, A]\rangle + \frac{1}{2}\sum_k \left\langle \left[L_k^\dagger,\, A\right] L_k + L_k^\dagger \left[A,\, L_k\right]\right\rangle \tag{1.45}$$

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 $\sigma^\dagger$ (at the rate γ, Eq.(**??**)) and to the damping of the inversion σ_3, Eq.(**??**), as we found in the previous chapter.

Rate equations in a thermal field

are generated by two Lindblad operators

$$L_{\rm em} = \sqrt{\gamma(\bar{n}+1)}\,\sigma, \qquad L_{\rm abs} = \sqrt{\gamma\bar{n}}\,\sigma^\dagger \tag{1.46}$$

where $\bar{n} = (\mathrm{e}^{\hbar\omega_{\rm A}/k_{\rm B}T} - 1)^{-1}$ is the average thermal photon number at the atomic transition frequency and temperature T of the radiation field. We recover the previous case for $T = 0$.

The operator $L_{\rm em}$ describes the emission of photons (spontaneous and stimulated) into the thermal field; the operator $L_{\rm abs}$ describes photon absorption. This can be easily checked by working out the equations of motion for the density matrix elements $\rho_{\rm gg}$ and $\rho_{\rm eg}$. (One gets the rate equations that have been used by Einstein in his proof of the Planck spectrum (*Physik Zeitschr* 1917).)

Both rates add up in the dynamics of the atomic dipole (the matrix elements $\rho_{\rm eg}$): their decay rate is $\gamma(2\bar{n}+1)$. 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

$$L_{\rm deph} = \sqrt{\kappa}\,\sigma_3 \tag{1.47}$$

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

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

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

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

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):

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

With the identification

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

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".

1.5 Exactly solvable open systems

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.

1.5.1 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.

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

$$H_{\mathrm{int}} = \sigma_3 \sum_k \left(g_k b_k^\dagger + g_k^* b_k \right) \tag{1.52}$$

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

$$S(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k) \tag{1.53}$$

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

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

where the "decoherence factor" is given by

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

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

$$\xi_k(t) = 2g_k \frac{1 - \mathrm{e}^{\mathrm{i}\omega_k t}}{\omega_k} \tag{1.56}$$

A proof of this result is sketched in Sec.1.5.2 below.

Discussion

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

$$t \to 0: \qquad \Gamma(t) \approx 2t^2 \sum_k |g_k(t)|^2 \coth(\beta\omega_k/2) = 2t^2 \int_0^\infty \mathrm{d}\omega \, S(\omega) \coth(\beta\omega/2) \tag{1.57}$$

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.(1.57) is often dominated by large frequencies, and can be made finite with a "UV cutoff frequency" $\omega_{\mathrm{c}} = 1/\tau_{\mathrm{c}}$. (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 $t < \tau_{\rm c}$ that are typically very short compared to the dissipative dynamics.

At larger times, we can make the approximation that $|\xi_k(t)|^2$ approaches a δ-function:[1]

$$t \to \infty : \qquad \left| \frac{1 - {\rm e}^{{\rm i}\omega_k t}}{\omega_k} \right|^2 \to 2\pi t \, \delta^{(1/t)}(\omega_k) \tag{1.59}$$

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 $\tau_{\rm c} \ll t \ll \hbar/k_{\rm B}T$). Then we can make the zero-temperature approximation $\coth(\beta\omega/2) \approx 1$ for the relevant modes and get

$$\tau_{\rm c} \ll t \ll \beta : \qquad \Gamma(t) \approx 4\pi S(0) t \tag{1.60}$$

hence an exponential decay with a rate $\kappa = 4\pi S(0)$ that involves the spectral strength at zero frequency (more precisely: at frequencies $T/\hbar \ll \omega \ll \omega_{\rm c}$). This behaviour is consistent with a Lindblad master equation because ${\rm e}^{-\Gamma t}$ becomes exponential in t. We thus see that the Lindblad form is not valid on the short time scale $\tau_{\rm c}$ that sets the correlation time of the bath fluctuations.

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

$$t \to \infty : \qquad \Gamma(t) \approx 4\pi t \sum_k |g_k(t)|^2 \delta^{(1/t)}(\omega_k) \coth(\beta\omega_k/2)$$

[1] This is based on the integral

$$\int_{-\infty}^{\infty} {\rm d}x \frac{\sin^2(x/2)}{x^2} = \frac{\pi}{2}. \tag{1.58}$$

$$\approx 4\pi t \int_0^\infty \mathrm{d}\omega\, \alpha\omega\, \delta^{(1/t)}(\omega) \frac{2T}{\hbar\omega} = 4\pi\alpha(T/\hbar)t \tag{1.61}$$

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

1.5.2 Calculation of the decoherence factor

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

$$H|\mathrm{g}\rangle = |\mathrm{g}\rangle H_\mathrm{g}, \qquad H_\mathrm{g} = -\frac{\hbar\omega_A}{2} + H_B - \sum_k \hbar(g_k b_k^\dagger + g_k^* b_k) \tag{1.62}$$

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

$$\begin{aligned}
\langle\sigma\rangle_t &= \mathrm{tr}_\mathrm{SB}[U^\dagger(t)|\mathrm{g}\rangle\langle\mathrm{e}|U(t)\rho(0)\otimes\rho_T(B)] &(1.63)\\
&= \mathrm{tr}_\mathrm{SB}[|\mathrm{g}\rangle\langle\mathrm{e}|\rho(0)\otimes U_\mathrm{g}^\dagger(t)U_\mathrm{e}(t)\rho_T(B)] &(1.64)\\
&= \langle\sigma\rangle_0 \mathrm{tr}_\mathrm{B}[U_\mathrm{g}^\dagger(t)U_\mathrm{e}(t)\rho_T(B)] &(1.65)
\end{aligned}$$

The bath trace can be taken for each mode separately since both $U_{\mathrm{g,e}}(t)$ 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)

$$\begin{aligned}
U_\mathrm{g}^\dagger(t) &= \exp[\mathrm{i}t(\omega b^\dagger b - gb - gb^\dagger)] = \exp[\mathrm{i}\omega t(b^\dagger-\gamma)(b-\gamma)]\,\mathrm{e}^{-\mathrm{i}tg^2/\omega} &(1.66)\\
U_\mathrm{e}(t) &= \exp[-\mathrm{i}t(\omega b^\dagger b - gb - gb^\dagger)] = \exp[-\mathrm{i}\omega t(b^\dagger+\gamma)(b+\gamma)]\,\mathrm{e}^{-\mathrm{i}tg^2/\omega}
\end{aligned}$$

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

$$D^\dagger(\gamma) f(b, b^\dagger) D(\gamma) = f(b+\gamma, b^\dagger+\gamma^*) \tag{1.67}$$

We can therefore write

$$\begin{aligned}
&U_\mathrm{g}^\dagger(t)U_\mathrm{e}(t)\rho_T(B)\\
&= D^\dagger(-\gamma)\exp(\mathrm{i}\omega t b^\dagger b)D(-\gamma)D^\dagger(\gamma)\exp(-\mathrm{i}\omega t b^\dagger b)D(\gamma) &(1.68)\\
&= D^\dagger(-\gamma)\exp(\mathrm{i}\omega t b^\dagger b)D(-2\gamma)\exp(-\mathrm{i}\omega t b^\dagger b)D(\gamma) &(1.69)
\end{aligned}$$

where in the last step, we have used $D^\dagger(\gamma) = D(-\gamma)$ and the composition law of the displacement operators. (The projective phase in QO I, Eq.(3.37) vanishes in this case.) We now use the identity, similar to Eq.(1.67)

$$U_0^\dagger(t) f(b, b^\dagger) U_0(t) = f(b\,\mathrm{e}^{-\mathrm{i}\omega t}, b^\dagger\,\mathrm{e}^{\mathrm{i}\omega t}) \tag{1.70}$$

where $U_0(t) = \exp(-\mathrm{i}\omega t b^\dagger b)$ is the 'free' time evolution operator. Applying this to the displacement operator $D(-2\gamma) = \exp(-2\gamma b^\dagger + 2\gamma^* b)$ that is 'sandwiched' in Eq.(1.69), we have

$$\exp(\mathrm{i}\omega t b^\dagger b) D(-2\gamma) \exp(-\mathrm{i}\omega t b^\dagger b) = D(-2\gamma\,\mathrm{e}^{\mathrm{i}\omega t}) =: D(-2\gamma(t)) \tag{1.71}$$

We end up with a product of three displacement operators

$$\begin{aligned} D(\gamma)D(-2\gamma(t))D(\gamma) &= \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\gamma^*\gamma(t)} D(\gamma - 2\gamma(t)) D(\gamma) && (1.72)\\ &= \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\gamma^*\gamma(t)} \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\gamma^*(t)\gamma} D(\xi_t) && (1.73)\\ \xi_t &= 2g\frac{1-\mathrm{e}^{\mathrm{i}\omega t}}{\omega} && (1.74) \end{aligned}$$

where the projective phases cancel and we recover the parameter $\xi_k(t)$ of Eq.(1.56).

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

$$\langle D(\xi_t)\rangle_{\mathrm{B}} = \mathrm{tr}\,[D(\xi_t)\rho_T] \tag{1.75}$$

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

$$\rho_T = \int \mathrm{d}^2\alpha |\alpha\rangle\langle\alpha| P_T(\alpha), \qquad P_T(\alpha) = \frac{\mathrm{e}^{-|\alpha|^2/\bar{n}}}{\pi\bar{n}} \tag{1.76}$$

and to calculate

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

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

$$\langle D(\xi_t)\rangle_{\mathrm{B}} = \mathrm{e}^{-|\xi_t|^2/2}\mathrm{e}^{-|\xi_t|^2\bar{n}} = \exp\left(-\tfrac{1}{2}|\xi_t|^2\coth\beta\omega/2\right) \tag{1.77}$$

Going back to $\langle\sigma\rangle_t$, we restore the factor $\mathrm{e}^{-\mathrm{i}\omega_A t}$ that we forgot in Eqs.(1.66) and take the product over all modes. This gives a sum in the exponent and hence

$$\langle\sigma\rangle_t = \mathrm{e}^{-\Gamma(t)}\langle\sigma\rangle_0 \tag{1.78}$$

$$\Gamma(t) = \sum_k \tfrac{1}{2}|\xi_k(t)|^2\coth(\beta\omega_k/2) \tag{1.79}$$

which is Eq.(1.80).

1.5.3 Long-time limit

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

$$\Gamma(t) = 8\alpha\int_0^\infty \mathrm{d}\omega\frac{\omega\omega_c^2}{\omega^2+\omega_c^2}\coth\frac{\omega}{2T}\frac{\sin^2(\omega t/2)}{\omega^2} \tag{1.80}$$

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

$$\coth\frac{\omega}{2T} = 2T\frac{\mathrm{d}}{\mathrm{d}\omega}\log\sinh\frac{\omega}{2T} \tag{1.81}$$

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

$$4\alpha T\,\mathrm{Re}\,\pi\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\omega}\frac{\omega_c^2}{\omega^2+\omega_c^2}(1-\mathrm{e}^{\mathrm{i}\omega t}) = 4\alpha T\,\mathrm{Re}\,\pi\mathrm{i}(-\mathrm{i}t) = 4\pi\alpha T t \tag{1.82}$$

This coincides with the term linear in t that we found with the approximation $\delta^{(t)}(\omega)$ to the $\sin^2$ function, Eq.(1.61). The contributions from the other poles give the sum

$$\Gamma(t) = \gamma t + 4\alpha\,\mathrm{Re}2\pi\mathrm{i}(\sum_{n=1}^{\infty}\frac{\omega_c^2}{\omega_c^2-\xi_n^2}\frac{T(1-\mathrm{e}^{-\xi_n t})}{\mathrm{i}\xi_n} + \frac{\omega_c^2}{2\mathrm{i}\omega_c}\coth\frac{\mathrm{i}\omega_c}{2T}\frac{1-\mathrm{e}^{-\omega_c t}}{\mathrm{i}\omega_c}) \quad (1.83)$$

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

$$K = 4\alpha(-\cot\pi N_c + \sum_{n=1}^{\infty}\frac{N_c^2}{n(N_c^2-n^2)}) \quad (1.84)$$

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

$$K \approx 4\alpha(\sum_{n=1}^{\lfloor N_c \rfloor}\frac{1}{n} - N_c^2\sum_{n=\lceil N_c \rceil}^{\infty}\frac{1}{n^3}) \quad (1.85)$$

Replacing the summations by integrations, we get

$$K \approx 4\alpha(\log N_c - N_c^2\frac{-3}{N_c^2}) = 4\alpha(\log\frac{\omega_c}{2\pi T} + 3) \quad (1.86)$$

up to corrections of order unity in the parenthesis.

1.5.4 Spontaneous decay

This model is studied in the exercises. A two-level atom is coupled to a bosonic environment within the rotating-wave approximation,

$$H_{\mathrm{int}} = \sum_k \left(g_k\sigma^\dagger a_k + g_k^* a_k^\dagger\sigma\right) \quad (1.87)$$

Since the quantum number "excitation" (see exercises) is conserved, the subspace spanned by the states by $|\mathrm{e},\mathrm{vac}\rangle$ and $|\mathrm{g},1_k\rangle$ (atom in ground state and one photon in mode k) is closed under time evolution. One can find a

closed integro-differential equation for the amplitude $c_{\rm e} = \langle {\rm e}, {\rm vac}|\psi(t)\rangle$ of the state vector and solve it with the Laplace transform. The result is a non-exponential decay. 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 $c_{\rm e}(t)$ that give interfering contributions in the backtransformation. A simple exponential decay emerges at long times when one single pole is located close to the imaginary axis (in the Laplace variable).

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. This feature has not yet been measured, 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.

1.6 Derivation of the quantum-optical master equation

Dephasing coupling. as done in the lecture.

Spontaneous emission. gives the Lindblad operator $L = \sqrt{\gamma}\,\sigma$ and an expression for the spontaneous decay rate γ that coincides with Fermi's Golden Rule.

Expression for frequency shift.

Remember coarse-grained time scale $1/\omega_A, \tau_c \ll \Delta t$: justifies the rotating-wave approximation. Consistent with an average of the microscopic atom-field dynamics over a time scale long compared to $1/\omega_A, \tau_c$ set by the free evolution. This temporal average is needed to give a positive (Lindblad) generator, see Dümcke & Spohn (1979) .

Motivation

Experimentally observed: excited states decay at some rate γ to the ground state. Evolution of population: *rate equation*

$$\begin{aligned} \dot{p}_e &= -\gamma p_e \\ \dot{p}_g &= \gamma p_e \end{aligned} \tag{1.88}$$

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

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

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

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:

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

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 perturbation theory — it allows to describe the atomic dynamics on slow 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.

1.6.1 Density matrix, interaction picture

Schrödinger equation for the atom+field density matrix

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

with the Hamiltonian

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

Atom plus laser mode: describe both by H_A.

Interaction picture: unitary transformation

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

gives Schrödinger equation

$$\frac{\mathrm{d}\tilde{\rho}}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\,[H_{\mathrm{int}}(t), \tilde{\rho}] \tag{1.89}$$

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

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

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

Formal solution to (1.89):

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

Iteration to second order:

$$\begin{aligned}\rho(t+\Delta t) &= \rho(t) + \frac{1}{\mathrm{i}\hbar}\int_t^{t+\Delta t} \mathrm{d}t_1\ [H_{\mathrm{int}}(t_1), \rho(t)] \\ &\quad - \frac{1}{\hbar^2}\int_t^{t+\Delta t} \mathrm{d}t_1 \int_t^{t_1} \mathrm{d}t_2\, [H_{\mathrm{int}}(t_1), [H_{\mathrm{int}}(t_2), \rho(t_2)]] \quad (1.90)\end{aligned}$$

1.6.2 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

  $$\rho(t) = \rho_A(t) \otimes \rho_F \quad (1.91)$$

  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

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

  The time-dependence is that of the free evolution.

Immediate consequence: the trace over the field of the first order term in (1.90) vanishes:

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

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 (1.90). 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 (1.91), 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

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

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

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

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

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

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

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

The term 1 is thus equal to

$$1: \quad C(\tau)|\mathbf{d}|^2\left(\sigma_+\sigma_-\mathrm{e}^{\mathrm{i}\omega_A\tau} + \sigma_-\sigma_+\mathrm{e}^{-\mathrm{i}\omega_A\tau}\right)\rho_A \tag{1.92}$$

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

$$\int_t^{t+\Delta t}\mathrm{d}t_1\int_t^{t_1}\mathrm{d}t_2 = \int_t^{t+\Delta t}\mathrm{d}t_1\int_0^{t_1-t}\mathrm{d}\tau = \int_0^{\Delta t}\mathrm{d}\tau\int_{t+\tau}^{t+\Delta t}\mathrm{d}t_1$$

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 1.1.

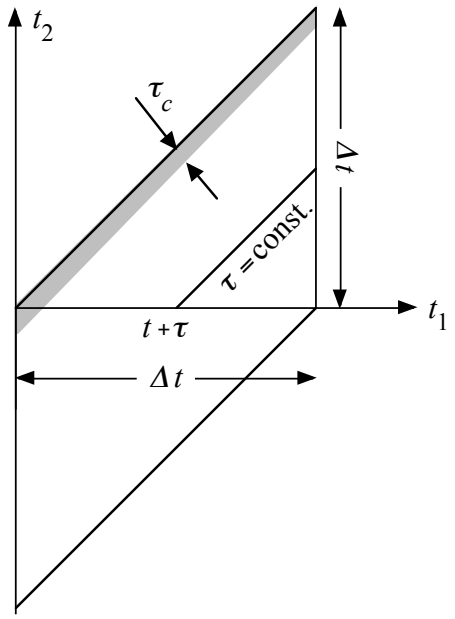


Figure 1.1: Domain of integration in the t_1, t_2-plane. Due to the short coherence time τ_c of the field, only the gray area just below the diagonal does contribute to the integral.

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. 1.1. This means that the integration limits for the t_1 integral change to

$$\int_0^{\Delta t} \mathrm{d}\tau \int_{t+\tau}^{t+\Delta t} \mathrm{d}t_1 \approx \int_0^{\Delta t} \mathrm{d}\tau \int_{t}^{t+\Delta t} \mathrm{d}t_1.$$

Since the term 1 (1.92) 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

$$\begin{aligned} 2: \qquad & -C(\tau)\left(d_i\sigma_+ \mathrm{e}^{\mathrm{i}\omega_A(t_1-\tau)} + d_i^*\sigma_- \mathrm{e}^{-\mathrm{i}\omega_A(t_1-\tau)}\right) \\ & \times\rho_A\left(d_i\sigma_+ \mathrm{e}^{\mathrm{i}\omega_A t_1} + d_i^*\sigma_- \mathrm{e}^{-\mathrm{i}\omega_A t_1}\right) \end{aligned}$$

The product gives either terms independent of t_1 or involving $\mathrm{e}^{\pm 2\mathrm{i}\omega_A t_1}$. 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:

$$2: \qquad -C(\tau)|\mathbf{d}|^2\left(\mathrm{e}^{\mathrm{i}\omega_A\tau}\sigma_-\rho_A\sigma_+ + \mathrm{e}^{-\mathrm{i}\omega_A\tau}\sigma_+\rho_A\sigma_-\right). \tag{1.93}$$

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

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

(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,

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

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

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

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

$$\Delta t \gg \tau_c : \qquad \int_0^{\Delta t} \mathrm{d}\tau\, C(\tau)\, \mathrm{e}^{\pm \mathrm{i}\omega_A \tau} = \frac{1}{2} S(\pm\omega_A) - \mathrm{i}\,\mathcal{P}\!\int \frac{\mathrm{d}\omega}{2\pi} \frac{S(\omega)}{\omega \mp \omega_A}. \quad (1.94)$$

To simplify the notation, we shall write the second term as $-\mathrm{i}R(\pm\omega_A)$.

The first and second terms are thus given by

$$\begin{aligned} 1: \quad & \tfrac{1}{2}|\mathbf{d}|^2 \left(S(\omega_A)\sigma_+\sigma_- + S(-\omega_A)\sigma_-\sigma_+\right)\rho_A \\ & -\mathrm{i}|\mathbf{d}|^2 \left(R(\omega_A)\sigma_+\sigma_- + R(-\omega_A)\sigma_-\sigma_+\right)\rho_A \qquad (1.95) \\ 2: \quad & -|\mathbf{d}|^2 \Big[\Big(\tfrac{1}{2}S(\omega_A) - \mathrm{i}R(\omega_A)\Big)\sigma_-\rho_A\sigma_+ \\ & + \Big(\tfrac{1}{2}S(-\omega_A) - \mathrm{i}R(-\omega_A)\Big)\sigma_+\rho_A\sigma_-\Big] \qquad (1.96) \end{aligned}$$

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.

1.6.3 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"

$$\frac{\Delta\rho_A}{\Delta t} = \frac{1}{\mathrm{i}\hbar}\left[H^{(2)}, \rho_A\right] + \mathcal{L}[\rho_A] \quad (1.97)$$

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

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

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 $\Delta\rho/\Delta t \mapsto \mathrm{d}\rho/\mathrm{d}t$, not making the difference between the ordinary derivative and its coarse grained average.

Level shifts

On the right hand side of the master equation (1.97), we have a "Hamiltonian-like" term that is given by

$$\begin{aligned} H^{(2)} &= -\frac{|\mathbf{d}|^2}{\hbar}\left(R(\omega_A)\sigma_+\sigma_- + R(-\omega_A)\sigma_-\sigma_+\right) \\ &= -\frac{|\mathbf{d}|^2}{\hbar}\left(R(\omega_A)|e\rangle\langle e| + R(-\omega_A)|g\rangle\langle g|\right) \end{aligned} \tag{1.98}$$

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

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

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

$$\begin{aligned} S_{ij}(\omega) &= \int \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega\tau}\langle E_i(\tau)E_j(0)\rangle \\ &= \sum_{\mathbf{k}\mu} E_k^2 \varepsilon^i_{\mathbf{k}\mu}\varepsilon^{j*}_{\mathbf{k}\mu}\underbrace{\langle a_{\mathbf{k}\mu}a^\dagger_{\mathbf{k}\mu}\rangle}_{=1}\int \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}(\omega-\omega_k)\tau} \\ &= 2\pi\sum_{\mathbf{k}\mu}\delta(\omega-\omega_k)E_k^2\varepsilon^i_{\mathbf{k}\mu}\varepsilon^{j*}_{\mathbf{k}\mu} \end{aligned} \tag{1.99}$$

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

$$\langle g|H^{(2)}|g\rangle = -\sum_{\mathbf{k}\mu}\frac{E_k^2|\mathbf{d}\cdot\boldsymbol{\varepsilon}|^2}{\hbar(\omega_k+\omega_A)}. \tag{1.100}$$

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.

For quantum optics applications, the level shift is typically taken into account when the atom is placed close to a mirror or other macroscopic

objects. The modification of the Lamb shift (the van der Waals potential) then enters the master equation as an additional potential and shifts the atomic transition frequency in a position-dependent way. (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 (1.97) 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

$$\begin{aligned} \mathcal{L}[\rho_A] &= -\frac{\gamma_e}{2}\left\{\sigma_+\sigma_-,\, \rho_A\right\} + \gamma_e \sigma_- \rho_A \sigma_+ \\ &\quad -\frac{\gamma_g}{2}\left\{\sigma_-\sigma_+,\, \rho_A\right\} + \gamma_g \sigma_+ \rho_A \sigma_- \end{aligned} \tag{1.101}$$

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

$$\gamma_{\,g}^{\,e} = \frac{|\mathbf{d}|^2}{\hbar^2} S(\pm\omega_A) \tag{1.102}$$

Note that the Liouvillian (1.101) 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

$$\begin{aligned} \dot{p}_e &= -\gamma_e p_e + \gamma_g p_g \\ \dot{p}_g &= -\gamma_g p_g + \gamma_e p_e \end{aligned} \tag{1.103}$$

We see here explicitly that the total population is conserved. We recover the rate equations (1.88) 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 (1.99):

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

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 (1.103) is attained at large times and reads

$$\begin{aligned} p_e(t\to\infty) &= \frac{\gamma_g}{\gamma_g+\gamma_e} \\ p_g(t\to\infty) &= \frac{\gamma_e}{\gamma_g+\gamma_e} \end{aligned} \tag{1.104}$$

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

$$\frac{p_e(t\to\infty)}{p_g(t\to\infty)} = \frac{\gamma_g}{\gamma_e} = \mathrm{e}^{-\hbar\omega_A/k_BT}$$

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 $\bar{n}(\omega_A)=(\mathrm{e}^{\hbar\omega_A/k_BT}-1)^{-1}$, we indeed get the Boltzmann factor:

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

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 (1.97), we get for example

$$\frac{\mathrm{d}\rho_{eg}}{\mathrm{d}t} = -\frac{\gamma_e+\gamma_g}{2}\rho_{eg} \tag{1.105}$$

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.

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 $1/\gamma_e \approx 10^{-9}\,\mathrm{s} \gg \tau_c \approx 10^{-12}\,\mathrm{s}$. 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".

1.7 Laser and micromaser

Introduction

What are the typical components of a laser[2]? Without going into details, we can identify two of them:

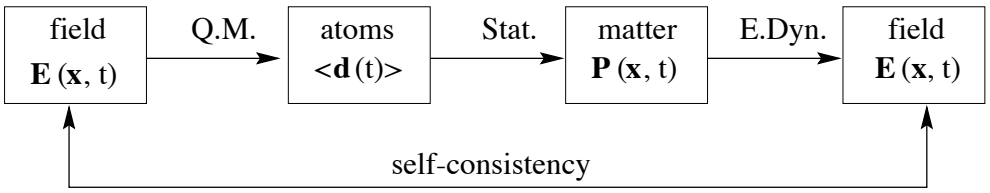
- some matter that amplifies light ("active medium");
- some device that traps the light around the space filled with the medium ("cavity")

In order to obtain an amplifying medium, one has to "pump" energy into it. The gain medium is thus a converter between the pump energy and the light emission. Quite often, the conversion efficiency is low, with values in the range 10–50% being considered "large".

The feedback mechanism is needed because the light would otherwise escape from the medium. An optical cavity like a Fabry-Pérot resonator (two mirrors) does this job because the light can travel back and forth between the mirrors a large number of times.

1.7.1 Idea of the theory

Sargent and Scully (1972) propose the following diagram that relates the different theories needed to describe a laser.



The electromagnetic field drives microscopic dipoles in the laser medium. This was the topic of the previous term. A statistical description gives, implicit in the density matrix approach we followed, links the dipoles to the macroscopic polarization of the medium [see Eq. (1.125) below]. The polarization enters the Maxwell equations for the electromagnetic field as a source and generates the field. In the end, a self-consistent

[2]Acronym of "Light Amplifier by Stimulated Emission of Radiation"

description is required: the fields at the left and right end should coincide. The condition of self-consistency allows to derive the following important quantities:

- the laser threshold,
- the laser intensity in steady state,
- the laser frequency.

This can be achieve even when one treats the field treated classically. For example, a "classical" or "coherent" field appeared via the Rabi frequency in the Bloch equations of the previous term. This approach is called "semi-classical laser theory". Note that nowhere in this approach does the word "photon" appear (if one is serious).

When a quantum-mechanical description is adopted, the photon finally comes into play and one may also derive

- the photon number probabability distribution ("photon statistics"),
- the intensity fluctuations and correlations of laser light,
- the phase fluctuations (related to the laser linewidth).

We shall illustrate this quantum theory by a calculation of the photon statistics and the laser linewidth.

We focus in these elementary considerations on a homogeneously distributed medium in the cavity made up from identical two-level systems ("homogeneous broadening"). Please refer to the experimental physics lectures for the discussion of "inhomogeneous" frequency broadening due to, for example, the atomic motion and other features.

Loss, gain, and nonlinearity. The quantum theory of a laser is a textbook example of a nonlinear problem that requires techniques from open quantum systems. The key issue is the nonlinearity in the gain of the laser medium, due to saturation, that leads to coupled nonlinear equations already at the semiclassical level. The quantum theory makes things worse by its use of non-commuting operators.

Recall that in the so-called semiclassical theory (see Sec.1.8), the following equation of motion for the intensity I the laser mode can be derived (Sargent III & Scully, 1972; Orszag, 2000):

$$\frac{\mathrm{d}I}{\mathrm{d}t} = -\kappa I + \frac{GI}{1+\beta I} \tag{1.106}$$

where κ is the loss rate, G is the linear gain, and β describes gain saturation for the laser medium. A quantum upgrade of this theory replaces the intensity by the photon number $a^\dagger a$ where the annihilation operator a describes the field amplitude of the laser mode. Mode loss is easy to handle by coupling the laser mode linearly to a mode continuum 'outside' the laser cavity (Walls & Milburn, 1994). This leads to a master equation for the density matrix in so-called Lindblad form [see Eq.(1.112)]

$$\left.\frac{\mathrm{d}\rho}{\mathrm{d}t}\right|_{\mathrm{loss}} = \kappa(L\rho L^\dagger - \tfrac{1}{2}\{L^\dagger L,\, \rho\}) \tag{1.107}$$

with a Lindblad operator $L_{\mathrm{loss}} = \sqrt{\kappa}\, a$. Linear gain can be handled in the same way, taking $L_{\mathrm{gain},0} = \sqrt{G}\, a^\dagger$, but gain saturation is more tricky. A heuristic conjecture is a Lindblad operator $L_{\mathrm{gain}} = \sqrt{G}\, a^\dagger (1+\beta a^\dagger a)^{-1/2}$. The operator ordering can only be ascertained *a posteriori*, and it is difficult to choose among the replacements $I \mapsto a^\dagger a$, $aa^\dagger$, or $\frac{1}{2}\{a^\dagger a + aa^\dagger\}$. We illustrate this difficulty in Sec.1.7.3 where the conventional quantum theory of the laser (due to Scully & Lamb) is presented.

In this section, we start with a microscopic model for the pumping process. This is motivated by experiments with so-called micromasers where a (microwave) cavity is crossed by a beam of excited two-level atoms. Nonlinear gain emerges from a treatment beyond second order in the atom-field coupling. Orszag (2000); Stenholm (1973) analyze a pumping model based on a dilute stream of excited two-level atoms that cross the laser cavity one by one and interact with the laser mode during some randomly distributed interaction time. This model can be largely handled exactly (Briegel & Englert, 1993), even in the presence of incoherent effects like cavity damping, imperfect atom preparation, and frequency-shifting collisions. The setup has become known as the 'micromaser' because of its experimental realization with a high-quality cavity (Meschede & al., 1985; Brune & al., 1987; Raizen & al., 1989). One line of research has focused

on the so-called 'strong coupling regime' that permits the laser mode to be driven into non-classical states (Weidinger & al., 1999; Varcoe & al., 2000).

We focus here on the 'weak coupling' regime. On the level of the master equation for the laser mode, this regime corresponds to a small product of coupling constant and elementary interaction time τ so that one can expand in this parameter. Mandel & Wolf (1995); Orszag (2000) consider a coupling to fourth order. For the description of a realistic experiment, one has to average the master equation with respect to a distribution of the interaction time τ (Sec. 1.7.2). It turns out, however, that the resulting master equation is not of the well-known Lindblad form, although it preserves the trace of the density matrix. This leads to conflicts with the positivity of the density operator, as is known since the original derivation of the master equation by Lindblad and by Gorini et al. (Lindblad, 1976; Gorini & al., 1976). We have shown that this problem can be cured by adding certain terms in sixth order to the master equation (Henkel, 2007). The material presented here is based on this reference. This problem provides us with an example where the Lindblad master equation can be derived from the Kraus-Stinespring representation of the finite-time evolution of the density matrix (Sec. **??**). The mathematical treatment is at the border of validity of the formal Lindblad theory since one has to deal with an infinite-dimensional Hilbert space and continuous sets of Kraus and Lindblad operators.

1.7.2 The micromaser model

Consider a two-level atom with states $|g\rangle$, $|e\rangle$ that is prepared at time t in its excited state $|e\rangle = (1,0)^T$ (density matrix $\rho_A = |e\rangle\langle e|$) and that interacts with a single mode (density matrix ρ) during a time τ. One adopts a Jaynes-Cummings-Paul Hamiltonian for the atom-field coupling

$$H_{\rm JCP} = \hbar g \left(a^\dagger \sigma + a \sigma^\dagger \right), \qquad \sigma = |g\rangle\langle e| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{1.108}$$

(this applies at resonance in a suitable interaction picture). Assume that the initial density operator of the atom+field-system factorizes into $P(t) = \rho(t) \otimes \rho_A$, compute $P(t+\tau)$ by solving the Schrödinger equation and get

the following reduced field density matrix (Orszag, 2000; Stenholm, 1973)

$$\rho(t+\tau) = \cos(g\tau\hat{\varphi})\rho(t)\cos(g\tau\hat{\varphi}) + (g\tau)^2 a^\dagger \operatorname{sinc}(g\tau\hat{\varphi})\rho(t)\operatorname{sinc}(g\tau\hat{\varphi})a \quad (1.109)$$

where $\operatorname{sinc}(x) \equiv \sin(x)/x$, and $\hat{\varphi}^2 = aa^\dagger$ is one plus the photon number operator. The operator-valued functions $\cos$ and sinc are defined by their series expansion. Only even powers of the argument occur, hence we actually never face the square root $\hat{\varphi}$ of the operator $aa^\dagger$. In the following, we abbreviate the mapping defined by Eq.(1.109) by $\mathbb{M}_\tau\rho(t)$ (this is sometimes called a superoperator).

The operation (1.109) describes an elementary 'pumping event' of the laser. We assume in the following that this event provides only a small change in the density operator, $(\mathbb{M}_\tau - \mathbb{1})\rho$ is 'small'. To provide a more realistic description, one introduces the following additional averages: excited atoms appear in the laser cavity at a rate r such that $r\tau \ll 1$. Over a time interval Δt, a number of $r\Delta t$ pumping events happens, and the accumulated change in the density operator is $\Delta\rho = r\Delta t(\mathbb{M}_\tau - \mathbb{1})\rho$. This will lead us to a differential equation when Δt is 'small enough'.

We make the additional assumption that the interaction time τ is distributed according to the probability measure $\mathrm{d}p(\tau)$ with mean value $\bar{\tau}$. This reflects the fact that atoms can cross the cavity mode with different velocities, at different positions etc. Also in a conventional laser, atoms interact with the laser mode only during some finite (and randomly distributed) time of the order of the lifetime of the excited state. Keeping the coarse-grained time step ($\Delta t \gg \bar{\tau}$), we thus get the difference equation (Orszag, 2000; Stenholm, 1973)

$$\frac{\Delta\rho}{\Delta t} = r\int \mathrm{d}p(\tau)\ (\mathbb{M}_\tau - \mathbb{1})\,\rho. \quad (1.110)$$

To simplify the superoperator appearing on the right hand side, Orszag (2000); Stenholm (1973) suggest an expansion in powers of $g\tau\hat{\varphi}$ up to the fourth order. Using an exponential distribution for $\mathrm{d}p(\tau)$, this leads to the approximate master equation

$$\begin{aligned}\frac{\mathrm{d}\rho}{\mathrm{d}t} &= G\left(a^\dagger\rho a - \tfrac{1}{2}\{aa^\dagger,\,\rho\}\right) \\ &\quad + \mathcal{B}\left(3aa^\dagger\rho aa^\dagger + \tfrac{1}{2}\{(aa^\dagger)^2,\,\rho\} - 2a^\dagger\{aa^\dagger,\,\rho\}a\right) \quad (1.111)\end{aligned}$$

where we followed the common practice of interpreting this as a differential equation. We use $\{\cdot,\cdot\}$ to denote the anticommutator. The linear gain is $G = 2r(g\bar{\tau})^2$, and $\mathcal{B} = (g\bar{\tau})^2 G$ is a measure of gain saturation. Indeed, the first line of Eq.(1.111) is in Lindblad form with $L_{\rm gain} = \sqrt{G}\, a^\dagger$ – applying this operator *increases* the photon number by one. It is easy to see that this leads, on average, to an increasing field amplitude, $(\mathrm{d}/\mathrm{d}t)\langle a\rangle_{\rm gain} = G\langle a\rangle$.

Losses from the laser mode can be included in the usual way by adding a term of the same structure as the first line of Eq.(1.111), but featuring the cavity decay rate κ, see Eq.(1.107) (Orszag, 2000; Stenholm, 1973) The same master equation as Eq.(1.111) is also found, using a different pumping model (Mandel & Wolf, 1995).

It is easy to check that Eq.(1.111) preserves the trace of ρ, using cyclic permutations. Nevertheless, it is not of the general form derived by Lindblad for master equations that preserve the complete positivity of density matrices Lindblad (1976); Gorini & al. (1976); Alicki & Lendi (1987). We shall show below [Eq.(1.118)] that Eq.(1.111) indeed leads to a density matrix with negative probabilities. Recall that the Lindblad form is given by

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \sum_\lambda \left(L_\lambda \rho L_\lambda^\dagger - \tfrac{1}{2}\left\{ L_\lambda^\dagger L_\lambda,\, \rho \right\} \right) \tag{1.112}$$

with a countable set of operators L_λ. One may think of an *ansatz* polynomial in the a and $a^\dagger$ for the L_λ, but it is difficult to see how to generate the mixed third order-first order terms $a^\dagger a a^\dagger \rho a$ in Eq.(1.111) without generating also contributions like $a^\dagger a a^\dagger \rho a a^\dagger a$. Note that this 'missing term' cannot disappear by cancellations: if we allow the L_λ operators to contain at maximum three factors of a or $a^\dagger$, then the highest order term generated by the 'sandwich' structure $L_\lambda \rho L_\lambda^\dagger$ is proportional to the squared coefficient of the highest order term of L_λ, and these terms cannot cancel out.

Of course, one can accept to work with this kind of 'post-Lindblad' master equations (as they appear frequently in the papers of Golubev and coworkers, see e.g. Golubev & Gorbachev (1986)). It is also possible to construct a set of Lindblad operators $\{L_\lambda\}$ such that adding a few additional terms to the master equation (1.111), it can be brought into the Lindblad form. For more details, see "Laser theory in manifest Lindblad form" Henkel (2007).

1.7.3 Scully-Lamb master equation

In this section, we outline a theory of the laser that starts from a quantum description of the cavity field. We still use for simplicity the single mode approximation — the basic observables are hence the annihilation and creation operators $a, a^\dagger$ for the field mode.

The laser is an *open quantum system* because energy is continuously fed into and removed from the cavity mode. We therefore have to use a density matrix description, as we did in the first part for a two-level atom. What are the "reservoirs" that the field mode is coupled to? First of all, the mode continuum outside the cavity: part of the cavity losses show up here (and permit to observe the laser dynamics). But in general, losses also occur in the material that makes up the cavity: mirrors and optical elements. We do not develop in this semester's course a detailed quantum theory of lossy optical elements (see chapter 4 of the SS 2002 version). Finally, the laser medium is also a reservoir of energy that may flow into the field mode — or not when the medium spontaneously emits photons into other modes.

In this section, we recall the master equation description for linear cavity loss and motivate the corresponding model for the gain medium. We shall derive a rate equation for the probabilities of finding n photons in the laser mode whose stationary solution gives the photon statistics. Finally, a sketch is given of the Schawlow-Townes limit for the laser linewidth.

Cavity damping

The density operator for the cavity field, $\rho(t)$, acts on the Hilbert space for the harmonic oscillator associated with the field mode. Taking the trace, we find the quantum expectation values of the quantities of interest. The average electric field, for example, is given by (we only write the positive frequency part)

$$\langle \mathbf{E}(\mathbf{x}, t) \rangle = \mathbf{e} f(\mathbf{x}) E_1 \langle a(t) \rangle = \mathbf{e} f(\mathbf{x}) E_1 \, \mathrm{tr} \, [a \, \rho(t)]$$

The trace can be performed in any basis, using photon number states or coherent states, for example. In the absence of any interaction, the Heisenberg operator a evolves freely at the frequency ω_c of the cavity. (We suppose for simplicity that this coincides with the laser frequency.)

We have seen in chap. 1 that the master equation to describe linear damping can be written in terms of Lindblad or jump operators. The one we need for cavity damping is given by $L = \sqrt{\kappa}\, a$, leading to

$$\left.\frac{\mathrm{d}\rho}{\mathrm{d}t}\right|_{\mathrm{damp}} = \kappa\, a\rho a^\dagger - \frac{\kappa}{2}\left\{a^\dagger a,\, \rho\right\}. \tag{1.113}$$

It is easy to check that the rate κ has the same meaning as in the semiclassical theory: it gives the (exponential) decay of the field's photon number if no other dynamics is present.

As an exercise, you may want to derive the rate equations for the diagonal elements $p_n(t) = \langle n|\rho(t)|n\rangle$ of the density matrix (these form the 'photon statistics'). The master equation (1.113) gives a transition rate between the photon number states $|n\rangle$ and $|n-1\rangle$ that is given by $n\kappa$, proportional to the number of photons that are presently in the cavity mode. One is tempted to interpret this as "each photon decides independently to leave the cavity." The final state is the vacuum state with zero photons — this is related to the implicit assumption that the reservoir is at zero temperature. It is a reasonable approximation at optical frequencies and room temperature.

Gain

In the previous semester, we used a model with a driven field mode where a "pump" generates a coherent state. We cannot use this model any longer because the laser medium does not provide, a priori, a fixed phase reference for the field it generates. At least the spontaneous emission of the pumped two-level atoms is "incoherent" (no fixed phase).

A suitable model for cavity gain in the linear regime is given by the jump operator $L_2 = \sqrt{G}\, a^\dagger$ and the master equation

$$\left.\frac{\mathrm{d}\rho}{\mathrm{d}t}\right|_{\mathrm{gain}} = G\, a^\dagger \rho a - \frac{G}{2}\left\{aa^\dagger,\, \rho\right\}, \tag{1.114}$$

where G is the gain rate coefficient and, up to the exchange of a and $a^\dagger$, no sign changes occur.

What about gain saturation? It is included in this theory if we allow G to depend on the instantaneous intensity of the cavity mode. The gain thus

depends on the photon number, $G = G(n)$. By analogy to the semiclassical gain, one can use the model

$$G(a^\dagger a) = \frac{G_0}{1 + Ba^\dagger a}$$

where $1/B$ plays the role of a saturation photon number. This actually leads to complications in the construction of suitable Lindblad operators. (How to take the square root here?) There are examples in textbooks that work with non-Lindblad forms and that need to be corrected afterwards to avoid unphysical results like negative probabilities.

1.7.4 Photon statistics

To start our analysis, let us compute the rate equations for the populations $p_n \equiv \rho_{nn}$ of finding n photons in the cavity mode. The sum of damping and gain gives the master equation Summarizing, we get the following master equation including damping and gain:

$$\begin{aligned}\frac{\mathrm{d}\rho}{\mathrm{d}t} = &-\mathrm{i}\omega_\mathrm{c}\left[a^\dagger a,\, \rho\right] - \frac{\kappa}{2}\left\{a^\dagger a,\, \rho\right\} + \kappa\, a\rho a^\dagger \\ &-\frac{G(a^\dagger a)}{2}\left\{aa^\dagger,\, \rho\right\} + G(a^\dagger a)\, a^\dagger \rho a. \end{aligned} \tag{1.115}$$

Taking the expectation value in the state $|n\rangle$ of the master equation (1.115), we get

$$\frac{\mathrm{d}p_n}{\mathrm{d}t} = -n\kappa\, p_n + (n+1)\kappa\, p_{n+1} - (n+1)G(n)\, p_n + nG(n-1)\, p_{n-1} \tag{1.116}$$

From the terms with a negative sign, we see that transitions leave the state $|n\rangle$ with rates $n\kappa$ and $(n+1)G(n)$. Looking at the rate equation for the state $|n-1\rangle$, we see that population from state $|n\rangle$ arrives at a rate $n\kappa$. We have thus identified a first process: the cavity field loses one photon at the rate $n\kappa$. This is the expected loss process. But there is also a transition from $|n\rangle$ to $|n+1\rangle$, occurring at a rate $(n+1)G(n)$. This is both spontaneous ("+1") and stimulated emission ("n") from the laser medium. Note that the present theory requires G to be positive (inverted medium) because transition rates are positive. The dependence of $G(n)$ on the photon number again models the gain saturation, as was the case in the semiclassical theory.

• Van Kampen's trick with the two-term recurrence relation **?**.

The transitions we have found are summarized in figure 1.2. We can

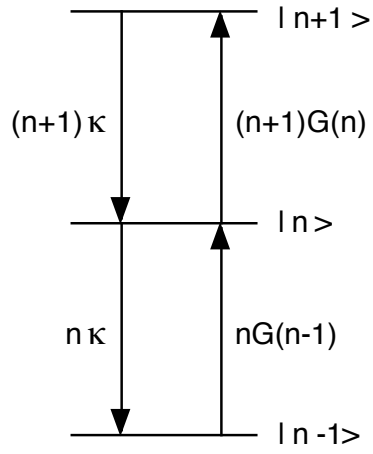


Figure 1.2: Transitions between photon number states.

now determine the stationary state of the laser. The probabilities p_n and p_{n+1}, say, then do not change with time, and therefore the probability current for the loss process $|n+1\rangle \to |n\rangle$ must be equal to the current for the emission process $|n\rangle \to |n+1\rangle$:

$$(n+1)\kappa p_{n+1} = (n+1)G(n)p_n \tag{1.117}$$

For the pair of levels $|n\rangle$ and $|n-1\rangle$, we get $n\kappa p_n = nG(n-1)p_{n-1}$ from the rate equation (1.116) which can also be found by shifting the label n in Eq.(1.117). We can check for the special case $|0\rangle \leftrightarrow |1\rangle$ that there is no saturation effect for the spontaneous emission rate into the empty cavity, which seems perfectly reasonable.[3]

We observe that the dynamic equilibrium between loss and gain processes gives a recurrence relation for the photon number probabilities in the stationary state. It is easily solved to give

$$p_{n+1} = \frac{G(n)}{\kappa}p_n \Rightarrow p_n = \mathcal{N}\prod_{m=0}^{n-1}\frac{G(m)}{\kappa} = \mathcal{N}\left(\frac{G_0}{\kappa}\right)^n \prod_{m=0}^{n-1}\frac{1}{1+Bm}, \tag{1.118}$$

[3]There are high Q cavity experiments where the field of a single photon suffices to saturate an atomic transition.

where $\mathcal{N}$ is a normalization constant. Below threshold, $G_0 < \kappa$, each of the ratios $G(n)/\kappa$ is smaller than unity, and the most probable state is the vacuum — perfectly reasonable because the laser intensity is damped away. Above threshold and for weak saturation, $G(n)/\kappa \approx G_0/\kappa > 1$, and photon numbers larger than zero are favoured. The maximum of the distribution is reached at a photon number $n_{\max}$ where $G(n_{\max})/\kappa = 1$. This equation can be solved to give

$$n_{\max} = \frac{G_0 - \kappa}{\kappa B}$$

which looks very similar to the steady state intensity of the semiclassical theory.

The photon statistics (1.118) is plotted in figure 1.3 for a laser below and above threshold. Note that below threshold, we do not have a thermal state (the probability is not an exponential $\propto \mathrm{e}^{-\beta n \hbar \omega_c}$), and that above threshold, the width of the number distribution is larger than for a coherent state with the same most probable photon number.

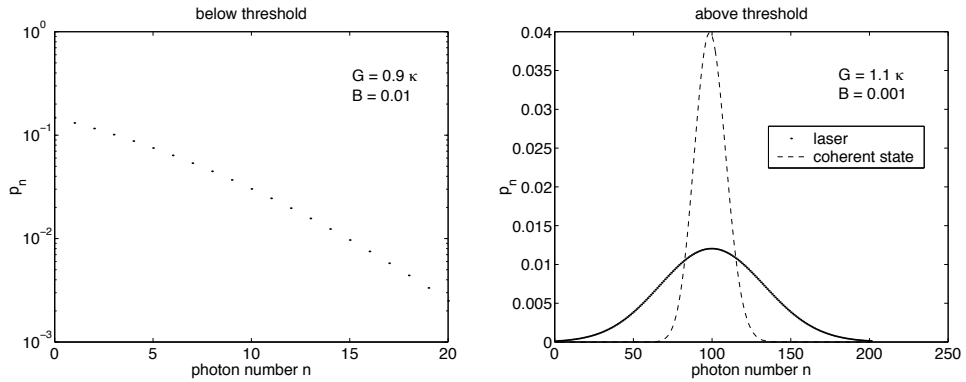


Figure 1.3: Photon statistics of a laser in steady state. Left: below threshold $G \equiv G_0 < \kappa$, right: above threshold.

As an exercise, you can use the following representation of the product in (1.118)

$$\prod_{m=0}^{n-1} \frac{1}{1+Bm} = B^{-n} \frac{\Gamma(1/B)}{\Gamma(1/B+n)}$$

where $\Gamma(\cdot)$ is now the gamma function. Using the Stirling formula for large values of n and $1/B$, show that p_n has the form of a truncated gaussian distribution and compute its width. You will find that the width approaches

that of a coherent state,

$$\Delta n^2 \to n_{\max}$$

when the laser is operating far above threshold. (This is difficult to achieve in practice, however.)

1.8 Semiclassical laser theory

We expose here, mainly for informative purposes, the so-called semiclassical theory of the laser. This section was not discussed in the SS 2010 course.

1.8.1 Wave equation for the field

We start with a reminder of the electrodynamics in a material with a given polarization. Let us recall that the polarization field enters the following Maxwell equation:

$$\frac{1}{\mu_0}\nabla \times \mathbf{B} = \mathbf{j} + \frac{\partial}{\partial t}\left(\varepsilon_0 \mathbf{E} + \mathbf{P}\right)$$

where it gives the "bound" part of the current density. We put in the following the "free" current density $\mathbf{j} = \mathbf{0}$ because we assume that the active material is globally neutral and the light only induces dipoles in it. Combining with the Faraday induction equation, $\nabla \times \mathbf{E} = -\partial_t \mathbf{B}$, one gets the wave equation for the electric field where the polarization enters as a source term:

$$\nabla \times \nabla \times \mathbf{E} + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E} = -\mu_0 \frac{\partial^2}{\partial t^2}\mathbf{P}. \tag{1.119}$$

We now make the approximation that in the cavity, a single mode is sufficient to capture the field dynamics. You have seen that one can then write for the field operator

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{e} E_1 \left[f(\mathbf{x}) a(t) + f^*(\mathbf{x}) a^\dagger(t) \right] \tag{1.120}$$

where $E_1 = (\hbar\omega_L / 2\varepsilon_0 V)^{1/2}$ is the "one-photon field amplitude", $a(t)$ is the annihilation operator for the mode (time-dependent in the Heisenberg picture), and $f(\mathbf{x})$ is the spatial mode function. It solves the homogeneous

equation

$$\nabla \times \nabla \times \mathbf{e}f - \frac{\omega_c^2}{c^2}\mathbf{e}f = \mathbf{0} \tag{1.121}$$

as you remember from the field quantization procedure. Here ω_c is one of the (empty) cavity resonance frequencies. For a planar cavity with axis along the z-direction, for example, we have

$$f(\mathbf{x}) = \sqrt{2}\sin(kz) \tag{1.122}$$

with $k = n\pi/L = \omega_c/c$ where n is a positive integer and L the cavity length. This mode function is normalized such that the integral of its square over the cavity volume V gives V. There are also lasers where propagating modes are a suitable description. In the photonics lectures, other cavity modes, including their transverse behaviour (perpendicular to the cavity axis) are introduced. For the semiclassical theory we develop here first, the product $E_1 a(t) = E(t)$ gives the (positive frequency) field amplitude. Its absolute square corresponds to the intensity, with $a^*(t)a(t)$ giving the "photon number" (although this is not required to be an integer in the semiclassical theory).

We now project the wave equation (1.119) onto the field mode $\mathbf{e}f(\mathbf{x})$. The term involving $f^*(\mathbf{x})a^\dagger(t)$ does not contribute when a propagating mode is used. We also make the approximation of slowly varying amplitudes for $E(t)$ that oscillates essentially at the frequency ω_L. The polarization field as well, $\mathbf{P}(\mathbf{x},t) = \mathbf{P}(\mathbf{x})\,\mathrm{e}^{-\mathrm{i}\omega_L t} + \mathrm{c.c.}$ This means that the time derivative of $\mathbf{P}(\mathbf{x})$ is much smaller than $\omega_L \mathbf{P}(\mathbf{x})$. (With this approximation and standing wave modes, the term $f^*(\mathbf{x})a(t)$ drops out at this point.) We get

$$\dot{E} = -\mathrm{i}(\omega_L - \omega_c)E - \frac{\kappa}{2}E + \mathrm{i}\frac{\omega_L}{2\varepsilon_0}\int \frac{\mathrm{d}^3x}{V} f^*(\mathbf{x})\mathbf{e}\cdot\mathbf{P}(\mathbf{x}), \tag{1.123}$$

where $\omega_L - \omega_c$ is the frequency detuning with respect to the cavity resonance and V the cavity volume. We have introduced the phenomenological decay rate κ for the energy of the cavity field. The quality factor of the cavity (often known experimentally) is given by $Q = \omega_c/\kappa$. Notice that the spatial integral is the overlap of the polarization field with the cavity mode. It is easy to see from this equation that the *real* part of the polarization

$\mathbf{P}$ determines a frequency shift of the laser (with respect to the cavity frequency), and that its *imaginary* part changes the energy $\propto |E|^2$ of the field. In particular, if $\mathrm{Im}\,\mathbf{P}$ is negative, the field energy increases (emission). We thus anticipate to find the absorption and emission of the medium in the imaginary part of the polarization.

1.8.2 Dipole moment and polarization

The "active medium" cavity inside the cavity that provides the polarization consists, in many cases, of a large number of atoms or molecules. These atoms are prepared in the excited state by some process that feeds energy into them ("pumping mechanism"), and then wait to release their energy in the form of photons into the cavity field. A two-level approximation for the atoms is a simple way to account for the sharp, nearly monochromatic emission spectrum of the laser. We could have used as well a harmonic oscillator[4], however, this does not reproduce some basic features of the laser like gain saturation. The quantum theory for the atom-light interaction gives us an expression for the "microscopic", average electric dipole $\langle \mathbf{d}(t) \rangle$. The polarization field is then simply the number density of these dipoles

$$\mathbf{P}(\mathbf{x}, t) = N(\mathbf{x}) \langle \mathbf{d}(t) \rangle. \tag{1.124}$$

In general, the density $N(\mathbf{x})$ is position dependent. In fact, also the induced dipole is because it involves the light field at the position $\mathbf{x}$.

The complex, slowly varying polarization field can be connected to the coherences of the density matrix in the rotating frame:

$$\begin{aligned} \mathbf{P}(\mathbf{x}, t) &= N(\mathbf{x}) \left[\langle \mathbf{d}^{(+)}(t) \rangle + \text{c.c.} \right] \\ &= N(\mathbf{x}) \mathbf{d} \left[\rho_{\text{eg}}(t) \mathrm{e}^{-\mathrm{i}\omega_L t} + \text{c.c.} \right] \end{aligned} \tag{1.125}$$

where $\mathbf{d}^{(+)}(t)$ is the positive frequency part of the atomic dipole operator, $\mathbf{d}$ is the fixed vector of dipole matrix elements and $\rho_{\text{eg}}(t)$ is the off-diagonal element ("optical coherence") of the atomic density matrix in the frame rotating at ω_L. A formula like (1.125) assumes that all dipoles in the medium are driven by a similar field and do not interact with each other. This is a

[4] This is a good model for antennas emitting at radio frequencies.

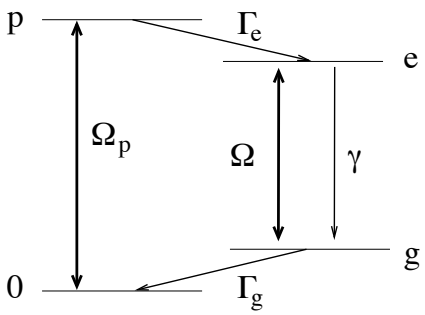


Figure 1.4: Four-level model to describe incoherent population pumping of the upper state e of the lasing transition e $\leftrightarrow$ g.

first starting point and leaves place for more elaborate theories, of course. We assume in particular that the resonance frequency is the same for all microscopic dipoles. This is not true for atoms in a (thermal) gas where the Doppler effect leads to a distribution of the resonance frequencies ("inhomogeneous broadening").

1.8.3 Dipole moment and atomic inversion

We now have to find a way to determine the dipole moment of the two-level atoms. Recall that its imaginary part is essential for light amplification. We shall see that it depends on the atomic inversion (population difference between upper and lower state). To this end, we use the optical Bloch equations for the atomic density matrix, with some modifications by adding additional energy levels. This model also provides a better understanding of the "pumping" mechanism, beyond some phenomenological rate equations. The modified two-level system is for example a four-level atom with fast relaxation in the two upper and two lower states. A simple model with four states as shown in figure 1.4 is outlined in the exercises. In this limit, the optical Bloch equations can be simplified, and one gets a justification for the often-used rate equations.

The next task is to compute the optical coherence $\rho_{\mathrm{eg}}(t)$ from the optical Bloch equations. Let us write down these equations for the two levels e and g involved in the laser transition. The rate equations for the populations ρ_{ee} and ρ_{gg} involve a pumping rate $\lambda_{\mathrm{e}} = \Gamma_{\mathrm{e}}\rho_{\mathrm{pp}}$ into the upper state (via rapid

decay from the pumped state p), the spontaneous decay rate γ and a decay rate $\Gamma_{\rm g}$ for the lower state. Including the Rabi frequency $\Omega = -(2/\hbar)\mathbf{d}\cdot\mathbf{E}$ for the laser field, as you have learned in the previous semester, this gives

$$\dot{\rho}_{\rm ee} = \lambda_{\rm e} - \gamma\rho_{\rm ee} + {\rm i}\frac{\Omega}{2}\left(\rho_{\rm eg} - \rho_{\rm ge}\right), \tag{1.126}$$

$$\dot{\rho}_{\rm gg} = \gamma\rho_{\rm ee} - \Gamma_{\rm g}\rho_{\rm gg} - {\rm i}\frac{\Omega}{2}\left(\rho_{\rm eg} - \rho_{\rm ge}\right). \tag{1.127}$$

Notice that the first equation gives an increase of the excited state population when the coherence $\rho_{\rm eg}$ has a positive imaginary part (recall that Ω is actually negative...). This is in agreement with the damping of the field energy in the wave equation derived before.

The last Bloch equation is for the coherence itself. The population decay rates γ and $\Gamma_{\rm g}$ lead to a decoherence rate $\Gamma = \frac{1}{2}(\gamma + \Gamma_{\rm g})$ as you have seen in the derivation of the Bloch equations. In the frame rotating at the laser frequency ω_L, the laser field detuning is $\Delta = \omega_L - \omega_{\rm eg}$, and we get

$$\dot{\rho}_{\rm eg} = {\rm i}\Delta\rho_{\rm eg} - \Gamma\rho_{\rm eg} + {\rm i}\frac{\Omega}{2}\left(\rho_{\rm ee} - \rho_{\rm gg}\right). \tag{1.128}$$

From this equation we learn that the optical dipole is created by the population difference (inversion) $\rho_{\rm ee} - \rho_{\rm gg}$. As discussed in the exercises, this equation can be solved approximately in the limit that the decay rate Γ is the largest time constant around (this solution also corresponds to the stationary state):

$$\rho_{\rm eg} = -\frac{\Omega/2}{\Delta + {\rm i}\Gamma}\left(\rho_{\rm ee} - \rho_{\rm gg}\right). \tag{1.129}$$

In particular, the imaginary part of the optical coherence is (we assume as usual a real Rabi frequency)

$${\rm Im}\,\rho_{\rm eg} = \frac{\Gamma\Omega/2}{\Delta^2 + \Gamma^2}\left(\rho_{\rm ee} - \rho_{\rm gg}\right).$$

Note that this expression is negative when the two-level system is inverted (upper level population $\rho_{\rm ee} > \rho_{\rm g}$), using again that actually $\Omega < 0$. This means that the medium amplifies the light via stimulated emission.

1.8.4 Medium polarization and saturation

Solving also the other Bloch equations in the stationary state, we can compute the inversion

$$\rho_{\mathrm{ee}} - \rho_{\mathrm{gg}} = \lambda_{\mathrm{e}} \left(1/\gamma - 1/\Gamma_{\mathrm{g}}\right) \frac{\Delta^2 + \Gamma^2}{\Delta^2 + \Gamma^2 + (\Gamma/\gamma)\Omega^2/2}. \tag{1.130}$$

The system is inverted when the lifetime $1/\gamma$ of the upper state exceeds the lifetime $1/\Gamma_{\mathrm{g}}$ of the lower state, which is perfectly reasonable.

The end result of the calculation is the following expression for the polarization field. We quote only the amplitude of the positive frequency component and assume that dipole moment and electric field are collinear:

$$\begin{aligned} \mathbf{P}(\mathbf{x}) &= N(\mathbf{x})(D^2/\hbar)\mathbf{e}E(\mathbf{x}) \frac{\lambda_{\mathrm{e}} \left(1/\gamma - 1/\Gamma_{\mathrm{g}}\right) (\Delta - \mathrm{i}\Gamma)}{\Delta^2 + \Gamma^2 + 2(\Gamma D^2/\gamma\hbar^2)|E(\mathbf{x})|^2} && (1.131) \\ &=: \frac{\varepsilon_0 \chi \mathbf{E}(\mathbf{x})}{1 + B|E(\mathbf{x})|^2}. && (1.132) \end{aligned}$$

In the last line, we have introduced the (linear) susceptibility χ of the laser medium and a coefficient B that takes into account the nonlinear response.

The most important result is that the imaginary part of the polarization is negative (*amplification* of the field) when the two-level system is inverted. The four-level scheme shown in fig. 1.4 is just one possibility to achieve inversion by a suitable pumping scheme. Refer to the experimental physics lectures for other, perhaps more efficient, pumping mechanisms.

The coefficient B in (1.132) describes the *saturation* of the medium: for very large laser intensity $|E|^2$, the induced polarization decreases proportional to $1/|E|$ instead of increasing. The physics behind saturation is characteristic for the two-level system: when the laser field gets extremely strong, the inversion vanishes (see Eq. (1.130)). We have already seen this behaviour when we considered Rabi oscillations with weak damping: the two-level system gets always re-excited by the laser and is finally with equal probability in the upper and lower states. For a harmonic oscillator, there is no saturation since arbitrarily high lying states can be populated.

1.8.5 Laser threshold and steady state

We now want an equation for the intensity $I(t) = |E(t)|^2$ (restoring a slow time-dependence) in the mode $\mathbf{e}f(\mathbf{x})$. To this end, we work out the spatial

overlap in Eq. (1.123) with a standing wave mode $f(\mathbf{x}) = \sqrt{2}\sin kz$:

$$\dot{E} = -\mathrm{i}(\omega_L - \omega_c)E - \frac{\kappa}{2}E + \mathrm{i}\frac{\omega_L \chi}{2}E(t)\int \frac{\mathrm{d}z}{L}\frac{2\sin^2(kz)}{1+2B|E(t)|^2\sin^2(kz)}$$

Here, L is the cavity length. The difficulty is the sine function in the denominator. In the exercises, you are asked to compute this integral analytically. Here, we adopt an approximate treatment that is also often used in the literature and assume that the saturation is weak. The denominator can then be expanded, and to first order in B, we get

$$\int \frac{\mathrm{d}z}{L} 2\sin^2(kz)\left[1 - 2B|E(t)|^2\sin^2(kz)\right] = 1 - \frac{3B}{2}|E(t)|^2$$

As an exercise, you can estimate the dimensionless quantity $B|E(t)|^2$ for typical parameter values. This result is often "resummed" to make the saturation effect more clear:

$$1 - \frac{3B}{2}|E(t)|^2 \approx \frac{1}{1+\frac{3B}{2}|E(t)|^2}$$

This procedure may seem strange, but reproduces quite well the exact result, as shown in figure 1.5.

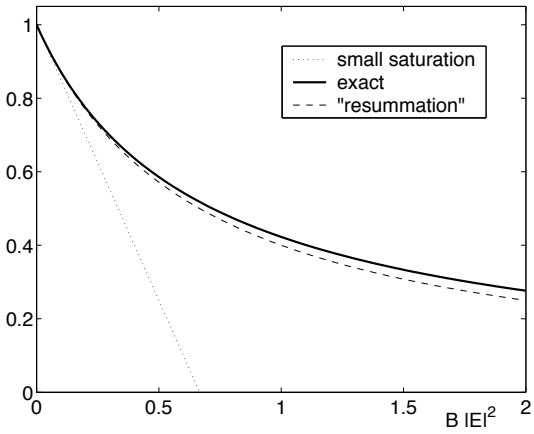


Figure 1.5: Different approximations for the gain saturation factor, integrated over the cavity mode.

The equation of motion for the intensity is now given by (for small gain saturation; check that B is real)

$$\frac{\mathrm{d}I}{\mathrm{d}t} = 2\,\mathrm{Re}\left(E^*\frac{\mathrm{d}E}{\mathrm{d}t}\right) = -\kappa I(t) - \omega_L(\mathrm{Im}\,\chi)I(t)\left[1 - (3B/2)I(t)\right]$$

This form suggests the introduction of an amplification rate ("gain") $G = -\omega_L(\mathrm{Im}\,\chi)$. Using also the conventional notation $\beta = 3GB/2$ (a rate per intensity) for the saturation coefficient, we obtain

$$\frac{\mathrm{d}I}{\mathrm{d}t} = (G - \kappa)I - \beta I^2 \tag{1.133}$$

as the fundamental equation of motion for the laser emission.

Threshold

The *laser threshold* is reached when the gain is sufficiently large to amplify the laser intensity: $G > \kappa$. In this case, stimulated emission overcomes the loss of the field due to cavity imperfections etc. If the gain is too small (or even negative), $G < \kappa$, then the field decays exponentially from its initial value. This remark points to a weakness of the semiclassical approach. It is in fact experimentally known that, once the laser is above threshold (gain exceeds loss), the laser field builds up — although one starts from an apparently empty cavity. What happens is that the spontaneous emission of the laser medium "ignites" the exponential growth of the laser field. But a model for this requires a quantum treatment of the laser, as we shall outline in the next session.

Steady state intensity

Once the laser is above threshold, the field does not grow indefinitely: the saturation of the medium, described by the coefficient β, stops the exponential growth. A steady state is reached at an intensity

$$I_{\mathrm{ss}} = \frac{G - \kappa}{\beta}.$$

This expression is valid not too far above threshold where the expansion of the saturation denominator is still accurate. Note that this increases linearly with the gain which is itself proportional to the pumping power. A typical diagram is shown in figure 1.6 where the steady state intensity is plotted vs. gain. Experimentalists often use instead of G the pump power.

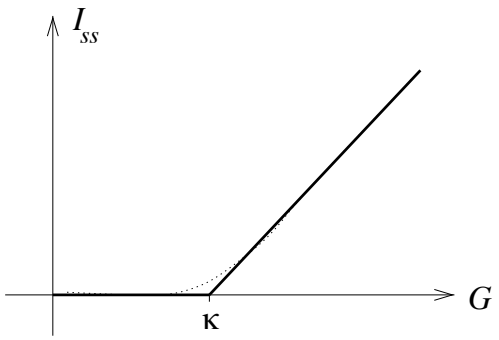


Figure 1.6: Intensity of laser emission vs. gain. The laser threshold is at $G = \kappa$ where κ is the loss rate. Solid line: semiclassical theory (1.134). The dotted line results from the quantum theory.

Phase transition analogy

To summarize, the laser intensity in steady state above and below threshold is given by

$$I_{\rm ss} = \begin{cases} 0 & \text{if } G < \kappa, \\ \dfrac{G-\kappa}{\beta} & \text{if } G > \kappa. \end{cases} \tag{1.134}$$

It has been noted that this behaviour is analogous to a phase transition: as a "control parameter" (gain, temperature) is scanned across a critical value, an "order parameter" (laser intensity, magnetization, long-range order) abruptly changes to a nonzero value. This way of thinking has been explored in depth in the school of H. Haken (Stuttgart), see, e.g., *Light*, vol. 2 (North-Holland, Amsterdam 1985), *Synergetics* (Springer, Berlin 1977), and *The Theory of Coherence, Noise and Photon Statistics of Laser Light*, chap. A3 in *Laser Handbook*, vol. 1, edited by F. T. Arecchi and E. O. Schulz-DuBois (North-Holland, Amsterdam 1972).

Other topics of semiclassical laser theory

These questions are deferred to other lectures:

- time evolution of the laser intensity ("relaxation oscillation") and chaos ("Lorenz model")

- stability analysis of the above threshold solution $I_{\rm ss} = 0$.
- inclusion of "inhomogeneous broadening" (dipoles in motion, distribution of transition frequencies, etc.)
- alternative pumping schemes (incoherent pumping, current injection and laser diodes etc.)
- multi-mode operation, frequency locking of different modes, "Q-switching" etc.

Exercises

Find reasonable values for the parameters gain G, cavity loss κ and saturation coefficient B. An often used quantity is the "saturation intensity" $I_{\rm sat} = 1/B$. It gives the typical order of magnitude for the intra-cavity field.

Compute the laser frequency shift with respect to the cavity resonance $\omega_{\rm c}$ (re-derive carefully the wave equation) and the medium resonance $\omega_{\rm eg}$.

Plot the gain spectrum (as a function of ω_L) for different laser powers $|E|^2$. At low power, you find a lorentzian whose width is given by the "dephasing rate" Γ (the relaxation rate of the optical dipole); at high power, the width increases — this is called "power broadening".

Try to solve the time-dependent nonlinear equation of motion (1.133), if nothing else works, at least numerically. How does one reach the steady state? Do the initial conditions matter?