



# **Chapter 7 (Quantum Dissipation)**

Lectures on Background to Quantum Information

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# 7. QUANTUM DISSIPATION

## 7.1 Introduction

### 7.1.1 Motivation

The goal of *dissipative quantum mechanics* or ‘quantum dissipation theory’ is to formulate microscopic theories of irreversible behaviour of quantum systems. Simply speaking, one would like to understand processes like, e.g., *friction* or ‘damping’ on a microscopic level. This requires at least two things: ‘friction’ means that physical objects interact with each other, i.e., we need to talk about interactions. Furthermore, this occurs as a function of time for systems which are usually out of equilibrium, i.e., we need to talk about dynamics.

A further, more ambitious goal is to better understand the relation between microscopic and macroscopic theories, e.g., the relation between mechanics (classical or quantum) and statistical mechanics (again classical or quantum).

Already in classical (Newtonian) mechanics, the description of irreversible behaviour is a non-trivial problem. One can often introduce dissipation into microscopic equations by adding phenomenological terms, such as the velocity-dependent damping term  $\gamma\dot{x}(t)$  ( $\gamma > 0$ ) in the damped (forced) harmonic oscillator,

$$\ddot{x}(t) + \gamma\dot{x}(t) + \omega^2x(t) = f(t). \quad (7.1)$$

In this example, one of the goals would be to derive this equation and to actually calculate  $\gamma$  from an underlying microscopic theory.

Other examples (some of these are very tough, some not so tough problems):

- What is the spontaneous photon emission rate of an atom in vacuum?
- What is the electrical resistance of a (small or large) piece of metal at very low temperatures?
- How does a Laser work?
- What is the typical time after which a given realisation of a qubit (a quantum two-level system as realised in, e.g., a linear ion trap, the charge or magnetic flux in superconducting junctions, the electron charge or spin in semiconductor quantum dots, the nuclear spin etc.) fails to operate in the desired manner?

### 7.1.2 Origin of Dissipation, System-Bath Theories

The most successful approach to quantum dissipation has been the use of *System-Bath Theories*, which will be the main topic of this chapter. The main idea is the following:

STEP 1: we divide the ‘world’ into two parts: a) the part we are really interested in (for example, all the conduction band electrons in a piece of metal), and b) the part we are not so

much interested in (for example, all the rest of the metal). This splitting obviously is a choice that depends on what we want to describe/calculate

STEP 2: Call these two parts ‘system’ and ‘reservoir’, identify the interaction between system and reservoir, and then derive an effective theory for the system only.

### Example

Single oscillator (‘system’) with angular frequency  $\omega_0$ , mass  $M$ , position  $x$ , coupled to  $N \gg 1$  oscillators (‘reservoir’)  $i = 1, \dots, N$  with angular frequencies  $\omega_i$ , masses  $m_i$ , position  $x_i$ , coupling of the form  $c_i x_i x$  via position coordinates.

Exercise: derive and solve the equations of motion a) for the *total system* (system plus reservoir) and b) for the system only.

The coupling leads to an effective dynamics of the system oscillator governed by the sum of many eigenmodes with eigenfrequencies. This sum is determined by the coupling constants  $c_i$ . For finite  $N$ , this is just a problem of coupled oscillators, and the motion of the system oscillator must therefore be periodic with a (large) period  $T$ . The time  $T$  after which the entire system returns back to its initial starting point is called *Poincaré* time.

The key point now is: 1. For times  $t \ll T$ , the effective dynamics of the system ( $x$  and  $p$  of the system oscillator) very much resembles the dynamics we would expect from a *damped* system: a sum of many oscillatory terms with ‘nearly random’ coefficients decays as a function of time  $t \ll T$ . 2. In most known cases,  $T$  is very, very large (‘larger than the age of the universe’). This means that one can safely neglect the periodic ‘Poincaré return’ of the system.

### Formal Splitting

The basic idea in microscopic theories of dissipation is a decomposition of a total system into a system  $S$  and a reservoir part  $R$  or  $B$ , ‘bath’. The (Hamiltonian) dynamics of the total system is reversible, but the dynamics of the system  $S$  is effectively not reversible for times  $t \ll T$ .

In this lecture, we formulate these ideas for quantum systems. The Hilbert space of the total system is defined by the tensor product

$$\mathcal{H}_{\text{total}} = \mathcal{H}_S \otimes \mathcal{H}_B. \quad (7.2)$$

The Hamiltonian of the total system is defined as

$$H_{\text{total}} \equiv H \equiv H_S + H_{SB} + H_B \quad (7.3)$$

Here and in the following, we will mostly discuss *time-independent* Hamiltonians. Time-dependent Hamiltonians  $H = H(t)$  can be treated as well but require additional techniques (e.g., Floquet theory for period time-dependence; adiabatic theorems for slow time-dependence).

#### 7.1.3 Overview

1. ‘Simple’ Systems with *few* degrees of freedom: typically quantum optics systems, atoms, few-level systems, cavity modes.

- Weak coupling approximation: Master Equation (Born and Markov Approximation)
- Damped harmonic oscillator.

- Solution methods: phase-space methods ( $P$ -representation etc.).
- Solution methods: quantum trajectories.
- Correlation Functions, Quantum Regression Theorem.
- Beyond weak coupling approximation: Feynman-Vernon influence functional (path integral) theories; R. P. Feynman, F. L. Vernon, *Ann. Phys. (N.Y.)* **24**, 118 (1963). Non-exponential decay laws at low temperatures.
- Exact solution of damped harmonic oscillator.
- Spin-Boson Problem, Two-Level System.
- Non-Markovian versus Markovian, Lindblad versus non-Lindblad.
- ‘Non-standard’ methods.

2. Systems with *many* degrees of freedom: typically condensed matter systems, electrons + phonons (particle statistics).

- Quasiclassical kinetic theories, Boltzmann equation.
- Quantum Many-Body Non-Equilibrium Methods. (Keldysh) Greens Function Methods, quantum Boltzmann equation.

In this chapter, we will concentrate on 1. (‘Simple’ Systems with *few* degrees of freedom). Also, not discussed in detail in this lecture are

- Nakajima-Zwanzig theories, Mori projection operator theories. These give a more formal approach towards system-bath theories.
- ‘Early approaches’ such as Wigner-Weisskopf theory of spontaneous emission.
- ...

Generally speaking, quantum dissipation can be regarded as a subfield of non-equilibrium quantum statistics/ non-equilibrium many-body theory.

#### 7.1.4 Literature

Quite a few text books are available:

H. Carmichael, ‘An Open System Approach to Quantum Optics’, Springer Lecture Notes in Physics m 18, (Berlin, Heidelberg, 1993): good introduction into Master equations, quantum trajectories, quantum optics.

D. F. Walls and G. J. Milburn, ‘Quantum Optics’, Springer (Berlin) 1994: quantum optics book; good reference book but very condensed.

U. Weiss, ‘Quantum Dissipative Systems’, World Scientific (Singapore) (1993): advanced methods (path integral) beyond Master equation approach.

H. Haug and A.-P. Jauho, ‘Quantum Kinetics in Transport and Optics of Semiconductors’, Springer 1996: non-equilibrium (Keldysh) Green’s function approach.

F. Haake, ‘Quantum Signatures of Chaos’, Springer (Berlin, Heidelberg) 2001: good chapter on dissipation.

A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, *Rev. Mod. Phys.* **59**, 1 (1987): famous review of dissipative two-level system.

## 7.2 Master Equation I: Derivation

### 7.2.1 Interaction Picture

We define an interaction picture by writing

$$H \equiv H_0 + V, \quad H_0 \equiv H_S + H_B, \quad V \equiv H_{SB} \quad (7.4)$$

with the Hamiltonian  $H_0$  describing the time evolution of the uncoupled system and bath, and the perturbation  $V$  describing the interaction  $H_{SB}$ .

We define  $\chi(t)$  as the total density matrix (system + bath) which obeys the Liouville-von-Neumann equation ,

$$\frac{d}{dt}\chi(t) = -i[H, \chi(t)] \rightsquigarrow \chi(t) = e^{-iHt}\chi(t=0)e^{iHt}, \quad (7.5)$$

where we start with the initial condition  $\chi(t=0)$  at time  $t=0$ . In the interaction picture,

$$\tilde{\chi}(t) \equiv e^{iH_0t}\chi(t)e^{-iH_0t} \quad (7.6)$$

$$\tilde{A}(t) \equiv e^{iH_0t}Ae^{-iH_0t}. \quad (7.7)$$

The equation of motion for the density operator in the interaction picture becomes

$$\begin{aligned} \frac{d}{dt}\tilde{\chi}(t) &= i[H_0, \tilde{\chi}(t)] + e^{iH_0t}\frac{d}{dt}\chi(t)e^{-iH_0t} \\ &= i[H_0, \tilde{\chi}(t)] - ie^{iH_0t}[H, \chi(t)]e^{-iH_0t} \\ &= i[H_0, \tilde{\chi}(t)] - ie^{iH_0t}[H_0 + V, \chi(t)]e^{-iH_0t} \\ &= i[H_0, \tilde{\chi}(t)] - i[H_0 + \tilde{V}(t), \tilde{\chi}(t)] \\ &= -i[\tilde{V}(t), \tilde{\chi}(t)]. \end{aligned} \quad (7.8)$$

In integral form, this can be written as

$$\tilde{\chi}(t) = \chi(t=0) - i \int_0^t dt' [\tilde{V}(t'), \tilde{\chi}(t')] \quad (7.9)$$

which we insert into Eq. (7.8) to obtain

$$\boxed{\frac{d}{dt}\tilde{\chi}(t) = -i[\tilde{V}(t), \chi(t=0)] - \int_0^t dt' [\tilde{V}(t), [\tilde{V}(t'), \tilde{\chi}(t')]]}. \quad (7.10)}$$

Up to here, everything is still exact.

### 7.2.2 Perturbation Theory in the System-Bath Coupling

#### Effective Density Matrix of the System

We wish to obtain an equation of motion for the *effective density matrix of the system* at time  $t > 0$ ,

$$\rho(t) \equiv \text{Tr}_B[\chi(t)]. \quad (7.11)$$



This object is sufficient to calculate expectation values of *system* operators  $A_S$ :

$$\begin{aligned}\langle A_S \rangle_t &\equiv \text{Tr}_{\text{total}}[\chi(t)A_S] \\ &= \text{Tr}_S [\text{Tr}_B \chi(t)] A_S = \text{Tr}_S [\rho(t)A_S].\end{aligned}\quad (7.12)$$

Now use

$$\begin{aligned}\text{Tr}_B[\tilde{\chi}(t)] &= \text{Tr}_B e^{iH_0 t} \chi(t) e^{-iH_0 t} \\ &= e^{iH_S t} (\text{Tr}_B e^{iH_B t} \chi(t) e^{-iH_B t}) e^{-iH_S t} = e^{iH_S t} \rho(t) e^{-iH_S t} \\ &\equiv \tilde{\rho}(t).\end{aligned}\quad (7.13)$$

Note that the interaction picture  $\rho(t) \leftrightarrow \tilde{\rho}(t)$  involves only the free *System* Hamiltonian  $H_S$  and not  $H_0$ ,

$$\tilde{\rho}(t) \equiv e^{iH_S t} \rho(t) e^{-iH_S t}.\quad (7.14)$$

Using

$$\tilde{A}_S(t) \equiv e^{iH_0 t} A_S e^{-iH_0 t} = e^{iH_S t} A_S e^{-iH_S t}\quad (7.15)$$

for system operators, one has

$$\langle A_S \rangle_t = \text{Tr}_S [\tilde{\rho}(t) \tilde{A}_S(t)] = \text{Tr}_S [\rho(t) A_S(t)].\quad (7.16)$$

Equation of Motion for  $\tilde{\rho}(t)$

This follows from Eq.(7.11) and (7.10) by taking the trace over the bath,

$$\boxed{\frac{d}{dt} \tilde{\rho}(t) = -i \text{Tr}_B [\tilde{V}(t), \chi(t=0)] - \int_0^t dt' \text{Tr}_B [\tilde{V}(t), [\tilde{V}(t'), \tilde{\chi}(t')]]}.\quad (7.17)$$

Assumption (factorising initial condition):

$$\begin{aligned}\chi(t=0) &= R_0 \otimes \rho(t=0) \\ R_0 &\equiv \text{Tr}_S [\chi(t=0)], \quad \rho(t=0) \equiv \text{Tr}_B [\chi(t=0)].\end{aligned}\quad (7.18)$$

This *factorisation assumption* is key to most of the results that follow. Its validity has been discussed and criticised in the past (see Weiss book for further references). Some of the issues are:

- Does the factorisation assumption only affect transient or also the long-time behaviour of the density matrix?
- Are there exactly solvable models where these issues can be clarified?

A theoretical formulation of time-evolution for arbitrary initial condition is sometimes possible: ‘preparation function’ (exact solution of dissipative quantum oscillator; Grabert, Ingold et al); generalisation of many-body Keldysh GF (three-by-three matrix instead of two-by-two matrix, M. Wagner).

## Born Approximation

In the interaction picture,

$$\tilde{\chi}(t') = R_0 \otimes \tilde{\rho}(t=0) \quad \text{to zeroth order in } V. \quad (7.19)$$

The Born approximation in the equation of motion Eq.(7.17) consists in

$$\tilde{\chi}(t') \approx R_0 \otimes \tilde{\rho}(t') \quad \text{Born approximation.} \quad (7.20)$$

This means one assumes that for all times  $t' > 0$ , the total density matrix remains a product of the initial bath density matrix  $R_0$  and the system density matrix  $\tilde{\rho}(t')$ . Intuitively, one argues that this is justified when the bath is ‘very large’ and the coupling  $H_{SB}$  ‘weak’, so that the back-action of the system onto the bath can be neglected. In practice, one usually assumes a thermal equilibrium for the bath,

$$R_0 = \frac{e^{-\beta H_B}}{\text{Tr} e^{-\beta H_B}}, \quad \text{thermal equilibrium bath,} \quad (7.21)$$

where  $\beta = 1/k_B T$  with  $T$  the bath equilibrium temperature.

**Remark:** A more detailed analysis of the Born approximation and alternative approximations can be done within the framework of the *Projection Operator formalism*.

Within the Born approximation, with Eq. (7.20), (7.18), and (7.17), one obtains a *closed integro-differential equation* for the reduced density operator  $\tilde{\rho}(t)$  of the system in the interaction picture,

$$\boxed{\begin{aligned} \frac{d}{dt} \tilde{\rho}(t) &= -i \text{Tr}_B [\tilde{V}(t), R_0 \otimes \tilde{\rho}(t=0)] \\ &- \int_0^t dt' \text{Tr}_B [\tilde{V}(t), [\tilde{V}(t'), R_0 \otimes \tilde{\rho}(t')]]. \end{aligned}} \quad (7.22)$$

**Remark:** Eq.(7.22) is exact up to second order in the perturbation  $V$ : set  $\tilde{\rho}(t') = \rho(0)$  on the r.h.s. of Eq.(7.22). Since  $\tilde{\rho}(t')$  in the double commutator on the r.h.s. of Eq.(7.22) depends on  $V$ , Eq.(7.22) is to infinite order in  $V$  though not exact. Diagrammatically this corresponds to a summation of an infinite series of diagrams. It is non-trivial to make this statement more precise, but roughly speaking these diagrams contain certain vertex corrections as can be seen from the fact that  $\rho(t)$  is a density matrix and not a wave function.

### 7.2.3 Explicit Form of Master Equation

The equation of motion Eq.(7.20) is pretty useless unless one specifies at least some more details for the interaction Hamiltonian  $V \equiv H_{SB}$ . Denoting system operators by  $S'_j$  and bath operators by  $B_k$ , the most general form of  $V$  is

$$V = \sum_{jk} c_{jk} S'_j \otimes B_k \equiv \sum_k S_k \otimes B_k, \quad (7.23)$$

where we have re-defined the sum over  $j$  as a new system operator ( $\rightarrow$  similarity to Schmidt-decomposition).

**Remark:** Note that  $S_k$  and  $B_k$  need not necessarily be hermitian. Inserting Eq.(7.23) into Eq.(7.22), we have

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}(t) &= -i \sum_k \text{Tr}_B [\tilde{S}_k(t) \tilde{B}_k(t), R_0 \rho(t=0)] \\ &- \int_0^t dt' \sum_{kl} \text{Tr}_B [\tilde{S}_k(t) \tilde{B}_k(t), [\tilde{S}_l(t') \tilde{B}_l(t'), R_0 \tilde{\rho}(t')]]. \end{aligned}$$

To simplify things, we will assume

$$\mathrm{Tr}_B \tilde{B}_k(t) R_0 = 0 \quad (7.24)$$

from now on. This is no serious restriction. We furthermore introduce the *bath correlation functions*

$$C_{kl}(t, t') \equiv \mathrm{Tr}_B \left[ \tilde{B}_k(t) \tilde{B}_l(t') R_0 \right]. \quad (7.25)$$

**Assumption 1:**

$$[R_0, H_B] = 0 \quad \text{bath in equilibrium.} \quad (7.26)$$

This means

$$C_{kl}(t, t') \equiv C_{kl}(t - t'). \quad (7.27)$$

We then have

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}(t) &= - \int_0^t dt' \sum_{kl} \left[ C_{kl}(t - t') \left\{ \tilde{S}_k(t) \tilde{S}_l(t') \tilde{\rho}(t') - \tilde{S}_l(t') \tilde{\rho}(t') \tilde{S}_k(t) \right\} \right. \\ &\quad \left. + C_{lk}(t' - t) \left\{ \tilde{\rho}(t') \tilde{S}_l(t') \tilde{S}_k(t) - \tilde{S}_k(t) \tilde{\rho}(t') \tilde{S}_l(t') \right\} \right]. \end{aligned} \quad (7.28)$$

**Assumption 2a (Markov approximation):** the bath correlation function  $C_{kl}(\tau)$  is strongly peaked around  $\tau \equiv t - t' = 0$  with a peak width  $\delta\tau \ll \gamma^{-1}$ , where  $\gamma$  is a ‘typical rate of change of  $\tilde{\rho}(t)$ .’ Note that the condition  $\delta\tau \ll \gamma^{-1}$  can only be checked *after* the equation of motion for  $\tilde{\rho}(t)$  has been solved. In the interaction picture, one then replaces  $\tilde{\rho}(t') \rightarrow \tilde{\rho}(t)$  under the integral to obtain

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}(t) &= - \int_0^t dt' \sum_{kl} \left[ C_{kl}(t - t') \left\{ \tilde{S}_k(t) \tilde{S}_l(t') \tilde{\rho}(t) - \tilde{S}_l(t') \tilde{\rho}(t) \tilde{S}_k(t) \right\} \right. \\ &\quad \left. + C_{lk}(t' - t) \left\{ \tilde{\rho}(t) \tilde{S}_l(t') \tilde{S}_k(t) - \tilde{S}_k(t) \tilde{\rho}(t) \tilde{S}_l(t') \right\} \right]. \end{aligned} \quad (7.29)$$

The important fact is that this approximation is carried out in the interaction (and not in the original Schrödinger) picture: in the interaction picture, the only relevant time-scale the change of the density matrix is  $\gamma^{-1}$  and not (the usually much faster) timescales from the free evolution with  $H_S$ . In fact, one now transforms back into the Schrödinger picture, using Eq.(7.14),

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}(t) &= i[H_S, \tilde{\rho}(t)] + e^{iH_S t} \frac{d}{dt} \rho(t) e^{-iH_S t} \\ \rightsquigarrow \frac{d}{dt} \rho(t) &= -i[H_S, \rho(t)] + e^{-iH_S t} \frac{d}{dt} \tilde{\rho}(t) e^{iH_S t} \end{aligned} \quad (7.30)$$

which leads to

$$\begin{aligned}
\rightsquigarrow \frac{d}{dt}\rho(t) &= -i[H_S, \rho(t)] \\
&- \int_0^t dt' \sum_{kl} \left[ C_{kl}(t-t') \left\{ e^{-iH_S t'} \tilde{S}_k(t) \tilde{S}_l(t') \tilde{\rho}(t) - \tilde{S}_l(t') \tilde{\rho}(t) \tilde{S}_k(t) \right\} e^{iH_S t} \right. \\
&+ \left. C_{lk}(t'-t) \left\{ e^{-iH_S t'} \tilde{\rho}(t) \tilde{S}_l(t') \tilde{S}_k(t) - \tilde{S}_k(t) \tilde{\rho}(t) \tilde{S}_l(t') \right\} e^{iH_S t} \right] \\
&= -i[H_S, \rho(t)] \\
&- \int_0^t dt' \sum_{kl} \left[ C_{kl}(t-t') \left\{ S_k \tilde{S}_l(t'-t) \rho(t) - \tilde{S}_l(t'-t) \rho(t) S_k \right\} \right. \\
&+ \left. C_{lk}(t'-t) \left\{ \rho(t) \tilde{S}_l(t'-t) S_k - S_k \rho(t) \tilde{S}_l(t'-t) \right\} \right]. \tag{7.31}
\end{aligned}$$

**Assumption 2b (Markov approximation):** the integral over  $t'$  can be carried out to  $t = \infty$ . This in fact is completely consistent with assumption 2a (see above). Defining

$$D_k \equiv \lim_{t \rightarrow \infty} \int_0^t d\tau \sum_l C_{kl}(\tau) \tilde{S}_l(-\tau), \quad E_k \equiv \lim_{t \rightarrow \infty} \int_0^t d\tau \sum_l C_{lk}(-\tau) \tilde{S}_l(-\tau), \tag{7.32}$$

we can write

$$\boxed{
\begin{aligned}
\frac{d}{dt}\rho(t) &= -i[H_S, \rho(t)] \\
&- \sum_k \left[ S_k D_k \rho(t) - D_k \rho(t) S_k + \rho(t) E_k S_k - S_k \rho(t) E_k \right].
\end{aligned}
} \tag{7.33}$$

## 7.3 Master Equation II: the Damped Harmonic Oscillator

### 7.3.1 Introduction

In the following, we will discuss two models for damped harmonic oscillators and derive the explicit forms for the corresponding Master equations.

#### Non-RWA Model

$$\begin{aligned}
H_{\text{total}} &\equiv H_S + H_{SB} + H_B \\
&= \Omega a^\dagger a + \sum_Q \gamma_Q (a_Q + a_Q^\dagger)(a + a^\dagger) + \sum_Q \omega_Q a_Q^\dagger a_Q.
\end{aligned} \tag{7.34}$$

Here,  $V \equiv H_{SB} = S \otimes B$  with  $S = a + a^\dagger$  and  $B = \sum_Q \gamma_Q (a_Q + a_Q^\dagger)$ . The indices  $k$  and  $l$  play no role here.

#### RWA-Model

$$\begin{aligned}
H_{\text{total}} &\equiv H_S + H_{SB} + H_B \\
&= \Omega a^\dagger a + \sum_Q \gamma_Q (a_Q a^\dagger + a_Q^\dagger a) + \sum_Q \omega_Q a_Q^\dagger a_Q.
\end{aligned} \tag{7.35}$$

Here,  $V \equiv H_{SB} = \sum_{i=1,2} S_i \otimes B_i$  with  $S_1 = a^\dagger$ ,  $S_2 = a$ , and  $B_1 = \sum_Q \gamma_Q a_Q$ ,  $B_2 = \sum_Q \gamma_Q a_Q^\dagger$ . The indices  $k$  and  $l$  now do play a role.

## 7.3.2 Master Equation (RWA)

We first derive the master equation for the RWA model.

## Thermal Bath Correlation Functions (RWA)

The bath correlation functions simply are

$$\begin{aligned}
C_{12}(t) &\equiv \text{Tr}_B \left[ \tilde{B}_1(t) B_2 R_0 \right] = \text{Tr}_B \left[ \sum_{QQ'} \gamma_Q \gamma_{Q'} a_Q e^{-i\omega_Q t} a_{Q'}^\dagger R_0 \right] \\
&= \sum_Q \gamma_Q^2 e^{-i\omega_Q t} (1 + n_B(\omega_Q)) = \int_0^\infty d\omega \rho(\omega) e^{-i\omega t} (1 + n_B(\omega)) \\
C_{21}(t) &\equiv \text{Tr}_B \left[ \tilde{B}_2(t) B_1 R_0 \right] = \text{Tr}_B \left[ \sum_{QQ'} \gamma_Q \gamma_{Q'} a_Q^\dagger e^{i\omega_Q t} a_{Q'} R_0 \right] \\
&= \sum_Q \gamma_Q^2 e^{i\omega_Q t} n_B(\omega_Q) = \int_0^\infty d\omega \rho(\omega) e^{i\omega t} n_B(\omega) \\
C_{11}(t) &= C_{22}(t) = 0,
\end{aligned} \tag{7.36}$$

where all the information on the microscopic coupling to the bath is now comprised within one single function, the bath *spectral density*  $\rho(\omega)$

$$\rho(\omega) \equiv \sum_Q \gamma_Q^2 \delta(\omega_Q - \omega). \tag{7.37}$$

Using  $\tilde{S}_1(t) = a^\dagger e^{i\Omega t}$ ,  $\tilde{S}_2(t) = a e^{-i\Omega t}$ , we have

$$\begin{aligned}
D_1 &\equiv \int_0^\infty d\tau C_{12}(\tau) \tilde{S}_2(-\tau) = \int_0^\infty d\tau C_{12}(\tau) a e^{i\Omega t} = \hat{C}_{12}(-i\Omega) a \\
D_2 &\equiv \int_0^\infty d\tau C_{21}(\tau) \tilde{S}_1(-\tau) = \int_0^\infty d\tau C_{21}(\tau) a^\dagger e^{-i\Omega t} = \hat{C}_{21}(i\Omega) a^\dagger \\
E_1 &\equiv \int_0^\infty d\tau C_{21}^*(\tau) \tilde{S}_2(-\tau) = \int_0^\infty d\tau C_{21}^*(\tau) a e^{i\Omega t} = [\hat{C}_{21}(i\Omega)]^* a = D_2^\dagger \\
E_2 &\equiv \int_0^\infty d\tau C_{12}^*(\tau) \tilde{S}_1(-\tau) = \int_0^\infty d\tau C_{12}^*(\tau) a^\dagger e^{-i\Omega t} = [\hat{C}_{12}(-i\Omega)]^* a^\dagger = D_1^\dagger
\end{aligned} \tag{7.38}$$

Here, we defined the Laplace transformation of a function  $f(t)$ ,

$$\hat{f}(z) = \int_0^\infty dt e^{-zt} f(t). \tag{7.39}$$

The Master equation therefore is

$$\begin{aligned}
\frac{d}{dt} \rho(t) &= -i[\Omega a^\dagger a, \rho(t)] \\
&- \sum \left\{ S_k D_k \rho(t) - D_k \rho(t) S_k + \rho(t) E_k S_k - S_k \rho(t) E_k \right\} \\
&= -i[\Omega a^\dagger a, \rho(t)] \\
&- \left\{ \left[ \hat{C}_{12}(-i\Omega) a^\dagger a + \hat{C}_{21}(i\Omega) a a^\dagger \right] \rho(t) + \rho(t) \left[ [\hat{C}_{21}(i\Omega)]^* a a^\dagger + [\hat{C}_{12}(-i\Omega)]^* a^\dagger a \right] \right. \\
&- \left. \hat{C}_{12}(-i\Omega) a \rho(t) a^\dagger - \hat{C}_{21}(i\Omega) a^\dagger \rho(t) a - [\hat{C}_{21}(i\Omega)]^* a^\dagger \rho(t) a - [\hat{C}_{12}(-i\Omega)]^* a \rho(t) a^\dagger \right\}.
\end{aligned} \tag{7.40}$$

### 7.3.3 Rates and Energy Shift (RWA)

Let us have a closer look at the expressions

$$\hat{C}_{12}(z) = \int_0^\infty d\omega \rho(\omega) [1 + n_B(\omega)] \int_0^\infty dt e^{-(z+i\omega)t}. \quad (7.41)$$

The Laplace transform exists for  $\text{Im}(z) > 0$  to ensure convergence of the integral, but in the expressions above we need  $\hat{C}_{12}(z = -i\Omega)$  etc., i.e. purely imaginary arguments! The limit  $t \rightarrow \infty$ , if explicitly written, reads

$$\hat{C}_{12}(z = -i\Omega) = \lim_{t \rightarrow \infty} \int_0^\infty d\omega \rho(\omega) [1 + n_B(\omega)] \int_0^t dt' e^{i(\Omega-\omega)t'}. \quad (7.42)$$

Now,

$$\lim_{t \rightarrow \infty} \int_0^t dt' e^{ixt'} = \lim_{t \rightarrow \infty} \left[ \frac{\sin xt}{x} + i \frac{1 - \cos xt}{x} \right] = \pi \delta(x) + iP \left( \frac{1}{x} \right), \quad (7.43)$$

where  $P$  denotes the principal value.

For the first term, we used a very useful

---

**Theorem:**

For any integrable, normalised function  $f(x)$  with  $\int_{-\infty}^\infty dx f(x) = 1$ ,

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} f\left(\frac{x}{\varepsilon}\right) = \delta(x). \quad (7.44)$$


---

Since  $\int_{-\infty}^\infty dx \sin(x)/x = \pi$ , this yields the Delta function above.

We split the two bath correlation functions into real and imaginary parts,

$$\begin{aligned} \hat{C}_{12}(-i\Omega) &\equiv \frac{1}{2}\gamma_+ + i\Delta_+, & \hat{C}_{21}(i\Omega) &\equiv \frac{1}{2}\gamma + i\Delta \\ \gamma_+ &\equiv \gamma_+(\Omega) \equiv 2\pi\rho(\Omega)[1 + n_B(\Omega)], & \gamma &\equiv \gamma(\Omega) \equiv 2\pi\rho(\Omega)n_B(\Omega) \\ \Delta_+ &\equiv P \int_0^\infty \frac{d\omega}{2\pi} \frac{\gamma_+(\omega)}{\Omega - \omega}, & \Delta &\equiv -P \int_0^\infty \frac{d\omega}{2\pi} \frac{\gamma(\omega)}{\Omega - \omega}. \end{aligned} \quad (7.45)$$

**Remarks:**

- Real and imaginary parts of the correlation functions are related to each other: Kramers-Kronig relations.
- Note the minus-sign in the definition of  $\Delta$ .

### 7.3.4 Final Form of Master Equation

Using these definitions, we can now write

$$\begin{aligned} \frac{d}{dt}\rho(t) &= -i[\Omega a^\dagger a, \rho(t)] - \frac{1}{2} \left\{ [(\gamma_+ + 2i\Delta_+)a^\dagger a + (\gamma + 2i\Delta)aa^\dagger] \rho(t) \right. \\ &\quad \left. + \rho(t) [(\gamma - 2i\Delta)aa^\dagger + (\gamma_+ - 2i\Delta_+)a^\dagger a] - 2\gamma_+ a \rho(t) a^\dagger - 2\gamma a^\dagger \rho(t) a \right\}. \end{aligned} \quad (7.46)$$

We write  $2i\Delta aa^\dagger = 2i\Delta(a^\dagger a + 1)$  and obtain

$$\begin{aligned} \frac{d}{dt}\rho(t) &= -i[(\Omega + \Delta_+ + \Delta)a^\dagger a, \rho(t)] \\ &- \frac{1}{2}\gamma_+ \left\{ a^\dagger a \rho(t) + \rho(t) a^\dagger a - 2a\rho(t)a^\dagger \right\} - \frac{1}{2}\gamma \left\{ aa^\dagger \rho(t) + \rho(t)aa^\dagger - 2a^\dagger \rho(t)a \right\}. \end{aligned} \quad (7.47)$$

This can be further re-arranged into

$$\boxed{\begin{aligned} \frac{d}{dt}\rho(t) &= -i\bar{\Omega}[a^\dagger a, \rho] - \kappa \left\{ a^\dagger a \rho + \rho a^\dagger a - 2a\rho a^\dagger \right\} \\ &- 2\kappa n_B(\Omega) \left\{ a^\dagger a \rho + \rho a a^\dagger - a\rho a^\dagger - a^\dagger \rho a \right\}, \end{aligned}} \quad (7.48)$$

where

$$\bar{\Omega} \equiv \Omega + P \int_0^\infty d\omega \frac{\rho(\omega)}{\Omega - \omega}, \quad \kappa \equiv \pi\rho(\Omega). \quad (7.49)$$

### Remarks

- This is the ‘standard’ Master equation for the damped harmonic oscillator, as discussed in many text books and used for many applications.
- Modifications appear if one uses the non-RWA model Hamiltonian instead of the RWA Hamiltonian.
- Eq.(7.48) is, of course, not exact because we have used 2nd order perturbation theory (in the system-bath coupling  $\gamma_Q$ ), and the Markov approximation.
- The oscillator energy  $\hbar\Omega$  is renormalised due to the coupling to the environment. The renormalised frequency  $\bar{\Omega}$  is *temperature independent*.
- The integral for the renormalised frequency  $\bar{\Omega}$  may diverge, depending on the form of the spectral density  $\rho(\omega)$ , Eq.(7.37), in which case this theory breaks down. We will make this statement more precise below.
- One can show that the Master equation Eq.(7.48) (and its non-RWA analogon, model 1) is indeed ‘wrong’ in the sense that there is an *exact* solution for the density operator  $\rho(t)$  within the same model, which is different from the solution of Eq.(7.48). This again will be discussed below.
- Comparing the exact  $\rho(t)$  with that obtained from Eq.(7.48), one could now discuss the ‘validity of the entire Master equation approach’. However, the damped harmonic oscillator is (with very few exceptions) the only quantum dissipative system where an exact solution exists.

#### 7.3.5 Expectation Values (RWA Model)

We would like to use our Master equation Eq.(7.48)

$$\begin{aligned} \frac{d}{dt}\rho(t) &= -i\bar{\Omega}[a^\dagger a, \rho] - \kappa \left\{ a^\dagger a \rho + \rho a^\dagger a - 2a\rho a^\dagger \right\} \\ &- 2\kappa n_B(\Omega) \left\{ a^\dagger a \rho + \rho a a^\dagger - a\rho a^\dagger - a^\dagger \rho a \right\} \end{aligned}$$

and calculate some ‘useful’ quantities as, for examples, expectation values of System (= oscillator) observables  $\hat{\theta}$ . Let us do this for the number operator,  $\hat{\theta} = \hat{n} = a^\dagger a$ . Multiplying with  $n$  and taking the trace, we obtain

$$\begin{aligned}
\frac{d}{dt}\langle n \rangle(t) &= -i\bar{\Omega}\text{Tr}\left(n[a^\dagger a, \rho]\right) - \kappa\text{Tr}\left\{a^\dagger a a^\dagger a \rho + \rho a^\dagger a a^\dagger a - 2a\rho a^\dagger a^\dagger a\right\} \\
&\quad - 2\kappa n_B(\Omega)\text{Tr}\left\{a^\dagger a a^\dagger a \rho + \rho a a^\dagger a^\dagger a - a^\dagger a a \rho a^\dagger - a^\dagger a a^\dagger \rho a\right\} \\
&= -i\bar{\Omega}\text{Tr}\left(a^\dagger a a^\dagger a \rho - a^\dagger a \rho a^\dagger a\right) - \kappa\text{Tr}\left\{2a^\dagger a a^\dagger a \rho - 2\rho a^\dagger (a a^\dagger - 1)a\right\} \\
&\quad - 2\kappa n_B(\Omega)\text{Tr}\left\{a^\dagger a a^\dagger a \rho + \rho(a^\dagger a + 1)a^\dagger a - a^\dagger(a a^\dagger - 1)a\rho - a a^\dagger a a^\dagger \rho\right\} \\
&= -2\kappa\text{Tr}\left\{\rho a^\dagger a\right\} \\
&\quad - 2\kappa n_B(\Omega)\text{Tr}\left\{a^\dagger a a^\dagger a \rho + \rho(a^\dagger a + 1)a^\dagger a - a^\dagger(a a^\dagger - 1)a\rho - (a^\dagger a + 1)(a^\dagger a + 1)\rho\right\} \\
&= -2\kappa\text{Tr}\left\{\rho a^\dagger a\right\} + 2\kappa n_B(\Omega) \\
&= -2\kappa(\langle n \rangle(t) - n_B(\Omega)). \tag{7.50}
\end{aligned}$$

This now is a simple first order differential equation which has the solution

$$\langle n \rangle(t) = \langle n \rangle(t=0)e^{-2\kappa t} + \kappa n_B(\Omega)(1 - e^{-2\kappa t}). \tag{7.51}$$

In particular, one has

$$\langle n \rangle(t \rightarrow \infty) = n_B(\Omega). \tag{7.52}$$

For large times, the occupation number is thus given by the thermal equilibrium Bose distribution, regardless of the initial condition  $\langle n \rangle(t=0)$ .

### 7.3.6 Master Equation (Non-RWA Model)

Let us re-call that now

$$\begin{aligned}
H_{\text{total}} &\equiv H_S + H_{SB} + H_B \\
&= \Omega a^\dagger a + \sum_Q \gamma_Q (a_Q + a_Q^\dagger)(a + a^\dagger) + \sum_Q \omega_Q a_Q^\dagger a_Q.
\end{aligned}$$

### 7.3.7 Thermal Bath Correlation Function (non-RWA)

In the following, we will have a closer look at the properties of bath correlation functions.

#### Definition

We first re-call the definition of the bath correlation function,

$$\begin{aligned}
C(t) &\equiv \text{Tr}_B \left[ \tilde{B}(t) B R_0 \right] = \text{Tr}_B \left[ \sum_{QQ'} \gamma_Q \gamma_{Q'} (a_Q e^{-i\omega_Q t} + a_Q^\dagger e^{i\omega_Q t})(a_{Q'} + a_{Q'}^\dagger) R_0 \right] \\
&= \sum_Q \gamma_Q^2 \left[ e^{-i\omega_Q t} (1 + n_B(\omega_Q)) + e^{i\omega_Q t} n_B(\omega_Q) \right] \\
&= \int_0^\infty d\omega \rho(\omega) \left[ e^{-i\omega t} (1 + n_B(\omega)) + e^{i\omega t} n_B(\omega) \right] = C^*(-t). \tag{7.53}
\end{aligned}$$

Furthermore,  $n_B(\omega) \equiv 1/[e^{\beta\omega} - 1]$  is the Bose function.



Bosonic Spectral Density  $\rho(\omega)$ 

All the dependence on the coupling constants  $\gamma_Q$  is encapsulated within the spectral density  $\rho(\omega)$ . The latter is often parametrised as

$$\rho(\omega) = 2\alpha\omega_c^{1-s}\omega^s e^{-\omega/\omega_c}, \quad (7.54)$$

where  $\alpha$  is the dimensionless *coupling parameter* and  $\omega_c$  is the *cutoff frequency*. Note that  $\rho(\omega)$  has the dimension  $[\omega]$  which is the reason for the pre-factor  $\omega_c^{1-s}$ . The parameter  $s$  determines the low-frequency behaviour of  $\rho(\omega)$ , and one calls couplings with

$$\begin{aligned} s < 1 & : & \text{sub-ohmic} \\ s = 1 & : & \text{ohmic} \\ s > 1 & : & \text{super-ohmic.} \end{aligned} \quad (7.55)$$

This classification has its origin in the analysis of the dissipative two-level (spin-boson) system which we will discuss below.

The case  $s = 1, \omega_c \rightarrow \infty$

$$\rho(\omega) = 2\alpha\omega \quad (7.56)$$

is called *scaling limit* of the ohmic bath and has the special property of homogeneity  $\rho(k\omega) = k\rho(\omega)$ .

Properties of  $C(t)$ 

One can write

$$C(t) = \int_0^\infty d\omega \rho(\omega) [\coth(\beta\omega/2) \cos(\omega t) - i \sin(\omega t)], \quad (7.57)$$

where we used the useful identity

$$\coth(\beta\omega/2) = 1 + 2n_B(\omega). \quad (7.58)$$

Calculation of the integral with  $\rho(\omega)$  given by Eq.(7.54) yields

$$\begin{aligned} C(t) = & 2\alpha\omega_c^{1-s}\beta^{-(s+1)} \times \\ & \Gamma(s+1) \left[ \zeta\left(s+1, \frac{1+\beta\omega_c - i\omega_c t}{\beta\omega_c}\right) + \zeta\left(s+1, \frac{1+i\omega_c t}{\beta\omega_c}\right) \right], \end{aligned} \quad (7.59)$$

where  $\Gamma$  is the Gamma function and

$$\zeta(z, u) \equiv \sum_{n=0}^{\infty} \frac{1}{(n+u)^z}, \quad u \neq 0, -1, -2, \dots \quad (7.60)$$

is the generalised Zeta function (cf. W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorem for the Special Functions of Mathematical Physics*, Springer, Berlin 1966). The zero temperature limit is obtained either from the  $\beta \rightarrow \infty$  limit of Eq.(7.59) or directly by calculating the integral,

$$C(t) = 2\alpha\omega_c^{s+1}\Gamma(s+1) (1+i\omega_c t)^{-(s+1)}. \quad (7.61)$$

### Validity of Markov Assumption

With explicit expressions like Eq. (7.59) and Eq. (7.61), one can now directly assess the validity of the Markov assumption (Assumption 2a above): ‘the bath correlation function  $C_{kl}(\tau)$  is strongly peaked around  $\tau = 0$  with a peak width  $\delta\tau \ll \gamma^{-1}$ , where  $\gamma$  is a typical rate of change of  $\tilde{\rho}(t')$ .’ For example, for  $T = 0$ ,  $\gamma = 2\pi\rho(\Omega)$ , and within the model  $\rho(\omega) = 2\alpha\omega_c^{1-s}\omega^s e^{-\omega/\omega_c}$ , Eq.(7.54), one has  $\delta\tau \sim \omega_c^{-1}$ , cf. Eq.(7.61). This would mean

$$\begin{aligned} \omega_c^{-1} 4\pi\alpha\omega_c^{1-s}\Omega^s e^{-\Omega/\omega_c} &\ll 1 \\ 4\pi\alpha(\Omega/\omega_c)^s e^{-\Omega/\omega_c} &\ll 1, \end{aligned} \quad (7.62)$$

which is fulfilled for large  $\omega_c$  ( $\Omega/\omega_c \lesssim 1$ ),  $s > 0$ , and small  $\alpha$ . The condition of small  $\alpha$  is consistent with the Born approximation (perturbation theory in the coupling to the bath).

### 7.3.8 Derivation of Master equation (non-RWA), secular approximation

We now move on to derive the Master equation for the non-RWA model. Using  $\tilde{S}(t) = ae^{-i\Omega t} + a^\dagger e^{i\Omega t}$ , we have

$$\begin{aligned} D &\equiv \int_0^\infty d\tau C(\tau) \tilde{S}(-\tau) = \int_0^\infty d\tau C(\tau) [ae^{i\Omega\tau} + a^\dagger e^{-i\Omega\tau}] \\ &= \hat{C}(-i\Omega)a + \hat{C}(i\Omega)a^\dagger \equiv c_- a + c_+ a^\dagger \\ E &\equiv \int_0^\infty d\tau C^*(\tau) \tilde{S}(-\tau) = \int_0^\infty d\tau C^*(\tau) \tilde{S}^\dagger(-\tau) = D^\dagger \\ &= c_+^* a + c_-^* a^\dagger, \end{aligned} \quad (7.63)$$

where we used the Laplace transform of  $C(\tau)$ ,

$$\hat{C}(z) \equiv \int_0^\infty d\tau e^{-z\tau} C(\tau). \quad (7.64)$$

#### ‘Secular approximation’

We note that  $\hat{C}(z) = \hat{C}_{12}(z) + \hat{C}_{21}(z)$ . In the secular approximation, one sets

$$\begin{aligned} \hat{C}_{12}(i\Omega) &\equiv \int_0^\infty d\omega \rho(\omega) e^{-i\omega t} e^{-i\Omega t} (1 + n_B(\omega)) \rightarrow 0 \\ \hat{C}_{21}(-i\Omega) &\equiv \int_0^\infty d\omega \rho(\omega) e^{i\omega t} e^{i\Omega t} n_B(\omega) \rightarrow 0. \end{aligned} \quad (7.65)$$

The real parts of  $\hat{C}_{12}(i\Omega)$  and  $\hat{C}_{21}(-i\Omega)$  are zero because  $\delta(\omega + \Omega)$  yields no contribution from the integral (remember that  $\Omega > 0$ ). This approximation therefore neglects the imaginary parts of  $\hat{C}_{12}(i\Omega)$  and  $\hat{C}_{21}(-i\Omega)$  which, however, do not lead to damping but only to a renormalisation of the system Hamiltonian  $H_S$ . For consistency, we therefore neglect the imaginary parts of  $\hat{C}_{12}(-i\Omega)$  and  $\hat{C}_{21}(i\Omega)$  as well. Therefore,

$$\begin{aligned} c_- + c_+ &\approx \frac{1}{2}(\gamma_+ + \gamma) = \pi\rho(\Omega)[1 + 2n_B(\omega)] \\ c_- - c_+ &\approx \frac{1}{2}(\gamma_+ - \gamma) = \pi\rho(\Omega). \end{aligned} \quad (7.66)$$

### $x$ - $p$ Representation

We now can write

$$D = \frac{1}{\sqrt{2}} ((c_- + c_+)x + i(c_- - c_+)p) \approx \frac{\pi\rho(\Omega)}{\sqrt{2}} \left( x \coth\left(\frac{\beta\Omega}{2}\right) + ip \right), \quad (7.67)$$

where we again used  $\coth(\beta\Omega/2) = 1 + 2n_B(\Omega)$ . Using  $E = D^\dagger$ , one obtains the *Master equation from the Non-RWA Model in secular approximation*,

$$\boxed{\begin{aligned} \frac{d}{dt}\rho &= -i[H_S, \rho] - \frac{\pi\rho(\Omega)}{2} \coth\left(\frac{\beta\Omega}{2}\right) (x^2\rho + \rho x^2 - 2x\rho x) \\ &- i\frac{\pi\rho(\Omega)}{2} (xp\rho - \rho px - p\rho x + x\rho p). \end{aligned}} \quad (7.68)$$

## 7.4 Master Equation IV: Phase Space Solution Methods

We discuss these methods here only for the Master equation of the damped harmonic oscillator in RWA,

$$\begin{aligned} \frac{d}{dt}\rho(t) &= -i\bar{\Omega}[a^\dagger a, \rho] - \kappa \left\{ a^\dagger a \rho + \rho a^\dagger a - 2a\rho a^\dagger \right\} \\ &- 2\kappa n_B(\Omega) \left\{ a^\dagger a \rho + \rho a a^\dagger - a\rho a^\dagger - a^\dagger \rho a \right\}. \end{aligned} \quad (7.69)$$

### 7.4.1 $P$ -representation

The idea here is to convert the operator equation into a partial differential equation (PDE) for the  $P$ -representation of the reduced density operator  $\rho$ .

Revision:  $P$ -representation

We recall that the  $P$ -representation of an operator  $\hat{\theta}$  was defined as (cf. 4.137)

$$\hat{\theta} = \int \frac{d^2z}{\pi} P(\hat{\theta}; z) |z\rangle\langle z|. \quad (7.70)$$

Remarks:

1. Other authors use a definition without the  $1/\pi$ .
2. Some books write  $P(z)$  (instead of  $P(\hat{\theta} = \rho; z)$ ) for the  $P$ -representation of the density operator, and use the form

$$P(z) \equiv P(z, z^*) = \text{Tr} [\rho \delta(z^* - a^\dagger) \delta(z - a)]. \quad (7.71)$$

(again multiply this by  $\pi$  to get our  $P$ ).

3. For coherent states  $\rho = |z_0\rangle\langle z_0|$ , one has  $P(z) = \pi\delta(z - z_0)$ .
4. We have the Metha-formula (4.149),

$$P(\hat{\theta}; z) = e^{|z|^2} \int \frac{d^2z'}{\pi} \langle -z' | \hat{\theta} | z' \rangle e^{|z'|^2} e^{zz'^* - z^*z'}. \quad (7.72)$$

5. The  $P$ -distribution can be highly singular. Example: number state.

## Derivation of the PDE

In order to transform the master equation, we require the  $P$ -representation of terms like  $a\rho a^\dagger$  etc. Let us start with  $a^\dagger\rho$ .

Method 1: We follow Walls/Milburn and introduce *Bargmann states*

$$||z\rangle \equiv e^{|z|^2/2}|z\rangle \equiv \sum_n \frac{z^n}{(n!)^{1/2}}|n\rangle, \quad (7.73)$$

(‘coherent states without the normalisation factor in front’). Therefore,

$$a^\dagger||z\rangle = \frac{\partial}{\partial z}||z\rangle, \quad \langle z||a = \frac{\partial}{\partial z^*}\langle z|. \quad (7.74)$$

We use this to write

$$\begin{aligned} \rho &= \int \frac{d^2z}{\pi} ||z\rangle\langle z| e^{-|z|^2} \underline{P(z)} \rightsquigarrow \\ a^\dagger\rho &= \int \frac{d^2z}{\pi} a^\dagger||z\rangle\langle z| e^{-|z|^2} P(z) = \int \frac{d^2z}{\pi} \left[ \frac{\partial}{\partial z} ||z\rangle \right] \langle z| e^{-|z|^2} P(z) \\ &= - \int \frac{d^2z}{\pi} ||z\rangle\langle z| \frac{\partial}{\partial z} e^{-zz^*} P(z) = \int \frac{d^2z}{\pi} ||z\rangle\langle z| \underline{\left( z^* - \frac{\partial}{\partial z} \right) P(z)}, \end{aligned} \quad (7.75)$$

using integration by parts,  $\frac{\partial}{\partial z}\langle z| = 0$ , and assuming the vanishing of  $P(z)$  at infinity. Comparison yields

$$a^\dagger\rho \leftrightarrow \left( z^* - \frac{\partial}{\partial z} \right) P(z). \quad (7.76)$$

Method 2: Use the Metha formula for  $\hat{\theta} = a^\dagger\rho$ ,

$$\begin{aligned} P(a^\dagger\rho; z) &= e^{|z|^2} \int \frac{d^2z'}{\pi} \langle -z'|a^\dagger\rho|z'\rangle e^{|z'|^2} e^{zz'^* - z^*z'} \\ &= e^{zz^*} \int \frac{d^2z'}{\pi} (-z'^*) \langle -z'|\rho|z'\rangle e^{|z'|^2} e^{zz'^* - z^*z'} = \\ &= \left[ -\frac{\partial}{\partial z} + z^* \right] (e^{zz^*}) \int \frac{d^2z'}{\pi} \langle -z'|\rho|z'\rangle e^{|z'|^2} e^{zz'^* - z^*z'}. \end{aligned} \quad (7.77)$$

Here, we generate  $-z'^*$  in the integral by differentiation with respect to the parameter  $z$  and subsequent compensation of the term arising from  $e^{zz^*}$ , thus arriving even faster at Eq.(7.76). Similarly,

$$\begin{aligned} P(\rho a; z) &= e^{zz^*} \int \frac{d^2z'}{\pi} \langle -z'|\rho|z'\rangle z' e^{|z'|^2} e^{zz'^* - z^*z'} = \\ &= \left[ -\frac{\partial}{\partial z^*} + z \right] (e^{zz^*}) \int \frac{d^2z'}{\pi} \langle -z'|\rho|z'\rangle e^{|z'|^2} e^{zz'^* - z^*z'}. \end{aligned} \quad (7.78)$$

For the terms  $a^\dagger a \rho$ , the first method is easier:

$$\begin{aligned}
a^\dagger a \rho &= \int \frac{d^2 z}{\pi} a^\dagger a ||z\rangle \langle z| e^{-|z|^2} P(z) = \int \frac{d^2 z}{\pi} \left[ \frac{\partial}{\partial z} ||z\rangle \right] \langle z| e^{-|z|^2} z P(z) \\
&= - \int \frac{d^2 z}{\pi} ||z\rangle \langle z| \frac{\partial}{\partial z} e^{-zz^*} z P(z) = \int \frac{d^2 z}{\pi} ||z\rangle \langle z| e^{-|z|^2} \left( z^* - \frac{\partial}{\partial z} \right) z P(z) \\
\rho a^\dagger a &= \int \frac{d^2 z}{\pi} ||z\rangle \langle z| a^\dagger a e^{-|z|^2} P(z) = \int \frac{d^2 z}{\pi} ||z\rangle \left[ \frac{\partial}{\partial z^*} \langle z| \right] e^{-|z|^2} z^* P(z) \\
&= - \int \frac{d^2 z}{\pi} ||z\rangle \langle z| \frac{\partial}{\partial z^*} e^{-zz^*} z^* P(z) = \int \frac{d^2 z}{\pi} ||z\rangle \langle z| e^{-|z|^2} \left( z - \frac{\partial}{\partial z^*} \right) z^* P(z) \\
a \rho a^\dagger &= \int \frac{d^2 z}{\pi} a ||z\rangle \langle z| a^\dagger e^{-|z|^2} P(z) = \int \frac{d^2 z}{\pi} ||z\rangle \langle z| e^{-|z|^2} z z^* P(z) \\
a^\dagger \rho a &= \int \frac{d^2 z}{\pi} \left[ \frac{\partial}{\partial z} ||z\rangle \right] \left[ \frac{\partial}{\partial z^*} \langle z| \right] e^{-|z|^2} P(z) = \int \frac{d^2 z}{\pi} ||z\rangle \langle z| \frac{\partial}{\partial z^*} \frac{\partial}{\partial z} e^{-|z|^2} P(z) \\
&= \int \frac{d^2 z}{\pi} ||z\rangle \langle z| e^{-|z|^2} \left( z - \frac{\partial}{\partial z^*} \right) \left( z^* - \frac{\partial}{\partial z} \right) P(z).
\end{aligned}$$

In particular, for the master equation we need

$$\begin{aligned}
&\left\{ a^\dagger a \rho + \rho a^\dagger a - 2a \rho a^\dagger \right\} \leftrightarrow \left\{ \left( z^* - \frac{\partial}{\partial z} \right) z + \left( z - \frac{\partial}{\partial z^*} \right) z^* - 2z z^* \right\} P(z) \\
&= - \left\{ \frac{\partial}{\partial z} z + \frac{\partial}{\partial z^*} z^* \right\} P(z) = - \left\{ z \frac{\partial}{\partial z} + z^* \frac{\partial}{\partial z^*} + 2 \right\} P(z) \\
&\left\{ a^\dagger a \rho + \rho (a^\dagger a + 1) - a \rho a^\dagger - a^\dagger \rho a \right\} \leftrightarrow \left\{ \left( z^* - \frac{\partial}{\partial z} \right) z + \left( z - \frac{\partial}{\partial z^*} \right) z^* + 1 \right. \\
&\quad \left. - z z^* - \left( z - \frac{\partial}{\partial z^*} \right) \left( z^* - \frac{\partial}{\partial z} \right) \right\} P(z) \\
&= \left\{ - \frac{\partial}{\partial z} z + z \frac{\partial}{\partial z} + 1 + \frac{\partial}{\partial z^*} \frac{\partial}{\partial z} \right\} P(z) = \frac{\partial}{\partial z^*} \frac{\partial}{\partial z} P(z) \\
&\quad [a^\dagger a, \rho] \leftrightarrow \left[ - \frac{\partial}{\partial z} z + \frac{\partial}{\partial z^*} z^* \right] P(z) = \left[ -z \frac{\partial}{\partial z} + z^* \frac{\partial}{\partial z^*} \right] P(z).
\end{aligned}$$

The whole master equation is therefore transformed into

$$\boxed{\frac{\partial}{\partial t} P(z, t) = \left\{ 2\kappa + i [\bar{\Omega} - i\kappa] z \frac{\partial}{\partial z} - i [\bar{\Omega} + i\kappa] z^* \frac{\partial}{\partial z^*} + 2\kappa n_B \frac{\partial^2}{\partial z^* \partial z} \right\} P(z, t)} \quad (7.79)$$

Here, we have explicitly indicated that the  $P$ -function depends both on  $z$  and on the time  $t$ .

**Remarks:**

- The first order derivate terms are called drift terms, the second order derivate terms diffusion term.
- This is not directly solvable by Fourier transformation:  $z, z^*$ -dependence of coefficients.
- Written in real coordinates, this has the form of a *Fokker-Planck equation*

$$\frac{\partial}{\partial t} P(\mathbf{x}) = \left( - \sum_j \frac{\partial}{\partial x_j} A_j(\mathbf{x}) + \frac{1}{2} \sum_{ij} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} D_{ij}(\mathbf{x}) \right) P(\mathbf{x}) \quad (7.80)$$

Solution of the PDE I: zero temperature  $T = 0 \rightsquigarrow n_B = 0$

In this case, we only have first order derivatives. There is a (more or less) complete theory of first order PDEs: they are solved by the method of characteristics (cf. Courant/Hilbert).

We write the PDE as

$$\left\{ \frac{\partial}{\partial t} - i [\bar{\Omega} - i\kappa] z \frac{\partial}{\partial z} + i [\bar{\Omega} + i\kappa] z^* \frac{\partial}{\partial z^*} \right\} P(z, z^*, t) = 2\kappa P(z, z^*, t) \quad (7.81)$$

and consider the function  $P(z, z^*, t)$  on *trajectories*  $z = z(t)$  and  $z^* = z^*(t)$  where  $P(z, z^*, t) = P(z(t), z^*(t), t)$ . We regard the l.h.s. of Eq.(7.81) as a total differential. Along the trajectories, the temporal change of  $P$  is

$$\begin{aligned} \frac{d}{dt} P(z(t), z^*(t), t) &= \{ \dot{z}(t) \partial_z + \dot{z}^*(t) \partial_{z^*} + \partial_t \} P(z(t), z^*(t), t) \\ &= 2\kappa P(z(t), z^*(t), t) \end{aligned} \quad (7.82)$$

Comparison yields

$$\begin{aligned} \dot{z}(t) &= -i [\bar{\Omega} - i\kappa] z(t) \rightsquigarrow z(t) = z_0 e^{-i[\bar{\Omega} - i\kappa]t} \\ \dot{z}^*(t) &= i [\bar{\Omega} + i\kappa] z^*(t) \rightsquigarrow z^*(t) = z_0^* e^{i[\bar{\Omega} + i\kappa]t}. \end{aligned} \quad (7.83)$$

On the other hand,  $\frac{d}{dt} P = 2\kappa P$  yields

$$P(z(t), z^*(t), t) = e^{2\kappa t} P_0(z_0, z_0^*). \quad (7.84)$$

Here,  $P_0$  is the initial condition for  $P$ , with  $z_0 = z(t=0)$  and  $z_0^* = z^*(t=0)$ . This looks very innocent but has a deep physical (and geometrical) meaning: we can trace back our trajectories  $z(t), z^*(t)$  to their origin  $z_0, z_0^*$ , writing

$$z_0 = z(t) e^{+i[\bar{\Omega} - i\kappa]t}, \quad z_0^* = z^*(t) e^{-i[\bar{\Omega} + i\kappa]t}. \quad (7.85)$$

We thus have expressed the initial values  $z_0, z_0^*$  in terms of the ‘final’ values  $z(t), z^*(t)$ . Insertion into Eq.(7.84) yields

$$P(z(t), z^*(t), t) = e^{2\kappa t} P_0 \left( z(t) e^{+i[\bar{\Omega} - i\kappa]t}, z^*(t) e^{-i[\bar{\Omega} + i\kappa]t} \right). \quad (7.86)$$

We now write again  $z$  and  $z^*$  instead of  $z(t), z^*(t)$ , and therefore have

$$P(z, z^*, t) = e^{2\kappa t} P_0 \left( z e^{+i[\bar{\Omega} - i\kappa]t}, z^* e^{-i[\bar{\Omega} + i\kappa]t} \right). \quad (7.87)$$

Solution of the PDE II: finite temperature  $T \geq 0 \rightsquigarrow n_B \geq 0$

Since we know the solution for  $n_B = 0$ , we perform a transformation of variables and seek the solution for  $n_B > 0$  in the form

$$P(z, z^*, t) = F(u, u^*, s), \quad u = z e^{+i[\bar{\Omega} - i\kappa]t}, u^* = z^* e^{-i[\bar{\Omega} + i\kappa]t}, s = t, \quad (7.88)$$

which leads to

$$\begin{aligned} \partial_t P &= \left( i [\bar{\Omega} - i\kappa] z e^{+i[\bar{\Omega} - i\kappa]t} \partial_u + -i [\bar{\Omega} + i\kappa] z^* e^{-i[\bar{\Omega} + i\kappa]t} \partial_{u^*} + \partial_s \right) F(u, u^*, s) \\ &= \left( i [\bar{\Omega} - i\kappa] z \partial_z - i [\bar{\Omega} + i\kappa] z^* \partial_{z^*} \right) P(z, z^*, t) + \partial_s F(u, u^*, s) \\ &\doteq \left( i [\bar{\Omega} - i\kappa] z \partial_z - i [\bar{\Omega} + i\kappa] z^* \partial_{z^*} + 2\kappa + 2\kappa n_B \partial_z \partial_{z^*} \right) P(z, z^*, t), \end{aligned} \quad (7.89)$$

where in the last line we compared with the original PDE. Therefore, one has

$$\begin{aligned}\partial_s F(u, u^*, s) &= 2\kappa F(u, u^*, s) + 2\kappa n_B \partial_z \partial_{z^*} P(z, z^*, t) \\ &= 2\kappa F(u, u^*, s) + 2\kappa n_B e^{2\kappa s} \partial_u \partial_{u^*} F(u, u^*, s),\end{aligned}\quad (7.90)$$

where we used  $\partial_z \partial_{z^*} = e^{2\kappa s} \partial_u \partial_{u^*}$ , cf. Eq.(7.88). The big advantage now is that we had got rid of the first order derivatives with the  $z, z^*$ -dependent coefficients. Eq.(7.90) is now a standard diffusion equation with time ( $s = t$ )-dependent coefficients, which can be solved by Fourier transformation:

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**Reminder:** Complex Fourier Transformation, cf (4.141)

$$\begin{aligned}\text{Fourier Trafo } \tilde{f}(w) &\equiv \int d^2 z e^{i\mathbf{z}\mathbf{w}} f(z), \quad f(z) = \int \frac{d^2 w}{(2\pi)^2} e^{-i\mathbf{z}\mathbf{w}} \tilde{f}(w) \\ \text{scalar product } \mathbf{z}\mathbf{w} &\equiv \frac{1}{2} (z w^* + z^* w) = (z_1, z_2) \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}\end{aligned}\quad (7.91)$$

**Reminder:** Gauß Integrals

$$\int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}, \quad \Re a > 0 \quad (7.92)$$

$$\int \frac{d^2 w}{(2\pi)^2} e^{-i\mathbf{z}\mathbf{w}} e^{-\frac{a}{4}\mathbf{w}\mathbf{w}} = \frac{1}{\pi a} e^{-\frac{|z|^2}{a}}. \quad (7.93)$$

---

We now Fourier-transform Eq.(7.90),  $\partial_s F = (2\kappa + 2\kappa n_B e^{2\kappa s} \partial_u \partial_{u^*}) F$ , to obtain

$$\partial_s \tilde{F}(w, w^*, s) = \left( 2\kappa + 2\kappa n_B e^{2\kappa s} \left( -\frac{1}{4} \mathbf{w}\mathbf{w} \right) \right) \tilde{F}(w, w^*, s) \quad (7.94)$$

$$\rightsquigarrow \tilde{F}(w, w^*, s) = \exp \left\{ 2\kappa s - \frac{1}{4} n_B (e^{2\kappa s} - 1) \mathbf{w}\mathbf{w} \right\} \tilde{F}(w, w^*, s=0)$$

$$\begin{aligned}\rightsquigarrow F(u, u^*, s) &= \int \frac{d^2 w}{(2\pi)^2} e^{-i\mathbf{u}\mathbf{w}} \exp \left\{ 2\kappa s - \frac{1}{4} n_B (e^{2\kappa s} - 1) \mathbf{w}\mathbf{w} \right\} \tilde{F}(w, w^*, s=0) \\ &= \int d^2 u' \int \frac{d^2 w}{(2\pi)^2} e^{-i(\mathbf{u}-\mathbf{u}')\mathbf{w}} e^{\{2\kappa s - \frac{1}{4} n_B (e^{2\kappa s} - 1) \mathbf{w}\mathbf{w}\}} F(u', u'^*, s=0) \\ &= \frac{e^{2\kappa s}}{\pi n_B (e^{2\kappa s} - 1)} \int d^2 u' \exp \left\{ -\frac{|u - u'|^2}{n_B (e^{2\kappa s} - 1)} \right\} F(u', u'^*, s=0)\end{aligned}$$

Now we remember  $u = z e^{+i[\bar{\Omega} - i\kappa]t}$ ,  $s = t$ , and write  $u' = z'$  in  $F(u', u'^*, s=0) = P(z', z'^*, t=0)$ , to find

$$\begin{aligned}P(z, z^*, t) &= \int d^2 z' \frac{1}{\pi n_B (1 - e^{2\kappa t})} \exp \left\{ -\frac{|z e^{+i[\bar{\Omega} - i\kappa]t} - z'|^2}{n_B (e^{2\kappa t} - 1)} \right\} P(z', z'^*, t=0) \\ &= \int d^2 z' \frac{1}{\pi n_B (1 - e^{-2\kappa t})} \exp \left\{ -\frac{|z - z' e^{-i[\bar{\Omega} - i\kappa]t}|^2}{n_B (1 - e^{-2\kappa t})} \right\} P(z', z'^*, t=0) \\ &\equiv \int d^2 z' G(z, z'; t) P(z', z'^*, t=0), \\ G(z, z'; t) &\equiv \frac{1}{\pi n_B (1 - e^{-2\kappa t})} \exp \left\{ -\frac{|z - z' e^{-i[\bar{\Omega} - i\kappa]t}|^2}{n_B (1 - e^{-2\kappa t})} \right\}.\end{aligned}\quad (7.95)$$

This is the solution of the *initial value problem* of the PDE: we have explicitly constructed the *propagator*  $G(z, z'; t)$  and expressed the solution of the PDE at times  $t > 0$  in terms of the *initial P-distribution*  $P(z', z'^*, t = 0)$ .

#### 7.4.2 $W$ -representation

An alternative phase-space method is to convert the operator master equation into a PDE for the Wigner function  $W(A; z)$  of an operator  $A$ . We recall Formula (4.177b) for the Wigner function of an *operator product*  $AB$ ,

$$W(AB; z) = W(A; z) \exp \left[ \frac{1}{2} \left( \overleftarrow{\partial}_z \overrightarrow{\partial}_{z^*} - \overleftarrow{\partial}_{z^*} \overrightarrow{\partial}_z \right) \right] W(B; z) \quad (7.96)$$

We obtain

$$\begin{aligned} W(a) &= z, & W(a^\dagger) &= z^* \\ W(a^\dagger a) &= z^* \left( 1 + \frac{1}{2} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) \right) z = z^* z - \frac{1}{2} \\ W(a^\dagger a \rho) &= \left( z^* z - \frac{1}{2} \right) \left( 1 + \frac{1}{2} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) + \frac{1}{8} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) \right) W(\rho) \\ &= \left( z^* z - \frac{1}{2} \right) W(\rho) + \frac{1}{2} z^* \partial_{z^*} W(\rho) - \frac{1}{2} z \partial_z W(\rho) - \frac{2}{8} \partial_z \partial_{z^*} W(\rho) \\ W(\rho a^\dagger a) &= W(\rho) \left( 1 + \frac{1}{2} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) + \frac{1}{8} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) \right) \left( z^* z - \frac{1}{2} \right) \\ &= \left( z^* z - \frac{1}{2} \right) W(\rho) - \frac{1}{2} z^* \partial_{z^*} W(\rho) + \frac{1}{2} z \partial_z W(\rho) - \frac{2}{8} \partial_z \partial_{z^*} W(\rho) \end{aligned} \quad (7.97)$$

Similarly,

$$\begin{aligned} W(a \rho) &= z \left( 1 + \frac{1}{2} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) \right) W(\rho) = z W(\rho) + \frac{1}{2} \partial_{z^*} W(\rho) \\ W(a \rho a^\dagger) &= \left( z W(\rho) + \frac{1}{2} \partial_{z^*} W(\rho) \right) \left( 1 + \frac{1}{2} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) \right) z^* \\ &= \left( z z^* W(\rho) + \frac{1}{2} z^* \partial_{z^*} W(\rho) \right) + \frac{1}{2} \partial_z (z W(\rho)) + \frac{1}{4} \partial_z \partial_{z^*} W(\rho) \\ W(a^\dagger \rho) &= z^* \left( 1 + \frac{1}{2} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) \right) W(\rho) = z^* W(\rho) - \frac{1}{2} \partial_z W(\rho) \\ W(a^\dagger \rho a) &= \left( z^* W(\rho) - \frac{1}{2} \partial_z W(\rho) \right) \left( 1 + \frac{1}{2} (\partial_z \partial_{z^*} - \partial_{z^*} \partial_z) \right) z \\ &= \left( z z^* W(\rho) - \frac{1}{2} z \partial_z W(\rho) \right) - \frac{1}{2} \partial_{z^*} (z^* W(\rho)) + \frac{1}{4} \partial_z \partial_{z^*} W(\rho) \end{aligned} \quad (7.98)$$

Thus,

$$\begin{aligned} \{a^\dagger a \rho + \rho a^\dagger a - 2a \rho a^\dagger\} &\leftrightarrow -\{2 + z \partial_z + z^* \partial_{z^*} + \partial_z \partial_{z^*}\} W(\rho) \\ \{a^\dagger a \rho + \rho (a^\dagger a + 1) - a \rho a^\dagger - a^\dagger \rho a\} &\leftrightarrow -\partial_z \partial_{z^*} W(\rho) \\ [a^\dagger a, \rho] &\leftrightarrow (z^* \partial_{z^*} - z \partial_z) W(\rho). \end{aligned} \quad (7.99)$$



Therefore, the master equation Eq.(7.69) is converted into

$$\begin{aligned} \frac{\partial}{\partial t} W(z, t) &= -i\bar{\Omega} (z^* \partial_{z^*} - z \partial_z) W(z, t) + \kappa \left\{ 2 + z \partial_z + z^* \partial_{z^*} + \partial_z \partial_{z^*} \right\} W(z, t) \\ &\quad + 2\kappa n_B(\Omega) \partial_z \partial_{z^*} W(z, t) \\ &= \left\{ 2\kappa + i [\bar{\Omega} - i\kappa] z \frac{\partial}{\partial z} - i [\bar{\Omega} + i\kappa] z^* \frac{\partial}{\partial z^*} + \kappa [1 + 2n_B] \frac{\partial^2}{\partial z^* \partial z} \right\} W(z, t). \end{aligned} \quad (7.100)$$

We compare this with the PDE for the  $P$ -function, Eq.(7.79):

$$\frac{\partial}{\partial t} P(z, t) = \left\{ 2\kappa + i [\bar{\Omega} - i\kappa] z \frac{\partial}{\partial z} - i [\bar{\Omega} + i\kappa] z^* \frac{\partial}{\partial z^*} + 2\kappa n_B \frac{\partial^2}{\partial z^* \partial z} \right\} P(z, t)$$

The difference is just in the diffusion term, i.e.,  $1 + 2n_B$  in the Wigner representation instead of  $2n_B$  in the  $P$  representation. In the Wigner representation, even at zero temperature  $T = 0$  ( $n_B = 0$ ) one has a diffusion term in the PDE. Technically, the solution proceeds as before: one first solves the first order part via characteristics and then the diffusive part via Fourier transformation.

- A similar derivation can be done for the  $Q$ -representation, cf. Walls/Milburn. The  $Q$ -representation is more convenient for systems where the initial oscillator state is squeezed, or the decay is into a bath not in thermal equilibrium but in a squeezed state.

### 7.4.3 Remarks

Phase space methods are powerful tools for solving Master equations. The resulting PDEs, however, are often non-trivial and cannot be solved exactly. This is particularly true if more than one degree of freedom is involved and one has to solve *systems of PDEs*.

Systems of partial differential equations are really complicated beasts: in contrast to systems of ordinary differential equations, they are not equivalent to a single PDE of higher order, cf. the discussion in Courant/Hilbert ‘Methoden der Mathematischen Physik’.

Related problems occur in the theory of the Laser, where one has to deal with PDEs containing derivatives up to infinite order. This is discussed in the book by Scully/Lamb. Another, very recent challenge are systems of Master equations with non-linear couplings between bosonic and electronic degrees of freedom in *nano-electromechanical systems*.

## 7.5 Correlation Functions and the Quantum Regression Theorem

### 7.5.1 Correlation Functions

Correlation functions are important since they can tell us a lot about the dynamics of dissipative systems. Moreover, they are often directly related to experimentally accessible quantities, such as photon or electron *noise*. In quantum optics, *fluctuations* of the photon field are expressed by correlations functions such as  $g^{(1)}(\tau)$  and  $g^{(2)}(\tau)$ .

We would like to calculate the correlation function of two *system* operators  $A$  and  $B$ ,

$$\boxed{C_{BA}(t, \tau) \equiv \langle B(t)A(t + \tau) \rangle \equiv \text{Tr}_{\text{total}} (\chi(0)B(t)A(t + \tau)), \quad \tau > 0.} \quad (7.101)$$

We insert the time evolution of the operators,

$$\chi(t) = e^{-iHt} \chi(0) e^{iHt}, \quad B(t) = e^{iHt} B e^{-iHt}, \quad A(t + \tau) = e^{iH(t+\tau)} A e^{-iH(t+\tau)} \quad (7.102)$$

to find

$$\begin{aligned} C_{BA}(t, \tau) &= \text{Tr}_{\text{total}} (\chi(0) B(t) A(t + \tau)) \\ &= \text{Tr}_{\text{total}} (e^{iHt} \chi(t) B e^{-iHt} e^{iH(t+\tau)} A e^{-iH(t+\tau)}) \\ &= \text{Tr}_{\text{total}} (e^{-iH\tau} \underline{\chi(t)} B e^{iH\tau} A) \\ &= \text{Tr}_{\text{total}} (e^{-iH\tau} \underline{\rho(t)} R_0 B e^{iH\tau} A) \quad \text{Born Approximation} \\ &\equiv \text{Tr}_S \left( A \text{Tr}_{\text{Bath}} \left\{ e^{-iH\tau} \underline{\underline{\rho(t)}} B R_0 e^{iH\tau} \right\} \right) \\ &\equiv \text{Tr}_S \left( A \text{Tr}_{\text{Bath}} \left\{ e^{-iH\tau} \underline{\underline{\rho_{B;t}}} R_0 e^{iH\tau} \right\} \right) \\ &\equiv \text{Tr}_S (A \rho_{B;t}(\tau)). \end{aligned} \quad (7.103)$$

The correlation function can therefore be written as an expectation value of  $A$  with a ‘modified system density matrix’  $\rho_{B;t}(\tau)$  which starts at  $\tau = 0$  as  $\rho_{B;t}(\tau = 0) = \rho(t)B$  and evolves as a function of time  $\tau > 0$ .

For the time-evolution of a *system* operator  $\hat{O}$  according to

$$\hat{O}(\tau) \equiv \text{Tr}_{\text{Bath}} \left\{ e^{-iH\tau} \hat{O} R_0 e^{iH\tau} \right\}, \quad (7.104)$$

we can write a formal operator equation

$$\frac{d}{d\tau} \hat{O}(\tau) \equiv \mathcal{L}_\tau \hat{O}(\tau), \quad (7.105)$$

where we introduced the *super-operator*  $\mathcal{L}_\tau$ .

Example: Master equation for  $\hat{O} = \rho(0)$  in Born and Markov approximation, cf. Eq.(7.33)

$$\begin{aligned} \frac{d}{dt} \rho(t) &= -i[H_S, \rho(t)] \\ &- \sum_k \left[ S_k D_k \rho(t) - D_k \rho(t) S_k + \rho(t) E_k S_k - S_k \rho(t) E_k \right]. \end{aligned}$$

It is important to realise that  $\mathcal{L}_\tau$  is a linear operator. We now assume that the system has a basis of kets  $\{|\alpha\rangle\}$  and express the linearity of  $\mathcal{L}_\tau$  by writing the matrix elements of  $\mathcal{L}_\tau \hat{O}(\tau)$ ,

$$\langle \alpha | \mathcal{L}_\tau \hat{O}(\tau) | \beta \rangle = \sum_{\gamma\delta} \int_0^\tau d\tau' M_{\gamma\delta}^{\alpha\beta}(\tau, \tau') \langle \gamma | \hat{O}(\tau') | \delta \rangle. \quad (7.106)$$

with a time-dependent *memory kernel* as a fourth-order tensor  $M(\tau, \tau')$  that relates the matrix elements of the system operator  $\hat{O}$  at earlier times to its matrix elements of the (time-evolved) system operator at later times.

Using now  $A = |\beta\rangle\langle\alpha|$  in  $C_{BA}$ , we have

$$\begin{aligned}
C_{B,|\beta\rangle\langle\alpha|}(t, \tau) &= \langle\alpha|\rho_{B;t}(\tau)|\beta\rangle, \\
\frac{d}{d\tau}C_{B,|\beta\rangle\langle\alpha|}(t, \tau) &= \frac{d}{d\tau}\langle\alpha|\rho_{B;t}(\tau)|\beta\rangle = \langle\alpha|\mathcal{L}_\tau\rho_{B;t}(\tau)|\beta\rangle \\
&= \sum_{\gamma\delta} \int_0^\tau d\tau' M_{\gamma\delta}^{\alpha\beta}(\tau, \tau') \langle\gamma|\rho_{B;t}(\tau')|\delta\rangle \\
&= \sum_{\gamma\delta} \int_0^\tau d\tau' M_{\gamma\delta}^{\alpha\beta}(\tau, \tau') C_{B,|\delta\rangle\langle\gamma|}(t, \tau')
\end{aligned} \tag{7.107}$$

Introducing

$$\begin{aligned}
k &\equiv (\alpha\beta), & l &\equiv (\gamma\delta) \\
A_k &\equiv |\beta\rangle\langle\alpha|, & M_{\gamma\delta}^{\alpha\beta}(\tau, \tau') &\equiv M_{kl}(\tau, \tau'),
\end{aligned} \tag{7.108}$$

we convert the tensor equation into a vector equation,

$$\frac{d}{d\tau}C_{B,A_k}(t, \tau) = \sum_l \int_0^\tau d\tau' M_{kl}(\tau, \tau') C_{B,A_l}(t, \tau') \tag{7.109}$$

which can be written in compact form using the *vector of operators*,

$$\mathbf{A} \equiv \begin{pmatrix} A_1 \\ A_2 \\ \dots \\ A_k \\ \dots \end{pmatrix}. \tag{7.110}$$

In vector and matrix notation, we thus obtain the *quantum regression theorem*,

$$\boxed{\frac{d}{d\tau}\langle B(t)\mathbf{A}(t+\tau)\rangle = \int_0^\tau d\tau' \underline{\underline{M}}(\tau, \tau') \langle B(t)\mathbf{A}(t+\tau')\rangle, \quad \tau > 0.} \tag{7.111}$$

**Remarks:**

- We have not made use of the *Markov* approximation here.
- Within the Markov approximation (assumptions 2a and 2b), one has a simple differential (tensor) equation instead of an integro-differential (tensor) equation:

$$\begin{aligned}
\langle\alpha|\mathcal{L}_\tau\hat{O}(\tau)|\beta\rangle &= \sum_{\gamma\delta} M_{\gamma\delta}^{\alpha\beta} \langle\gamma|\hat{O}(\tau)|\delta\rangle \\
\rightsquigarrow \frac{d}{d\tau}\langle B(t)\mathbf{A}(t+\tau)\rangle &= \underline{\underline{M}}\langle B(t)\mathbf{A}(t+\tau')\rangle, \quad \tau > 0.
\end{aligned} \tag{7.112}$$

This is the usual form of the quantum regression theorem as discussed in many textbooks.

- For  $\tau < 0$ , the derivation of the quantum regression theorem is analogous to the case  $\tau > 0$  (exercise!)
- The first derivation of the quantum regression theorem has been given by Melvin Lax, Phys. Rev. **129**, 2342 (1963). He emphasises that the only approximation one needs is the factorisation (in our notation  $\chi(t) = \rho(t)R_0$ , Born approximation). In the ‘Note added in proof’ in his paper he states that the derivation therefore is correct even for non-Markoffian systems.

## 7.6 The Two-Level System I

### 7.6.1 Generic Model: Two-Level System Interacting with Bosonic Modes

#### System

Assume a system with Hilbert space  $\mathcal{H} = C^2$  with basis vectors  $(1, 0)^\dagger$  and  $(0, 1)^\dagger$ . In general, a ‘System’-Hamiltonian will have the form of the Hamiltonian of a *Pseudo Spin*  $\frac{1}{2}$  in a (time-dependent) *classical pseudo magnetic field*  $\mathbf{B}(t)$  (c-number),

$$H_S(t) \equiv \mathbf{B}(t)\vec{\sigma}, \quad \vec{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}. \quad (7.113)$$

- Note that for a time-dependent  $\mathbf{B}(t)$ , the free Schrödinger equation with  $H_S(t)$  only is in general not analytically solvable. For an isolated two-level system ( $H_S(t)$  only), this is not a problem because one can easily solve a two-by-two differential equation on a computer. However, problems start when it comes to system-bath Hamiltonians. Many of the ‘simpler’ system bath theories implicitly assume that the time-evolution under  $H_s$  is trivial (which it is for constant  $\mathbf{B}(t) = \mathbf{B}$ ).
- Some special cases are analytically solvable: Landau-Zener-Rosen tunneling (Landau 1932).
- For a periodic time-dependence of  $\mathbf{B}(t)$ : Floquet theory (Shirley 1965).
- The wave function can acquire a geometrical phase (Berry phase, Berry 1984).

#### System-Bath Interaction

Assume a ‘bath’ of bosonic modes  $Q$  (the index  $Q$  contains all quantum numbers of that mode) with creation operator  $a_Q^\dagger$ . The simplest interaction between the two-level system and the bath is *linear* in  $a_Q^\dagger$  and  $a_Q$  and can be written with coupling constant vectors  $\mathbf{g}_Q(t)$ ,

$$H_{SB}(t) \equiv \hat{\mathbf{A}}(t)\vec{\sigma} \equiv \sum_Q \left( \mathbf{g}_Q(t)a_Q^\dagger + \mathbf{g}_Q^\dagger(t)a_Q \right) \vec{\sigma}. \quad (7.114)$$

Note that  $\hat{\mathbf{A}}(t)$  can be regarded as a *fluctuating (quantum operator) pseudo magnetic field*.

#### Bath

The simplest Hamiltonian for a bosonic bath is

$$H_B = \sum_Q \omega_Q a_Q^\dagger a_Q. \quad (7.115)$$

- Example: free photons,  $\omega_Q = c|Q|$ .
- Example: phonons in crystals. However, more realistic Hamiltonians would contain phonon-phonon interaction. In particular, in order to explain the thermal expansion of materials one needs boson-boson interaction ( $\rightsquigarrow$  ‘Grüneisen parameter’), cf. N. W. Ashcroft and N. D. Mermin, ‘*Solid State Physics*’, Saunders College (Philadelphia, 1976).

- Photonic or phononic crystals or cavities have more complicated bandstructures and nontrivial dispersion relations  $\omega = \omega_Q$ . Example: Phonon cavities in 2-dimensional thin elastic plate, Rayleigh-Lamb waves; cf. L. D. Landau and E. M. Lifshitz, ‘*Theory of Elasticity*’, Vol. 7 of Landau and Lifshitz, Course of Theoretical Physics (Pergamon Press, 1970); B. Auld, ‘*Acoustic Fields and Waves*’, (Wiley, New York, 1973).

### Further Remarks

1. Coupling to non-bosonic baths: this is a relatively unexplored field. The most prominent examples are *spin-baths*, where the system is coupled to a collection of spins or other two-level systems. Connection to theory of glasses.
2. Dissipative dynamics of qubit with geometrical phase: this is the topic of some current activities, cf. (Y. Makhlin *et al.* etc.)

### 7.6.2 Atom + Electrical Field

#### Model Atom

Assume a single electron within an atom, described as a two-level system with states  $|g\rangle$  (ground state),  $|e\rangle$  (excited state), and energy difference  $\hbar\omega_0$  between ground and excited state. Then,

$$H_{\text{atom}} = \frac{\hbar\omega_0}{2}\sigma_z, \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv |e\rangle\langle e| - |g\rangle\langle g|. \quad (7.116)$$

Remember

$$\begin{aligned} \sigma_x &\equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \sigma_y &\equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, & \sigma_z &\equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \sigma_- &\equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, & \sigma_+ &\equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \sigma_{\pm} &= \frac{1}{2}(\sigma_x \pm i\sigma_y), & \sigma_x &= \sigma_+ + \sigma_-, & \sigma_y &= -i(\sigma_+ - \sigma_-) \\ [\sigma_+, \sigma_-] &= \sigma_z, & [\sigma_z, \sigma_{\pm}] &= \pm 2\sigma_{\pm}. \end{aligned} \quad (7.117)$$

#### Dipole Approximation

Consider an electrical field in the form of a linearly polarised, monochromatic plain wave with wave vector  $\mathbf{k}$ ,

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E} \cos(\mathbf{k}\mathbf{r} - \omega t). \quad (7.118)$$

Describe the interaction of the atom with the electrical field in *dipole approximation*: the energy of a dipole  $\mathbf{d}$  in a field  $\mathbf{E}(\mathbf{r}, t)$  is given by  $-\mathbf{d}\mathbf{E}(\mathbf{r}, t)$ . Treating the field classically, we obtain the time-dependent dipole Hamiltonian

$$\begin{aligned} H_L(t) &= -\langle g|\mathbf{d}\mathbf{E}(\mathbf{r}, t)|e\rangle\langle g| - \langle e|\mathbf{d}\mathbf{E}(\mathbf{r}, t)|g\rangle\langle e| \\ &\approx -(\hbar\Omega\sigma_- + \hbar\Omega^*\sigma_+) \cos(\omega t), \end{aligned} \quad (7.119)$$

where we used  $\mathbf{k}\mathbf{r} \ll 1$  in the overlap integral (wave length  $\gg$  dimension of atom, ‘*dipole approximation*’), and introduced

$$\sigma_- \equiv |g\rangle\langle e|, \quad \sigma_+ \equiv |e\rangle\langle g|. \quad (7.120)$$

and the *Rabi frequency*

$$\Omega \equiv \frac{1}{\hbar} \langle g | \mathbf{dE} | e \rangle, \quad (7.121)$$

which in general is a complex number. The total system Hamiltonian therefore is

$$H_S(t) = H_{\text{atom}} + H_L(t) = \frac{\hbar\omega_0}{2} \sigma_z - (\hbar\Omega\sigma_- + \hbar\Omega^*\sigma_+) \cos(\omega t). \quad (7.122)$$

One usually assumes real  $\Omega = \Omega^*$ , in this case we can formally write  $H_S(t) = \mathbf{B}(t)\vec{\sigma}$  with

$$\mathbf{B}(t) = \begin{pmatrix} -\hbar\Omega \cos(\omega t) \\ 0 \\ \frac{1}{2}\hbar\omega_0 \end{pmatrix}. \quad (7.123)$$

### Rotating Wave Approximation (RWA)

We introduce the System Hamiltonian  $H_S^{\text{RWA}}(t)$  in rotating wave approximation (RWA) by writing  $\cos(\omega t) = \frac{1}{2}(e^{i\omega t} + e^{-i\omega t})$  and neglecting the counter-rotating terms  $\sigma_- e^{-i\omega t}$  and  $\sigma_+ e^{i\omega t}$

$$H_S^{\text{RWA}}(t) \equiv \frac{\hbar\omega_0}{2} \sigma_z - \left( \frac{\hbar\Omega}{2} \sigma_- e^{i\omega t} + \frac{\hbar\Omega}{2} \sigma_+ e^{-i\omega t} \right). \quad (7.124)$$

In this case,  $H_S^{\text{RWA}}(t) = \mathbf{B}^{\text{RWA}}(t)\vec{\sigma}$  with

$$\mathbf{B}^{\text{RWA}}(t) = \begin{pmatrix} -\frac{1}{2}\hbar\Omega \cos(\omega t) \\ -\frac{1}{2}\hbar\Omega \sin(\omega t) \\ \frac{1}{2}\hbar\omega_0 \end{pmatrix} \quad (7.125)$$

### 7.6.3 Spontaneous Emission (Atom without Driving Field)

#### Model for $H_{SB}$ : Two-Level System Coupled to Photon Bath in RWA

The microscopic interaction between a two-level *atom* and a photon bath is via a coupling

$$(a_Q + a_Q^\dagger)(\sigma_+ + \sigma_-) = (a_Q + a_Q^\dagger)\sigma_x, \quad (7.126)$$

cf. Walls/Milburn, Carmichael, Baym or other quantum optics (quantum mechanics) books. Comparing with our generic form Eq.(7.114),

$$H_{SB}(t) \equiv \hat{\mathbf{A}}(t)\vec{\sigma} \equiv \sum_Q \left( \mathbf{g}_Q(t) a_Q^\dagger + \mathbf{g}_Q^\dagger(t) a_Q \right) \vec{\sigma},$$

this case would correspond to a (time-independent) coupling vector  $\mathbf{g}_Q(t) = \mathbf{g}_Q^\dagger(t) = (g_Q, 0, 0)$ . Within the RWA, this interaction is further simplified by neglecting the ‘counter-rotating’ terms and by writing

$$\mathbf{g}_Q = \frac{1}{2}\gamma_Q \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}, \gamma_Q \text{real}. \quad (7.127)$$

Assuming a *free photon* bath, the total Hamiltonian then is

$$\begin{aligned} H_{\text{total}} &\equiv H_S + H_{SB} + H_B \\ &= H_S + \sum_Q \gamma_Q (a_Q \sigma_+ + a_Q^\dagger \sigma_-) + \sum_Q \omega_Q a_Q^\dagger a_Q. \end{aligned} \quad (7.128)$$

### Mapping onto harmonic oscillator master equation

We now use the fact that  $H_{SB}$  has the same form as for the damped single bosonic mode if we identify  $\sigma_+ \rightarrow a^\dagger$ ,  $\sigma_- \rightarrow a$ . We can therefore ‘copy’ the derivation of the master equation of the damped harmonic oscillator, as long as no commutation relations are used! This is the case up to Eq.(7.46),

$$\begin{aligned} \frac{d}{dt}\rho(t) &= -i[\Omega a^\dagger a, \rho(t)] \\ &- \frac{1}{2} \left\{ [(\gamma_+ + 2i\Delta_+)a^\dagger a + (\gamma + 2i\Delta)aa^\dagger] \rho(t) \right. \\ &+ \rho(t) [(\gamma - 2i\Delta)aa^\dagger + (\gamma_+ - 2i\Delta_+)a^\dagger a] \\ &\left. - 2\gamma_+ a \rho(t) a^\dagger - 2\gamma a^\dagger \rho(t) a \right\}, \quad \text{harmonic oscillator.} \end{aligned}$$

The interaction picture for the two-level atom is with respect to the Hamiltonian

$$H_0 \equiv \frac{\omega_0}{2}\sigma_z + H_B \rightsquigarrow \tilde{\sigma}_\pm(t) = \sigma_\pm e^{\pm i\omega_0 t}, \quad \tilde{\sigma}_z(t) = \sigma_z. \quad (7.129)$$

In the interaction picture, the Master equation for the two-level atom therefore reads

$$\begin{aligned} \frac{d}{dt}\tilde{\rho}(t) &= -\frac{1}{2} \left\{ [(\gamma_+ + 2i\Delta_+)\sigma_+\sigma_- + (\gamma + 2i\Delta)\sigma_-\sigma_+] \tilde{\rho}(t) \right. \\ &+ \tilde{\rho}(t) [(\gamma - 2i\Delta)\sigma_-\sigma_+ + (\gamma_+ - 2i\Delta_+)\sigma_+\sigma_-] \\ &\left. - 2\gamma_+\sigma_-\tilde{\rho}(t)\sigma_+ - 2\gamma\sigma_+\tilde{\rho}(t)\sigma_- \right\}. \end{aligned} \quad (7.130)$$

We now use

$$\sigma_+\sigma_- = \frac{1}{2}(1 + \sigma_z), \quad \sigma_-\sigma_+ = \frac{1}{2}(1 - \sigma_z), \quad (7.131)$$

re-arrange and transform back into the Schrödinger picture,

$$\boxed{\begin{aligned} \frac{d}{dt}\rho(t) &= -i\frac{1}{2}(\omega_0 + \Delta_+ - \Delta)[\sigma_z, \rho] - \frac{1}{2}\gamma_+ \left\{ \sigma_+\sigma_-\rho + \rho\sigma_+\sigma_- - 2\sigma_-\rho\sigma_+ \right\} \\ &- \frac{1}{2}\gamma \left\{ \sigma_-\sigma_+\rho + \rho\sigma_-\sigma_+ - 2\sigma_+\rho\sigma_- \right\}. \end{aligned}} \quad (7.132)$$

We recall (note that the harmonic oscillator frequency  $\Omega$  has to be replaced by  $\omega_0$ )

$$\begin{aligned} \gamma_+ &\equiv 2\pi\rho(\omega_0)[1 + n_B(\omega_0)], \quad \gamma \equiv 2\pi\rho(\omega_0)n_B(\omega_0) \\ \Delta_+ - \Delta &\equiv \delta\omega_0 \equiv P \int_0^\infty d\omega \frac{\rho(\omega)[1 + 2n_B(\omega)]}{\omega_0 - \omega}. \end{aligned} \quad (7.133)$$

### Remarks:

- In contrast to the harmonic oscillator, the energy shift  $\hbar\delta\omega_0$  is now *temperature dependent*.
- The  $T = 0$  contribution is the *Lamb-shift* within RWA.

### 7.6.4 Expectation Values, Einstein Equations, Bloch Equations

We can write the Master equation with the help of

$$\begin{aligned}
\sigma_- &\equiv |g\rangle\langle e|, \quad \sigma_+ \equiv |e\rangle\langle g|, \quad \sigma_- \sigma_+ = |g\rangle\langle g|, \quad \sigma_+ \sigma_- = |e\rangle\langle e| \\
\rightsquigarrow \frac{d}{dt}\rho(t) &= -i\frac{1}{2}\bar{\omega}_0[|e\rangle\langle e| - |g\rangle\langle g|, \rho] \\
&\quad - \frac{1}{2}\gamma_+ \left\{ |e\rangle\langle e|\rho + \rho|e\rangle\langle e| - 2|g\rangle\langle e|\rho|e\rangle\langle g| \right\} \\
&\quad - \frac{1}{2}\gamma \left\{ |g\rangle\langle g|\rho + \rho|g\rangle\langle g| - 2|e\rangle\langle g|\rho|g\rangle\langle e| \right\}.
\end{aligned} \tag{7.134}$$

Taking matrix elements, we obtain

$$\frac{d}{dt}\langle e|\rho|e\rangle = -\gamma_+\langle e|\rho|e\rangle + \gamma\langle g|\rho|g\rangle \tag{7.135}$$

$$\frac{d}{dt}\langle g|\rho|g\rangle = +\gamma_+\langle e|\rho|e\rangle - \gamma\langle g|\rho|g\rangle \tag{7.136}$$

$$\frac{d}{dt}\langle e|\rho|g\rangle = \left(-i\bar{\omega}_0 - \frac{\gamma_+ + \gamma}{2}\right)\langle e|\rho|g\rangle \tag{7.137}$$

$$\frac{d}{dt}\langle g|\rho|e\rangle = \left(+i\bar{\omega}_0 - \frac{\gamma_+ + \gamma}{2}\right)\langle g|\rho|e\rangle. \tag{7.138}$$

The first two equations for the *diagonal elements* (which are linearly dependent because  $\langle e|\rho|e\rangle + \langle g|\rho|g\rangle = 1$ ) are called *Einstein equations*. We can re-write the four equations, subtracting the second from the first, as three equations,

$$\boxed{
\begin{aligned}
\frac{d}{dt}\langle \sigma_z \rangle &= -(\gamma_+ + \gamma)\langle \sigma_z \rangle + (\gamma - \gamma_+) \\
\frac{d}{dt}\langle \sigma_+ \rangle &= \left(+i\bar{\omega}_0 - \frac{\gamma_+ + \gamma}{2}\right)\langle \sigma_+ \rangle \\
\frac{d}{dt}\langle \sigma_- \rangle &= \left(-i\bar{\omega}_0 - \frac{\gamma_+ + \gamma}{2}\right)\langle \sigma_- \rangle.
\end{aligned}
} \tag{7.139}$$

These equations are called *Bloch equations*. Introducing the *relaxation time*  $T_1$  and the *decoherence time*  $T_2$ ,

$$T_1 = \frac{1}{2}T_2 \equiv (\gamma_+ + \gamma)^{-1}, \tag{7.140}$$

we can write

$$\begin{aligned}
\frac{d}{dt}\langle \sigma_z \rangle &= -\frac{1}{T_1} (\langle \sigma_z \rangle - \langle \sigma_z \rangle_\infty), \quad \langle \sigma_z \rangle_\infty \equiv \frac{\gamma - \gamma_+}{\gamma + \gamma_+} \\
\frac{d}{dt}\langle \sigma_+ \rangle &= \left(+i\bar{\omega}_0 - \frac{1}{T_2}\right)\langle \sigma_+ \rangle \\
\frac{d}{dt}\langle \sigma_- \rangle &= \left(-i\bar{\omega}_0 - \frac{1}{T_2}\right)\langle \sigma_- \rangle.
\end{aligned} \tag{7.141}$$

## 7.7 The Quantum Jump (Quantum Trajectory) Approach

References: M. B. Plenio and P. L. Knight, Rev. Mod. Phys. **70**, 101 (1998); H. Carmichael ‘An Open System Approach to Quantum Optics’, Springer Lecture Notes in Physics *m18*, Springer (Berlin, Heidelberg, 1993).



### 7.7.1 Introduction

- Method for numerically solving Master equations in a Monte-Carlo-like simulation: wave functions instead of density matrix  $\rightsquigarrow$  computational advantages.
- Restricted to Markovian Master equations of Lindblad form.
- Some regard it as more physical than usual density operator theory.

Motivation: telegraphic fluorescence (driven spontaneous emission) of single atoms

Example single V-systems: two upper levels 1 (fast spontaneous emission) and 2 (slow spontaneous emission), one lower level 0 driven by two lasers. Transition  $0 \rightarrow 2$  traps the system in 2 for a long time. Resonance fluorescence intensity  $I(t)$  therefore exhibits jumps: ‘telegraphic fluorescence’ with random switching between bright and dark periods. Aim: calculate distribution of dark periods.

Length  $T_D$  of dark period can be simply calculated from the density matrix element  $\rho_{22}$

$$T_D^{-1} = \dot{\rho}_{22}(t=0), \quad \rho_{22} = 0, \quad (7.142)$$

where the derivative is calculated from the underlying equation of motion (Master equation). However, the calculation of other, more complicated quantities related to the description of telegraphic fluorescence turns out to be technically complicated within the Master equation formalism. Example: ‘exclusive probability’  $P_0(t)$  that, after an emission at time  $t = 0$ , no other photon has been emitted in the time interval  $[0, t]$ .

- Some people raise ‘objections’ against the traditional Master equation approach: the density operator  $\rho$  describes *ensembles* of quantum systems and is therefore inappropriate to describe *single* quantum systems such as a single ion in an ion trap. However, these objections are unjustified; as long as one sticks with the probabilistic interpretation of Quantum Mechanics, the density operator description is perfectly valid for a *single* quantum system.
- ‘Single quantum systems’ can not only be realised in ion traps, but also in ‘artificial atoms’ and ‘artificial molecules’ (solid state based quantum dots, superconducting charge or flux qubits). These will be discussed in a later chapter.

### 7.7.2 Unravelling and Decomposition into Histories

#### Super-Operators

We have another look at the (Markoffian) Master equation of the damped harmonic oscillator at zero temperature  $T = 0$  (spontaneous emission only);

$$\frac{d}{dt}\rho(t) = -i\bar{\Omega}[a^\dagger a, \rho] - \kappa \left\{ a^\dagger a \rho + \rho a^\dagger a - 2a\rho a^\dagger \right\}. \quad (7.143)$$

Suppose we started from a pure state  $\rho(0) = |\Psi\rangle\langle\Psi|$  at time  $t = 0$ : after a short time  $\Delta t$ , this would evolve according to

$$\begin{aligned} |\Psi\rangle\langle\Psi| &\rightarrow |\Psi\rangle\langle\Psi| + \Delta t \left\{ (-i\bar{\Omega}a^\dagger a - \kappa a^\dagger a \rho) |\Psi\rangle\langle\Psi| (i\bar{\Omega}a^\dagger a - \kappa a^\dagger a \rho) \right\} \\ &\quad + 2\kappa a |\Psi\rangle\langle\Psi| a^\dagger \\ &\equiv |\Psi\rangle\langle\Psi| + \Delta t \left\{ \mathcal{L}_0 |\Psi\rangle\langle\Psi| + \mathcal{L}_1 |\Psi\rangle\langle\Psi| \right\}, \end{aligned} \quad (7.144)$$

where we defined the *super-operators* via

$$\begin{aligned}\mathcal{L}_0\rho &\equiv -iH_{\text{eff}}\rho + \rho iH_{\text{eff}}^\dagger, & H_{\text{eff}} &\equiv H - i\kappa a^\dagger a = \bar{\Omega}a^\dagger a - i\kappa a^\dagger a \\ \mathcal{L}_1\rho &\equiv 2\kappa a\rho a^\dagger.\end{aligned}\tag{7.145}$$

For pure states  $|\Psi\rangle\langle\Psi|$ :  $\mathcal{L}_0$  generates time-evolution with non-hermitian Hamiltonian  $H_{\text{eff}}$ , but  $\mathcal{L}_1$  generates a *quantum jump*;

$$\begin{aligned}\mathcal{L}_0 &: |\Psi\rangle \rightarrow -iH_{\text{eff}}|\Psi\rangle \\ \mathcal{L}_1 &: |\Psi\rangle \rightarrow \sqrt{2\kappa}a|\Psi\rangle.\end{aligned}\tag{7.146}$$

The state  $a|\Psi\rangle$  corresponds to a state with one photon less.

### Decomposition into Histories

We may write the Master equation Eq.(7.143) as

$$\frac{d}{dt}\rho(t) = (\mathcal{L}_0 + \mathcal{L}_1)\rho(t).\tag{7.147}$$

This can be formally solved as follows: we define

$$\begin{aligned}\bar{\rho}(t) &\equiv e^{-\mathcal{L}_0 t}\rho(t), & \bar{\mathcal{L}}_1(t) &\equiv e^{-\mathcal{L}_0 t}\mathcal{L}_1e^{\mathcal{L}_0 t} \\ \rightsquigarrow \frac{d}{dt}\bar{\rho}(t) &= -\mathcal{L}_0\bar{\rho}(t) + e^{-\mathcal{L}_0 t}(\mathcal{L}_0 + \mathcal{L}_1)e^{\mathcal{L}_0 t}\bar{\rho}(t) = \bar{\mathcal{L}}_1(t)\bar{\rho}(t) \\ \rightsquigarrow \bar{\rho}(t) &= \rho(0) + \int_0^t dt_1 \bar{\mathcal{L}}_1(t_1)\bar{\rho}(t_1) \\ &= \rho(0) + \int_0^t dt_1 \bar{\mathcal{L}}_1(t_1)\rho(0) + \int_0^t dt_1 \int_0^{t_1} dt_2 \bar{\mathcal{L}}_1(t_1)\bar{\mathcal{L}}_1(t_2)\bar{\rho}(t_2) \\ &\dots \\ &= \rho(0) + \sum_{n=1}^{\infty} \int_0^t dt_1 \dots \int_0^{t_n} dt_n \bar{\mathcal{L}}_1(t_1)\dots\bar{\mathcal{L}}_1(t_n)\rho(0).\end{aligned}\tag{7.148}$$

Transforming back to  $\rho(t)$ , we can explicitly write this as

$$\begin{aligned}\rho(t) &= e^{\mathcal{L}_0 t}\rho(0) \\ &+ \sum_{n=1}^{\infty} \int_0^t dt_1 \dots \int_0^{t_n} dt_n e^{\mathcal{L}_0 t} e^{-\mathcal{L}_0 t_1} \mathcal{L}_1 e^{\mathcal{L}_0 t_1} e^{-\mathcal{L}_0 t_2} \mathcal{L}_1 e^{\mathcal{L}_0 t_2} \dots e^{-\mathcal{L}_0 t_n} \mathcal{L}_1 e^{\mathcal{L}_0 t_n} \rho(0) \\ &= e^{\mathcal{L}_0 t}\rho(0) \\ &+ \sum_{n=1}^{\infty} \int_0^t dt_1 \dots \int_0^{t_n} dt_n \underline{e^{\mathcal{L}_0(t-t_1)} \mathcal{L}_1 e^{\mathcal{L}_0(t_1-t_2)} \mathcal{L}_1 e^{\mathcal{L}_0(t_2-t_3)} \dots e^{\mathcal{L}_0(t_{n-1}-t_n)} \mathcal{L}_1 e^{\mathcal{L}_0 t_n} \rho(0)} \\ &\equiv e^{\mathcal{L}_0 t}\rho(0) + \sum_{n=1}^{\infty} \int_0^t dt_1 \dots \int_0^{t_n} dt_n \underline{\rho_c(t; t_1, \dots, t_n)},\end{aligned}\tag{7.150}$$

where we defined the un-normalised, *conditioned* ‘density matrix’  $\rho_c(t; t_1, \dots, t_n)$  at time  $t$  with  $n$  quantum jumps occurring at times  $t_1, \dots, t_n$ . This object (the underlined term in Eq.(7.150)) indeed corresponds to the original density matrix  $\rho(0)$ , ‘freely’ time-evolved with the effective Hamiltonian  $H_{\text{eff}}$  during the time intervals  $(0, t_n]$ ,  $(t_n, t_{n-1}]$ ,... interrupted by  $n$  ‘jumps’ at times  $t_n, t_{n-1}, \dots, t_1$ . The total density matrix  $\rho(t)$  at time  $t$  then is the sum over all possible ‘trajectories’ with  $n = 0, \dots, \infty$  jumps occurring in between a ‘free’, effective time evolution.

### 'Monte Carlo' Procedure

The decomposition of histories can now be simulated on a computer in order to actually solve the Master equation. Here, we only describe the simplest version (spontaneous emission, no driving field), starting from a pure state  $|\Psi\rangle$  of the total system. For more details, see Carmichael or Plenio/Knight.

Step 1: Fix a time step  $\Delta t$ . Calculate the probability  $\Delta P$  of photon emission;

$$\Delta P \equiv \gamma \Delta t \langle \Psi | a^\dagger a | \Psi \rangle. \quad (7.151)$$

Step 2: Compare  $\Delta P$  with a random number  $0 \leq r \leq 1$

- For  $\Delta P > r$ : 'emission', replace

$$|\Psi\rangle \rightarrow \frac{a|\Psi\rangle}{\|a|\Psi\rangle\|} \quad (7.152)$$

- For  $\Delta P \leq r$ : no emission but time-evolution under effective Hamiltonian  $H_{\text{eff}}$ ,

$$|\Psi\rangle \rightarrow \frac{(1 - i\Delta t H_{\text{eff}})|\Psi\rangle}{(1 - \Delta P)^{1/2}} \quad (7.153)$$

Step 3: Go back to Step 1.

This procedure (performed with small time-steps  $\Delta t$  up to a final time  $t_{\text{final}}$ ) yields a 'curve' of simulated states  $|\Psi(t)\rangle$ ,  $t \in [0, t_{\text{final}}]$  in the system Hilbert space  $\mathcal{H}_S$ . The procedure is then repeated many times in order to obtain time-dependent averages  $\langle \Psi | \hat{\theta} | \Psi \rangle$  of observables  $\hat{\theta}$ .

The entire procedure yields a density operator  $\rho(t) = |\Psi\rangle\langle\Psi|$  that solves the original Master equation, Eq.(7.143): in one time step  $\Delta t$ , we have

$$\begin{aligned} \rho(t + \Delta t) &= \Delta P \frac{a|\Psi(t)\rangle\langle\Psi(t)|a^\dagger}{\|a|\Psi(t)\rangle\|^2} + (1 - \Delta P) \frac{(1 - i\Delta t H_{\text{eff}})|\Psi(t)\rangle\langle\Psi(t)|(1 + i\Delta t H_{\text{eff}}^\dagger)}{(1 - \Delta P)^{1/2}(1 - \Delta P)^{1/2}} \\ &= \gamma \Delta t a \rho(t) a^\dagger + \rho(t) - i\Delta t [H, \rho(t)] + \kappa \Delta t (a^\dagger a \rho(t) + \rho(t) a^\dagger a) + O(\Delta t)^2 \\ \rightsquigarrow \frac{d}{dt} \rho(t) &= -i[H, \rho(t)] - \kappa \left\{ a^\dagger a \rho + \rho a^\dagger a - 2a \rho a^\dagger \right\}. \end{aligned} \quad (7.154)$$

### Remarks:

- The splitting of  $\mathcal{L}$  as  $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$  is not unique, there are usually several ways of how to 'unravel' the Master equation.
- For more complicated Master equations, one has to extend and modify the above procedure.

## 7.8 Feynman-Vernon Influence Functional Theories

### 7.8.1 Introduction, Motivation

This is a technique to solve the Liouville-von-Neumann Equation,

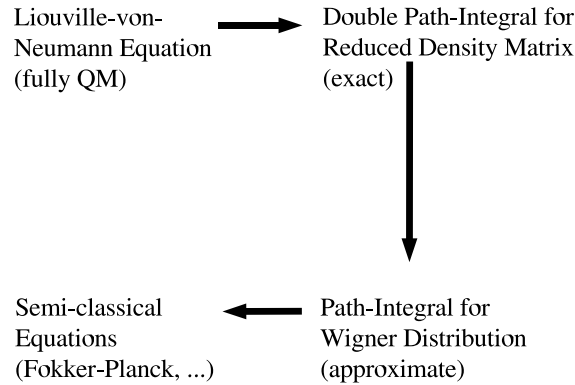
$$\frac{d}{dt}\chi(t) = -i[H, \chi(t)], \rightsquigarrow \chi(t) = e^{-iHt}\chi(t=0)e^{iHt}, \quad (7.155)$$

for the time-dependent density matrix  $\rho(t)$  of system-bath Hamiltonians

$$H \equiv H_S + H_B + H_{SB}, \quad (7.156)$$

cf. Eq. (7.4). It is mainly useful for cases where the system Hamiltonian  $H_S$  refers to a single (or a few) degrees of freedom, coupled via  $H_{SB}$  to a bath  $H_B$  of many degrees of freedom. The technique is based on **double path integrals**. The original reference is R. P. Feynman, F. L. Vernon, Ann. Phys. (N. Y.) **24**, 118 (1963).

One of the applications of influence functional theories is the systematic derivation of a semiclassical dynamics (Fokker-Planck equations, ...) from an exact quantum-mechanical theory:



### 7.8.2 Single Path Integrals

We assume a time-independent Hamiltonian for a particle of mass  $M$  in a one-dimensional potential  $V(x)$  (the generalisation to larger than one dimension is easy),

$$H \equiv T + V, \quad T \equiv \frac{p^2}{2M}. \quad (7.157)$$

The solution of the Schrödinger equation can be written as

$$|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle, \quad \langle x|\Psi(t)\rangle = \int dx' G(x, t; x', t' = 0) \langle x'|\Psi(0)\rangle, \quad t > 0 \quad (7.158)$$

with the help of the **propagator**

$$G(x, t; x') \equiv G(x, t; x', t' = 0) \equiv \langle x|e^{-iHt}|x'\rangle. \quad (7.159)$$

We now use the Trotter product formula

$$e^{-\lambda(T+V)} = \left( e^{-\frac{\lambda}{N}(T+V)} \right)^N = \lim_{N \rightarrow \infty} \left( e^{-\frac{\lambda}{N}T} e^{-\frac{\lambda}{N}V} \right)^N \quad (7.160)$$

with  $\lambda = it$  ( $\hbar = 1$ ) and write (inserting the identity  $N - 1$  times)

$$\begin{aligned} G(x, t; x') &= \lim_{N \rightarrow \infty} \int dx_1 \dots dx_{N-1} \prod_{j=0}^{N-1} \langle x_{j+1} | e^{-\frac{\lambda}{N}T} e^{-\frac{\lambda}{N}V} | x_j \rangle, \quad x_N \equiv x, x_0 \equiv x' \\ &= \lim_{N \rightarrow \infty} \int dx_1 \dots dx_{N-1} \prod_{j=0}^{N-1} \langle x_{j+1} | e^{-\frac{\lambda}{N}T} | x_j \rangle e^{-\frac{\lambda}{N}V(x_j)}. \end{aligned} \quad (7.161)$$

Now use (cf. p 1.15, 1.17),

$$\begin{aligned} \int \frac{dp}{(2\pi)} |p\rangle \langle p| &= 1, \quad \langle x|p\rangle = e^{ipx} \rightsquigarrow \\ \langle x|e^{-\frac{\lambda}{N}T}|y\rangle &= \langle x|e^{-\frac{\lambda}{2MN}p^2}|y\rangle \\ \int \frac{dp}{2\pi} \langle x|p\rangle e^{-\frac{\lambda}{2MN}p^2} \langle p|y\rangle &= \int \frac{db}{2\pi} e^{-\frac{\lambda}{2MN}p^2 + LP(x-y)} = \sqrt{\frac{MN}{2\pi\lambda}} e^{-MN(x-y)^2/2\lambda}, \end{aligned} \quad (7.162)$$

where we analytically continued the formula for Gaussian integrals

$$\boxed{\int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}, \quad \text{Re } a > 0,} \quad (7.163)$$

$a \rightarrow ia + \eta, \eta > 0$ , cf. Fresnel integrals and the book by H. Kleinert, ‘*Path Integrals*’ 2nd edition, World Scientific (Singapore, 1995).

We now introduce  $\varepsilon = t/N = \lambda/iN$  and have

$$\begin{aligned} G(x, t; x') &= \lim_{N \rightarrow \infty} \int dx_1 \dots dx_{N-1} \left( \frac{MN}{2\pi\lambda} \right)^{\frac{N}{2}} \prod_{j=0}^{N-1} \exp \left[ -\frac{MN(x_j - x_{j+1})^2}{2\lambda} - \frac{\lambda V(x_j)}{N} \right] \\ &= \lim_{N \rightarrow \infty} \int dx_1 \dots dx_{N-1} \left( \frac{M}{2\pi i \varepsilon} \right)^{\frac{N}{2}} \exp \left[ i\varepsilon \sum_{j=0}^{N-1} \left[ \frac{M}{2} \frac{(x_j - x_{j+1})^2}{\varepsilon^2} - V(x_j) \right] \right] \\ &\equiv \int_{x'}^x \mathcal{D}x e^{i \int_0^t dt' \mathcal{L}(x, \dot{x})}, \quad \mathcal{L}(x, \dot{x}) = \frac{1}{2} M \dot{x}^2 - V(x). \end{aligned} \quad (7.164)$$

Here, we have defined the **Lagrange Function**  $\mathcal{L}$  for the **path**  $x(t'), 0 \leq t' \leq t, x(0) \equiv x', x(t) \equiv x$  with start point  $x$  and end point  $x'$  in configuration space. The **Feynman path integral measure**  $\mathcal{D}x$  is a symbolic way of writing the limit  $N \rightarrow \infty$ ,

$$\mathcal{D}x = \lim_{N \rightarrow \infty} \int dx_1 \dots dx_{N-1} \left( \frac{M}{2\pi i \varepsilon} \right)^{\frac{N}{2}}. \quad (7.165)$$

- When calculating the path integral explicitly, one always has to go back to the finite  $N$  version and then take  $N \rightarrow \infty$ .

- The path integral represents an integration over *all* paths of the particle starting at  $x'$  and ending at  $x$ , not only the ones allowed by the Euler-Lagrange equations of classical mechanics. Each path is weighted with the factor  $\exp(iS_{\text{cl}})$ , where

$$S_{\text{cl}} \equiv \int_0^t dt' \frac{1}{2} M \dot{x}(t')^2 - V(x(t')) \quad (7.166)$$

is the classical action integral of the individual path  $x(t')$ . We therefore can write

$$\boxed{G(x, t; x') = \int_{x'}^x \mathcal{D}x \exp(iS_{\text{cl}})}. \quad (7.167)$$

Note, however, that this is only a shorthand notation for the discretised version in the  $N \rightarrow \infty$  limit.

### 7.8.3 Double Path Integrals

Now let us come back to our density operator for our system-bath Hamiltonian,

$$H \equiv H_S + H_B + H_{SB}, \chi(t) = e^{-iHt} \chi(t=0) e^{iHt}. \quad (7.168)$$

For the moment, let us assume that the system has one degree of freedom  $q$  and the bath the degree of freedom  $x$  (the generalisation to many bath degrees of freedom  $x_i$  is straightforward). We then use a representation of  $\chi(t)$  in spatial coordinates,

$$\begin{aligned} \langle x, q | \chi(t) | q', x' \rangle &= \int dq_0 dq'_0 dx_0 dx'_0 \langle x, q | e^{-iHt} | q_0, x_0 \rangle \langle x_0 q_0 | \chi(t=0) | q'_0, x'_0 \rangle \\ &\times \langle x'_0 q'_0 | e^{iHt} | q', x' \rangle. \end{aligned} \quad (7.169)$$

We trace out the bath degree of freedoms to obtain an effective density matrix

$$\rho(t) \equiv \text{Tr}_B \chi(t) \quad (7.170)$$

of the system,

$$\begin{aligned} \langle q | \rho(t) | q' \rangle &= \int dq_0 dq'_0 dx_0 dx'_0 dx \langle x, q | e^{-iHt} | q_0, x_0 \rangle \langle x_0 q_0 | \chi(t=0) | q'_0, x'_0 \rangle \\ &\times \langle x'_0 q'_0 | e^{iHt} | q', x \rangle. \end{aligned} \quad (7.171)$$

Now we realise that the Hamiltonian  $H \equiv H_S + H_B + H_{SB}$  induces a classical action  $S_{\text{total}} \equiv S_S[q] + S_B[x] + S_{SB}[xq]$ , where in the following for notational simplicity we omit indices at the

three  $S$ . We use the path integral representation for the propagator matrix elements,

$$\begin{aligned}
\langle q|\rho(t)|q'\rangle &= \int dq_0 dq'_0 dx_0 dx'_0 dx \int_{q_0}^q \mathcal{D}q \int_{x_0}^x \mathcal{D}x \int_{q'_0}^{q'} \mathcal{D}^*q' \int_{x'_0}^{x'=x} \mathcal{D}^*x' \\
&\times \exp [i (S[q] + S[x] + S[xq]) - i (S[q'] + S[x'] + S[x'q'])] \\
&\times \langle x_0 q_0 | \chi(t=0) | q'_0, x'_0 \rangle \\
&= \int dq_0 dq'_0 \int_{q_0}^q \mathcal{D}q \int_{q'_0}^{q'} \mathcal{D}^*q' \exp [i (S[q] - S[q'])] \\
&\times \int dx_0 dx'_0 dx \int_{x_0}^x \mathcal{D}x \int_{x'_0}^x \mathcal{D}^*x' \exp [i (S[x] + S[xq]) - i (S[x'] + S[x'q'])] \\
&\times \langle x_0 q_0 | \chi(t=0) | q'_0, x'_0 \rangle \\
&= [\text{assume } \chi(t=0) = \rho(0) \otimes \rho_B] \\
&= \int dq_0 dq'_0 \langle q_0 | \rho(0) | q'_0 \rangle \int_{q_0}^q \mathcal{D}q \int_{q'_0}^{q'} \mathcal{D}^*q' \exp [i (S[q] - S[q'])] \underline{\mathcal{F}[q(t'), q'(t')]} \\
\mathcal{F}[q(t'), q'(t')] &\equiv \int dx_0 dx'_0 dx \langle x_0 | \rho_B | x'_0 \rangle \\
&\times \int_{x_0}^x \mathcal{D}x \int_{x'_0}^x \mathcal{D}^*x' \exp [i (S[x] + S[xq]) - i (S[x'] + S[x'q'])]
\end{aligned}$$

- In the original Feynman-Vernon method, one assumes a *factorising initial condition*  $\chi(t=0) = \rho(0) \otimes \rho_B$ , although that can be generalised to non-factorising initial density matrices  $\chi(t=0)$ , cf. for example H. Grabert, P. Schramm, G. L. Ingold, Phys. Rep. **168**, 115 (1988), or the book by Weiss.
- The functional  $\mathcal{F}[q(t'), q'(t')]$  is called **influence functional**. It describes the effect of the bath on the time-evolution of the system density matrix.
- For zero system-bath coupling  $H_{SB} = 0$ ,  $\mathcal{F}[q(t'), q'(t')] = 1$

#### 7.8.4 The Influence Functional

Let us assume that we can write

$$H_{SB} = H_{SB}[q] = f(\hat{q})\hat{X} \quad (7.172)$$

with some given bath operator  $\hat{X}$  and some given function  $f(\hat{q})$  of the system coordinate  $\hat{q}$ . The influence functional can then be written as

$$\begin{aligned}
\mathcal{F}[q(t'), q'(t')] &\equiv \int dx_0 dx'_0 dx \langle x_0 | \rho_B | x'_0 \rangle \\
&\times \int_{x_0}^x \mathcal{D}x \exp [i (S[x] + S[xq])] \int_{x'_0}^x \mathcal{D}^*x' \exp [-i (S[x'] + S[x'q'])] \\
&= \int dx_0 dx'_0 dx \langle x_0 | \rho_B | x'_0 \rangle \langle x | U_B[q] x_0 \rangle [\langle x | U_B[q'] x'_0 \rangle]^* \\
&= \text{Tr}_B \left( \rho_B U_B^\dagger[q'] U_B[q] \right), \quad (7.173)
\end{aligned}$$

where  $U_B[q]$  is the unitary time-evolution operator for the time-dependent Hamiltonian  $H_B + H_{SB}[q]$  with a given  $q(t')$ ,  $0 \leq t' \leq t$ . Note that  $q(t')$  and  $q'(t')$  are independent paths, they

enter as ‘external’ parameters into the influence functional which then in the final expression for  $\langle q|\rho(t)|q'\rangle$  is integrated over all paths  $q(t')$  and  $q'(t')$ . This form is useful to recognise general properties of  $\mathcal{F}[q(t'), q'(t')]$ ,

- $q(t') = q'(t') \rightsquigarrow \mathcal{F}[q(t'), q'(t')] = 1$ .
- $|\mathcal{F}[q(t'), q'(t')]| \leq 1$ .

The

$$\boxed{\begin{aligned} &\text{Operator Form of Influence Functional} \\ &\mathcal{F}[q(t'), q'(t')] \equiv \text{Tr}_B \left( \rho_B U_B^\dagger[q'] U_B[q] \right), \end{aligned}} \quad (7.174)$$

is particularly useful for discussing the coupling to other baths (spin-baths, Fermi baths etc.)

### 7.8.5 Influence Functional for Coupling to Harmonic Oscillators

We start with the coupling of the system to a single harmonic oscillator,

$$H_B + H_{SB}[q] \equiv H_B(t) \equiv \frac{p^2}{2M} + \frac{1}{2}M\Omega^2 x^2 + g(t)x, \quad (7.175)$$

where without loss of generality we set  $f[q(t)] = g(t)$ .

Time-evolution operator  $U_B[q] \equiv U_B(t)$

This is given by the solution of the Schrödinger equation,

$$i\frac{\partial}{\partial t}U_B(t) = H_B(t)U_B(t), \quad U_B(0) = 1, \quad (7.176)$$

the formal solution of which is

$$U_B(t) = \text{T}e^{-i\int_0^t dt' H_B(t')} \quad (7.177)$$

with the time-ordering operator T. Now,  $U_B(t)$  can't be directly calculated from Eq. (7.177) because the  $H_B(t')$  do not commute with each other at different times<sup>1</sup>. One solution is to calculate  $U_B(t)$  by direct evaluation of the path integral which is tedious but can be done. Here, we show an alternative solution: introduce the interaction picture and write

$$\begin{aligned} H_B(t) &= H_0 + g(t)x \equiv H_0 + V(t) \\ U_B(t) &= e^{-iH_0 t} \tilde{U}(t), \quad i\partial_t \tilde{U}(t) = \tilde{V}(t) \tilde{U}(t) \\ \tilde{V}(t) &= e^{iH_0 t} V(t) e^{-iH_0 t} = g(t) \left( \hat{x} \cos \Omega t + \frac{\hat{p}}{M\Omega} \sin \Omega t \right). \end{aligned} \quad (7.178)$$

We solve for  $\tilde{U}(t)$  by making the general *ansatz*

$$\tilde{U}(t) = e^{-iA(t)} e^{-iB(t)\hat{x}} e^{-iC(t)\hat{p}} \quad (7.179)$$

<sup>1</sup> This is a dangerous source of mistakes, cf. J. H. Reina, L. Quiroga, and N. F. Johnson, ‘Decoherence of quantum registers’, Phys. Rev. A **65**, 032326 (2002)



with functions  $A(t)$  etc to be determined by taking the time-derivative of  $\tilde{U}(t)$ . This yields

$$\begin{aligned}
i\frac{\partial}{\partial t}\tilde{U}(t) &= \dot{A}(t)\tilde{U}(t) + \hat{x}\dot{B}(t)\tilde{U}(t) + \dot{C}(t)e^{-iA(t)}\underline{e^{-iB(t)\hat{x}}\hat{p}e^{-iC(t)\hat{p}}} \\
&= \dot{A}(t)\tilde{U}(t) + \hat{x}\dot{B}(t)\tilde{U}(t) + \dot{C}(t)e^{-iA(t)}\left(\underline{\hat{p}e^{-iB(t)\hat{x}} + [e^{-iB(t)\hat{x}}, \hat{p}]}\right)e^{-iC(t)\hat{p}} \\
&= \text{use } [e^{-i\alpha x}, p] = i\partial_x e^{-i\alpha x} = \alpha e^{-i\alpha x} \\
&= \left(\dot{A}(t) + \hat{x}\dot{B}(t) + \hat{p}\dot{C}(t) + B(t)\dot{C}(t)\right)\tilde{U}(t) \equiv \tilde{V}(t)\tilde{U}(t). \tag{7.180}
\end{aligned}$$

Therefore, comparing with the expression for  $\tilde{V}(t)$  yields

$$\begin{aligned}
B(t) &= \int_0^t dt' g(t') \cos \Omega t', \quad C(t) = \frac{1}{M\Omega} \int_0^t dt' g(t') \sin \Omega t' \\
A(t) &= -\frac{1}{M\Omega} \int_0^t dt' \int_0^{t'} ds g(t') g(s) \cos \Omega s \sin \Omega t' \tag{7.181}
\end{aligned}$$

and therefore,

$$\begin{aligned}
\langle x|U_B(t)|x'\rangle &= \langle x|e^{-iH_0 t} e^{-iA(t)} e^{-iB(t)\hat{x}} e^{-iC(t)\hat{p}}|x'\rangle \\
&= e^{-iA(t)} \langle x|e^{-iH_0 t} e^{-iB(t)\hat{x}}|x' + C(t)\rangle \\
&= e^{-iA(t)} \langle x|e^{-iH_0 t}|x' + C(t)\rangle e^{-iB(t)[x'+C(t)]} \tag{7.182}
\end{aligned}$$

In order to get explicit results here, we now need the propagator matrix elements for the harmonic oscillator,

$$\boxed{\langle x|e^{-iH_0 t}|x'\rangle = \sqrt{\frac{M\Omega}{2\pi i \sin \Omega t}} \exp \left\{ \frac{iM\Omega}{2 \sin \Omega t} [(x^2 + x'^2) \cos \Omega t - 2xx'] \right\}. \tag{7.183}}$$

These again can either be obtained by direct evaluation of the single path integral for the harmonic oscillator or (somewhat simpler) by using the stationary eigenstates. The matrix element for the driven harmonic oscillator,  $\langle x|U_B(t)|x'\rangle$ , can then after some transformations (straightforward algebra with trig functions) be written as

$$\begin{aligned}
\langle x|U_B(t)|x'\rangle &= \sqrt{\frac{M\Omega}{2\pi i \sin \Omega t}} \exp \{iS(x, t; x')\} \\
S(x, t; x') &\equiv \frac{iM\Omega}{2 \sin \Omega t} \left[ (x^2 + x'^2) \cos \Omega t - 2xx' \right. \\
&\quad - \frac{2x}{M\Omega} \int_0^t dt' g(t') \sin \Omega t' - \frac{2x'}{M\Omega} \int_0^t dt' g(t') \sin \Omega(t - t') \\
&\quad \left. - \frac{2}{M^2\Omega^2} \int_0^t \int_0^{t'} dt' ds g(t') g(s) \sin \Omega(t - t') \sin \Omega s \right]. \tag{7.184}
\end{aligned}$$

This coincides with the result given in L. S. Schulman, *Techniques and Applications of Path Integration*, Wiley (1981).

## Influence Phase

The influence phase can be obtained directly from its definition, Eq. (7.173),

$$\begin{aligned}
\mathcal{F}[q(t'), q'(t')] &\equiv \text{Tr}_B \left( \rho_B U_B^\dagger[q'] U_B[q] \right) = \text{Tr}_B \left( \rho_B \tilde{U}^\dagger[q'] e^{iH_0 t'} e^{-iH_0 t} \tilde{U}[q] \right) \\
&= \text{Tr}_B \left( \rho_B e^{iC' \hat{p}} e^{iB' \hat{x}} e^{iA'} e^{-iA} e^{-iB \hat{x}} e^{-iC \hat{p}} \right) \\
&= e^{i(A'-A)} \int dx \langle x | \rho_B | e^{iC' \hat{p}} e^{i(B'-B) \hat{x}} e^{-iC \hat{p}} | x \rangle \\
&= e^{i(A'-A)} \int dx \langle x | \rho_B | x + C - C' \rangle e^{i(B'-B)(x+C)},
\end{aligned}$$

where for a moment we abbreviated  $A, A'$  etc. for the integrals Eq. (7.181) with  $g(t') \equiv f(q(t'))$  in the undashed and  $g'(t') \equiv f(q'(t'))$  in the dashed (not the derivative) quantities. We now assume a *thermal equilibrium* for the density operator  $\rho_B$ ,

$$\rho_B = \frac{e^{-\beta H_0}}{Z}, \quad Z = \text{Tr} e^{-\beta H_0} = \frac{1}{2 \sinh \beta \Omega / 2} \quad (7.185)$$

$$\langle x | \rho_B | x' \rangle = \frac{1}{Z} \sqrt{\frac{M\Omega}{2\pi \sinh \Omega \beta}} \exp \left\{ \frac{-M\Omega}{2 \sinh \beta \Omega} [(x^2 + x'^2) \cosh \beta \Omega - 2xx'] \right\},$$

where we used the matrix elements of the propagator  $\langle x | e^{-iH_0 t} | x' \rangle$  for  $it = \beta$  (Wick rotation of the time  $t$ ). Doing the Gaussian integral yields

$$\begin{aligned}
\mathcal{F}[q(t'), q'(t')] &= e^{i(A'-A)} \int dx \langle x | \rho_B | x + C - C' \rangle e^{i(B'-B)(x+C)} \\
&= e^{i(A'-A)} \frac{1}{Z} \sqrt{\frac{M\Omega}{2\pi \sinh \Omega \beta}} \int dx e^{i(B'-B)(x+C)} \\
&\times \exp \left\{ -\frac{M\Omega}{2 \sinh \beta \Omega} [(x^2 + (x + C - C')^2) \cosh \beta \Omega - 2x(x + C - C')] \right\} \\
&= \left[ \text{use } \tanh \frac{x}{2} = \frac{\cosh x - 1}{\sinh x}, \quad \coth x - \frac{1}{2} \tanh \frac{x}{2} = \frac{1}{2} \coth \frac{x}{2} \right] \\
&= \exp \left\{ i(A' - A) + \frac{i}{2}(B' - B)(C + C') \right\} \\
&\times \exp \left\{ -\frac{1}{4M\Omega} \coth \frac{\beta \omega}{2} [(B' - B)^2 + M^2 \Omega^2 (C - C')^2] \right\}. \quad (7.186)
\end{aligned}$$

the last step now is to re-insert the definitions of  $A, B, C, A', B', C'$ . The resulting long expression

$$\mathcal{F}[q(t'), q'(t')] \quad (7.187)$$

$$\begin{aligned}
&= \exp \left\{ -\frac{1}{4M\Omega} \coth \frac{\beta \omega}{2} \int_0^t dt' \int_0^t ds (g_{t'}' - g_{t'}) (g_s' - g_s) \cos \Omega(t' - s) \right\} \\
&\times \exp \left\{ -\frac{i}{M\Omega} \int_0^t dt' \int_0^t ds (g_{t'}' g_s' - g_{t'} g_s) \cos \Omega s \sin \Omega t' \right\} \\
&\times \exp \left\{ \frac{i}{2M\Omega} \int_0^t dt' \int_0^t ds (g_{t'}' g_s' - g_{t'} g_s) \cos \Omega t' \sin \Omega s \right\} \\
&\times \exp \left\{ \frac{i}{2M\Omega} \int_0^t dt' \int_0^t ds (g_{t'}' g_s - g_{t'} g_s') \cos \Omega t' \sin \Omega s \right\} \quad (7.188)
\end{aligned}$$

can be further simplified with  $\sin \alpha \cos \beta = \frac{1}{2}[\sin(\alpha - \beta) + \sin(\alpha + \beta)]$  and carefully considering the limits of the integrals and the symmetry of the integrands. Re-installing furthermore  $g_{t'} \equiv g(t') \equiv f[q_{t'}]$  (we write the time-arguments as an index to avoid bulky expressions with too many brackets), the result can be written in a compact form, the Feynman-Vernon Influence Functional for the coupling of a single particle to a single harmonic oscillator in thermal equilibrium,

$$\begin{aligned}
H &= H_S[q] + H_B[x] + H_{SB}[xq] = H_S[q] + \frac{p^2}{2M} + \frac{1}{2}M\Omega^2 x^2 + f[q]x \\
\langle q|\rho(t)|q' \rangle &= \int dq_0 dq'_0 \langle q_0|\rho(0)|q'_0 \rangle \int_{q_0}^q \mathcal{D}q \int_{q'_0}^{q'} \mathcal{D}^* q' \exp [i(S[q] - S[q'])] \underline{\mathcal{F}[q_{t'}, q'_{t'}]} \\
\mathcal{F}[q_{t'}, q'_{t'}] &= \exp \{-\Phi[q_{t'}, q'_{t'}]\} \quad \text{Influence Functional} \\
\Phi[q_{t'}, q'_{t'}] &= \int_0^t dt' \int_0^{t'} ds \{f[q_{t'}] - f[q'_{t'}]\} \{L(t' - s)f[q_s] - L^*(t' - s)f[q'_s]\} \\
L(\tau) &= \frac{1}{2M\Omega} \left( \coth \frac{\beta\Omega}{2} \cos \Omega\tau - i \sin \Omega\tau \right). \tag{7.189}
\end{aligned}$$

Linear Response, Fluctuation-Dissipation Theorem for  $L(t)$

We first check that

$$L(t) = \langle x(t)x \rangle_0, \tag{7.190}$$

the (van-Hove) position correlation function of the harmonic oscillator with co-ordinate  $x$  in thermal equilibrium: write

$$\begin{aligned}
x &= \sqrt{\frac{1}{2M\Omega}} (a + a^\dagger), \quad x(t) = \sqrt{\frac{1}{2M\Omega}} (ae^{-i\Omega t} + a^\dagger e^{i\Omega t}) \\
L(t) &= \langle x(t)x \rangle_0 = \frac{1}{2M\Omega} \langle aa^\dagger e^{-i\Omega t} + a^\dagger a e^{i\Omega t} \rangle = \frac{1}{2M\Omega} \{(1 + n_B)e^{-i\Omega t} + n_B e^{i\Omega t}\} \\
&= \frac{1}{2M\Omega} \{(1 + 2n_B) \cos \Omega t - i \sin \Omega t\} = \frac{1}{2M\Omega} \left\{ \coth \frac{\beta\Omega}{2} \cos \Omega t - i \sin \Omega t \right\} \tag{7.191}
\end{aligned}$$

where we again have used the relation

$$1 + 2n_B = 1 + \frac{2}{e^{\beta\Omega} - 1} = \frac{e^{\beta\Omega} + 1}{e^{\beta\Omega} - 1} = \coth \frac{\beta\Omega}{2}. \tag{7.192}$$

Now let us have another look at this function. Consider the Hamiltonian

$$H_B[x] + H_{SB}[xq] \equiv H(t) = \frac{p^2}{2M} + \frac{1}{2}M\Omega^2 x^2 + f(t)x, \tag{7.193}$$

where we consider the function  $f[q_t] = f(t)$  for a fixed path  $q_t$  as an external classical force acting on the oscillator. The density matrix  $\rho_B(t)$  of the oscillator in the interaction picture fulfills, cf Eq.(7.9),

$$\begin{aligned}
\tilde{\rho}_B(t) &= \rho_0 - i \int_0^t dt' f(t') [\tilde{x}(t'), \tilde{\rho}_B(t')] \\
&\approx \rho_0 - i \int_0^t dt' f(t') [\tilde{x}(t'), \rho_0] \quad \text{1st order,} \tag{7.194}
\end{aligned}$$

where  $\rho_0 = \rho_B(t=0)$  is assumed to be the thermal equilibrium density matrix. The expectation value of the position is then

$$\begin{aligned}\langle x \rangle_t &\equiv \text{Tr} \rho_B(t) x = \text{Tr} \tilde{\rho}_B(t) \tilde{x}(t) \\ &= \langle x \rangle_0 - i \int_0^t dt' f(t') \text{Tr} [\tilde{x}(t'), \rho_0] \tilde{x}(t) = \langle x \rangle_0 - i \int_0^t dt' f(t') \text{Tr} \rho_0 [\tilde{x}(t), \tilde{x}(t')] \\ &= \langle x \rangle_0 - i \int_0^t dt' f(t') \langle [\tilde{x}(t), \tilde{x}(t')] \rangle_0, \quad \text{1st order.}\end{aligned}$$

We check that

$$\langle [\tilde{x}(t), \tilde{x}(t')] \rangle_0 = \langle [\tilde{x}(t-t'), \tilde{x}(0)] \rangle_0 \quad (7.195)$$

(definition of  $\rho_0$  !) and define the **linear susceptibility**

$$\chi_{xx}(t-t') \equiv i\theta(t-t') \langle [\tilde{x}(t-t'), \tilde{x}(0)] \rangle_0, \quad (7.196)$$

so that we can write

$$\langle x \rangle_t = \langle x \rangle_0 - i \int_0^t dt' \chi_{xx}(t-t') f(t'). \quad (7.197)$$

The theta function in  $\chi_{xx}(t-t')$  guarantees causality: the *response* of  $x$  at time  $t$  is determined by the system at *earlier* times  $t' \leq t$  only.

Define additional functions and their symmetric and antisymmetric (in time) linear combinations,

$$\begin{aligned}C^+(t) &\equiv \langle \tilde{x}(t)x \rangle_0, \quad C^-(t) \equiv \langle \tilde{x}(-t)x \rangle_0 = \langle x\tilde{x}(t) \rangle_0 \\ C^\pm(t) &\equiv S(t) \pm iA(t) \\ S(t) &= S(-t) = \frac{1}{2} \langle \tilde{x}(t)x + x\tilde{x}(t) \rangle_0, \quad A(t) = -A(-t) = \frac{1}{2i} \langle \tilde{x}(t)x - x\tilde{x}(t) \rangle_0.\end{aligned} \quad (7.198)$$

We thus have

$$\chi_{xx}(t) = -2\theta(t)A(t) \quad (7.199)$$

We define the Fourier transforms,

$$\begin{aligned}\hat{C}^\pm(\omega) &\equiv \int_{-\infty}^{\infty} dt C^\pm(t) e^{i\omega t}, \quad \hat{S}(\omega) \equiv \int_{-\infty}^{\infty} dt S(t) e^{i\omega t}, \quad \hat{A}(\omega) \equiv \int_{-\infty}^{\infty} dt A(t) e^{i\omega t} \\ \hat{\chi}(\omega) &\equiv \int_0^{\infty} dt \chi(t) e^{i\omega t}\end{aligned} \quad (7.200)$$

and use

$$\begin{aligned}\text{Tr}(e^{-\beta H_B} x \tilde{x}(t)) &= \text{Tr}(e^{-\beta H_B} x e^{\beta H_B} e^{-\beta H_B} \tilde{x}(t)) = \text{Tr}(\tilde{x}(i\beta) e^{-\beta H_B} \tilde{x}(t)) \\ &= \text{Tr}(e^{-\beta H_B} \tilde{x}(t) \tilde{x}(i\beta)) = \text{Tr}(e^{-\beta H_B} \tilde{x}(t-i\beta) x) \\ &\rightsquigarrow C^-(t) = C^+(t-i\beta),\end{aligned} \quad (7.201)$$

and therefore in the Fourier transform

$$C^-(\omega) = C^+(\omega) e^{-\beta\omega} \quad (\text{detailed balance relation}). \quad (7.202)$$

We now define real and imaginary part of the Fourier transform of the susceptibility,

$$\hat{\chi}_{xx}(\omega) \equiv \hat{\chi}'_{xx}(\omega) + i\hat{\chi}''_{xx}(\omega). \quad (7.203)$$

Then,

$$\begin{aligned} \hat{\chi}''(\omega) &= \text{Im} \int_0^\infty dt \chi(t) e^{i\omega t} = -2\text{Im} \int_0^\infty dt A(t) e^{i\omega t} = -2\frac{1}{2i} \int_0^\infty dt (A(t) e^{i\omega t} - A(t) e^{-i\omega t}) \\ &= i \int_0^\infty dt \left( A(t) e^{i\omega t} - \int_{-\infty}^0 dt A(-t) e^{i\omega t} \right) = [A(t) = -A(-t)] = i \int_{-\infty}^\infty dt A(t) e^{i\omega t} \\ &= i\hat{A}(\omega) = i\frac{1}{2i} (\hat{C}^+(\omega) - \hat{C}^-(\omega)) = \frac{1}{2} (1 - e^{-\beta\omega}) \hat{C}^+(\omega) \end{aligned} \quad (7.204)$$

The relation

$$\hat{\chi}''(\omega) = \frac{1}{2} (1 - e^{-\beta\omega}) \hat{C}^+(\omega) \quad (7.205)$$

is called **Fluctuation-Dissipation Theorem (FDT)** (Callen, Welton 1951) and can be re-written, using

$$\hat{S}(\omega) = \frac{1}{2} (\hat{C}^+(\omega) + \hat{C}^-(\omega)) = \frac{1}{2} (1 + e^{-\beta\omega}) \hat{C}^+(\omega), \quad (7.206)$$

leading to

$$\boxed{\hat{S}(\omega) = \hat{\chi}''(\omega) \coth \frac{\beta\omega}{2}.} \quad (7.207)$$

Example- harmonic oscillator: we have

$$\begin{aligned} \chi(t) &= i\theta(t) \langle [x(t), x] \rangle_0 = \frac{i\theta(t)}{2M\Omega} (e^{-i\Omega t} - e^{i\Omega t}) \\ \rightsquigarrow \hat{\chi}_{xx}(\omega) &= \text{Im} \frac{i}{2M\Omega} \int_0^\infty dt (e^{-i\Omega t} - e^{i\Omega t}) e^{i\omega t} \\ &= \frac{1}{2M\Omega} \int_0^\infty dt \{ \cos(\omega - \Omega)t - \cos(\omega + \Omega)t \} \\ &= \frac{1}{2M\Omega} \frac{1}{2} \int_{-\infty}^\infty dt \{ \cos(\omega - \Omega)t - \cos(\omega + \Omega)t \}, \end{aligned} \quad (7.208)$$

therefore

$$\hat{\chi}_{xx}(\omega) = \frac{1}{2M\Omega} \frac{2\pi}{2} \{ \delta(\omega - \Omega) - \delta(\omega + \Omega) \}. \quad (7.209)$$

On the other hand,

$$\begin{aligned} C(t) &\equiv L(t) = \langle \tilde{x}(t)x \rangle_0 = \frac{1}{2M\Omega} \left\{ \coth \frac{\beta\Omega}{2} \cos \Omega t - i \sin \Omega t \right\} \\ \rightsquigarrow S(t) &= \frac{1}{2M\Omega} \coth \frac{\beta\Omega}{2} \cos \Omega t \\ \rightsquigarrow S(\omega) &= \frac{1}{2M\Omega} \pi \{ \delta(\omega + \Omega) + \delta(\omega - \Omega) \} \coth \frac{\beta\Omega}{2} \\ &= \frac{1}{2M\Omega} \pi \{ -\delta(\omega + \Omega) + \delta(\omega - \Omega) \} \coth \frac{\beta\omega}{2} = \hat{\chi}_{xx}(\omega) \coth \frac{\beta\omega}{2}, \end{aligned} \quad (7.210)$$

which is consistent with the FDT.

## 7.8.6 Applications: Linear Coupling, Damped Harmonic Oscillator

Our result for the influence phase can immediately be generalised to a single particle, coupled to a system of  $N > 1$  harmonic oscillators in thermal equilibrium,

$$\begin{aligned}
H &= H_S[q] + H_B[x] + H_{SB}[xq] = H_S[q] + \sum_{\alpha=1}^N \frac{p_\alpha^2}{2M_\alpha} + \frac{1}{2}M_\alpha\Omega_\alpha x^2 + f_\alpha[q]x_\alpha \\
\mathcal{F}[q', q'_t] &= \exp\{-\Phi[q', q'_t]\} \quad \text{Influence Functional} \\
\Phi[q', q'_t] &= \sum_{\alpha=1}^N \int_0^t dt' \int_0^{t'} ds \{f_\alpha[q_{t'}] - f_\alpha[q'_{t'}]\} \{S_\alpha(t' - s)f_\alpha[q_s] - S_\alpha^*(t' - s)f_\alpha[q'_s]\} \\
S_\alpha(\tau) &= \frac{1}{2M_\alpha\Omega_\alpha} \left( \coth \frac{\beta\Omega_\alpha}{2} \cos \Omega_\alpha\tau - i \sin \Omega_\alpha\tau \right). \tag{7.211}
\end{aligned}$$

## Linear Coupling

In many applications, one assumes (often for simplicity) a *linear coupling* to the bath,

$$\begin{aligned}
H_B[x] + H_{SB}[xq] &= \sum_{\alpha=1}^N \left[ \frac{p_\alpha^2}{2M_\alpha} + \frac{1}{2}M_\alpha\Omega_\alpha^2 \left( x_\alpha - \frac{c_\alpha}{M_\alpha\Omega_\alpha^2}q \right)^2 \right] \\
&= \sum_{\alpha=1}^N \left[ \frac{p_\alpha^2}{2M_\alpha} + \frac{1}{2}M_\alpha\Omega_\alpha^2 x_\alpha^2 - c_\alpha q x_\alpha + \frac{1}{2} \frac{c_\alpha^2}{M_\alpha\Omega_\alpha^2} q^2 \right] \\
\mathcal{F}[q', q'_t] &= \exp\{-\Phi[q', q'_t]\} \quad \text{Influence Functional} \\
\Phi[q', q'_t] &= \int_0^t dt' \int_0^{t'} ds \{q_{t'} - q'_{t'}\} \{L(t' - s)q_s - L^*(t' - s)q'_s\} \\
&\quad + i \frac{\mu}{2} \int_0^t dt' \{q_{t'}^2 - (q'_{t'})^2\} \tag{7.212}
\end{aligned}$$

Here, the kernel  $L(t)$  and the spectral density  $J(\omega)$  are

$$\begin{aligned}
L(\tau) &\equiv \frac{1}{\pi} \int_0^\infty d\omega J(\omega) \left( \coth \frac{\beta\omega}{2} \cos \omega\tau - i \sin \omega\tau \right) \\
J(\omega) &\equiv \frac{\pi}{2} \sum_{\alpha=1}^N \frac{c_\alpha^2}{M_\alpha\Omega_\alpha} \delta(\omega - \Omega_\alpha). \tag{7.213}
\end{aligned}$$

Note that in this form, an additional term appears in  $H_{SB}$  as a potential

$$V_{\text{counter}}(q) \equiv \frac{1}{2}\mu q^2, \quad \mu \equiv \frac{1}{2} \sum_{\alpha} \frac{c_\alpha^2}{M_\alpha\Omega_\alpha^2} = \frac{2}{\pi} \int_0^\infty \frac{J(\omega)}{\omega}. \tag{7.214}$$

Since the action  $S$  appears as  $\exp(iS[q])$  in the path integral for  $q$  and  $\exp(-iS[q])$  in the path integral for  $q'$ , we could absorb the counter term into the influence phase as

$$\exp\left(i \frac{\mu}{2} \int_0^t dt' \{q_{t'}^2 - (q'_{t'})^2\}\right).$$

Note that the entire information on the coupling to the bath is now contained in the spectral density  $J(\omega)$ , which we have defined following the notation of Weiss, ‘Quantum Dissipative Systems’.

### Propagator for Damped Harmonic Oscillator

One now has to face the tedious task to (exactly) evaluate the double path integral, which can be done because it is Gaussian. Reference: H. Grabert, P. Schramm, and G.-L. Ingold, Phys. Rep. **168**, 115 (1988).

Comparison to Master Equation Approach: R. Karrlein, H. Grabert, Phys. Rev. E **55**, 153 (1997).

#### 7.8.7 Another Look at Influence Functionals for General Baths

(This sub-section is partly due to private communications from W. Zwerger). Feynman and Vernon realised that the coupling of a system  $S$  to *any* bath  $B$  can be mapped onto the coupling to an equivalent oscillator bath, if the coupling is weak and second order perturbation theory can be applied: let us have another look at the operator form of the influence functional, Eq. (7.174),

$$\begin{aligned} \mathcal{F}[q(t'), q'(t')] &\equiv \text{Tr}_B \left( \rho_B U_B^\dagger[q'] U_B[q] \right) \\ H_B(t) &= H_0 + V(t), \quad H'_B(t) = H_0 + V'(t), \end{aligned} \quad (7.215)$$

where  $U_B[q]$  is the time-evolution operator for  $H_B(t)$  and  $U_B^\dagger[q']$  the (backwards in time) evolution operator for  $H'_B(t)$ . Here,  $H_B(t)$  and  $H'_B(t)$  refer to different paths  $q$  and  $q'$ .

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Example: For a Fermi bath, we could have

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k, \quad V(t) \equiv V[q_t] = \sum_{kk'} M_{kk'} \exp(i(k - k')q_t) c_{k'}^\dagger c_k. \quad (7.216)$$

where  $c_k^\dagger$  creates a Fermion with quantum number  $k$ .

---

We again introduce the interaction picture and write

$$\begin{aligned} U_B[q] &= e^{-iH_0 t} \left\{ 1 + i \int_0^t dt' \tilde{V}(t') - \int_0^t \int_0^{t'} dt' ds \tilde{V}(t') \tilde{V}(s) + \dots \right\} \\ U_B^\dagger[q'] &= \left\{ 1 - i \int_0^t dt' \tilde{V}'(t') - \int_0^t \int_0^{t'} dt' ds \tilde{V}'(s) \tilde{V}'(t') + \dots \right\} e^{iH_0 t} \end{aligned} \quad (7.217)$$

The product of the two time-evolution operators therefore becomes

$$\begin{aligned}
U_B^\dagger[q']U_B[q] &= 1 - i \int_0^t dt' \left\{ \tilde{V}'(t') - \tilde{V}(t') \right\} + \int_0^t dt' \tilde{V}'(t') \int_0^t ds \tilde{V}(s) \\
&\quad - \int_0^t \int_0^{t'} dt' ds \left\{ \tilde{V}'(s) \tilde{V}'(t') + \tilde{V}(t') \tilde{V}(s) \right\} + \dots \\
&= 1 - i \int_0^t dt' \left\{ \tilde{V}'(t') - \tilde{V}(t') \right\} + \frac{1}{2} \int_0^t \int_0^t dt' ds \left\{ \tilde{V}'(t') \tilde{V}(s) + \tilde{V}'(s) \tilde{V}(t') \right\} \\
&\quad - \int_0^t \int_0^{t'} dt' ds \left\{ \tilde{V}'(s) \tilde{V}'(t') + \tilde{V}(t') \tilde{V}(s) \right\} + \dots \\
&= 1 - i \int_0^t dt' \left\{ \tilde{V}'(t') - \tilde{V}(t') \right\} + \int_0^t \int_0^{t'} dt' ds \left\{ \tilde{V}'(t') \tilde{V}(s) + \tilde{V}'(s) \tilde{V}(t') \right\} \\
&\quad - \int_0^t \int_0^{t'} dt' ds \left\{ \tilde{V}'(s) \tilde{V}'(t') + \tilde{V}(t') \tilde{V}(s) \right\} + \dots \\
&= 1 - i \int_0^t dt' \left\{ \tilde{V}'(t') - \tilde{V}(t') \right\} + \int_0^t \int_0^{t'} dt' ds \left\{ \left[ \tilde{V}'(t') - \tilde{V}(t') \right] \tilde{V}(s) \right\} \\
&\quad - \int_0^t \int_0^{t'} dt' ds \left\{ \tilde{V}'(s) \left[ \tilde{V}'(t') - \tilde{V}(t') \right] \right\} + \dots \tag{7.218}
\end{aligned}$$

In order to be a little bit more definite, a useful parametrisation of the interaction operators might be

$$\hat{V}(t) \equiv \sum_{\alpha\beta} g_{\alpha\beta}(t) \hat{X}_{\alpha\beta}, \quad \hat{V}'(t) \equiv \sum_{\alpha\beta} g'_{\alpha\beta}(t) \hat{X}_{\alpha\beta}, \tag{7.219}$$

with bath operators  $\hat{X}_{\alpha\beta}$ . Note that this comprises the cases considered so far (harmonic oscillator, Fermi bath). Taking the trace over  $\rho_B$ , we obtain

$$\begin{aligned}
\mathcal{F}[q(t'), q'(t')] &\equiv \text{Tr}_B \left( \rho_B U_B^\dagger[q'] U_B[q] \right) \equiv \langle U_B^\dagger[q'] U_B[q] \rangle_0 \\
&= 1 - i \sum_{\alpha\beta} \int_0^t dt' \left\{ g'_{\alpha\beta}(t') - g_{\alpha\beta}(t') \right\} \langle \tilde{X}_{\alpha\beta}(t') \rangle_0 \\
&\quad + \sum_{\alpha\beta\gamma\delta} \int_0^t \int_0^{t'} dt' ds \left\{ g'_{\alpha\beta}(t') - g_{\alpha\beta}(t') \right\} \left[ g_{\gamma\delta}(s) \langle \tilde{X}_{\alpha\beta}(t') \tilde{X}_{\gamma\delta}(s) \rangle_0 \right. \\
&\quad \left. - g'_{\gamma\delta}(s) \langle \tilde{X}_{\gamma\delta}(s) \tilde{X}_{\alpha\beta}(t') \rangle_0 \right] + \dots \tag{7.220}
\end{aligned}$$

Introducing the correlation tensor

$$L_{\alpha\beta\gamma\delta}(t', s) \equiv \langle \tilde{X}_{\alpha\beta}(t') \tilde{X}_{\gamma\delta}(s) \rangle_0, \tag{7.221}$$

this can be written as

$$\begin{aligned}
\mathcal{F}[q(t'), q'(t')] &= 1 - i \sum_{\alpha\beta} \int_0^t dt' \left\{ g'_{\alpha\beta}(t') - g_{\alpha\beta}(t') \right\} \langle \tilde{X}_{\alpha\beta}(t') \rangle_0 \\
&\quad + \sum_{\alpha\beta\gamma\delta} \int_0^t \int_0^{t'} dt' ds \left\{ g'_{\alpha\beta}(t') - g_{\alpha\beta}(t') \right\} \left[ g_{\gamma\delta}(s) L_{\alpha\beta\gamma\delta}(t', s) - g'_{\gamma\delta}(s) L_{\gamma\delta\alpha\beta}(s, t') \right] \\
&\quad + \dots \tag{7.222}
\end{aligned}$$



## 'Re-Exponentiation'

So far this expression for the influence functional is very general, but it is only to second order in the system-bath interaction! In principle, one should write down the entire Dyson series for  $U_B^\dagger[q']$  and  $U_B[q]$  and sum up all the terms of the resulting expression in order to obtain the final result for the influence functional. Clearly, this is in general not possible, and it is even not guaranteed that such an expression would be convergent and mathematically meaningful.

For simplicity, let us assume that the linear term vanishes,

$$\langle \tilde{X}_{\alpha\beta}(t') \rangle_0 \equiv 0. \quad (7.223)$$

For example, this is fulfilled for coupling to a linear harmonic oscillator,  $\hat{X}_{\alpha\beta} \equiv \delta_{\alpha\beta} \hat{x}$  with  $\hat{x}$  the oscillator coordinate.

At least some contributions to the infinite series for  $\mathcal{F}[q(t'), q'(t')]$  can be summed up in closed form: this is done by 're-exponentiation'. In fact, up to second order in the system-bath interaction, we can write (summarising all our definitions so far)

$$\begin{aligned} \hat{V}[q_t] &\equiv \sum_{\alpha\beta} g_{\alpha\beta}[q_t] \hat{X}_{\alpha\beta}, & L_{\alpha\beta\gamma\delta}(t', s) &\equiv \langle \tilde{X}_{\alpha\beta}(t') \tilde{X}_{\gamma\delta}(s) \rangle_0 \\ \mathcal{F}^{\text{pert}}[q(t'), q'(t')] &= \exp\{-\Phi^{\text{pert}}[q(t'), q'(t')]\}, \\ \Phi^{\text{pert}}[q(t'), q'(t')] &= \sum_{\alpha\beta\gamma\delta} \int_0^t \int_0^{t'} dt' ds \{g_{\alpha\beta}[q_{t'}] - g_{\alpha\beta}[q'_{t'}]\} \\ &\quad \times \left[ g_{\gamma\delta}[q_s] L_{\alpha\beta\gamma\delta}(t', s) - g_{\gamma\delta}[q'_s] L_{\gamma\delta\alpha\beta}(s, t') \right] \end{aligned} \quad (7.224)$$

by simply expanding the exponential. The 're-exponentiation' automatically sums up an infinite number of terms. Such 'exponentiation' schemes are known, e.g., from cluster expansions of the statistical operator  $e^{-\beta\hat{H}}$ . The important observation here is that for the harmonic oscillator case, this re-exponentiation becomes exact: with  $\hat{V} = f[q]\hat{x}$  and  $\hat{V}' = f[q']\hat{x}$ , we recognise

$$\begin{aligned} \Phi[q(t'), q'(t')] &= \int_0^t \int_0^{t'} dt' ds \{f[q_{t'}] - f[q'_{t'}]\} \{L(t', s)f[q_s] - L(s, t')f[q'_s]\}, \quad (7.225) \\ L(t', s) &= \langle x(t')x(s) \rangle_0 = \langle x(t' - s)x \rangle_0 = L(t' - s) \\ L(s, t') &= \langle x(s)x(t') \rangle_0 = \langle x(t')x(s) \rangle_0^* = L^*(t' - s), \end{aligned} \quad (7.226)$$

and therefore by comparison with Eq. (7.189) we find that both expressions coincide.

## 7.8.8 'Semiclassical' Limit for Damped Single Particle Motion

References: A. Schmid, *J. Low Temp. Phys.* **49**, 609 (1982); W. Zwerger, *Phys. Rev. B* **35**, 4737 (1987); N. Janssen and W. Zwerger, *Phys. Rev. B* **52**, 9406 (1995); U. Weiss, 'Quantum Dissipative Systems' (2nd ed.), World Scientific (Singapore) (1999), ch. 5.5.

Let us assume a single particle in a potential  $V(q)$ ,

$$H_S = \frac{p^2}{2m} + V(q). \quad (7.227)$$

We consider the reduced density matrix  $\rho(t)$  of the system  $S$ ,

$$\rho(x, y, t) \equiv \langle x + y/2 | \rho(t) | x - y/2 \rangle, \quad (7.228)$$

where we set

$$q = x + y/2, \quad q' = x - y/2; \quad x = \frac{1}{2}(q + q'), \quad y = q - q', \quad (7.229)$$

thus introducing the ‘center-of-mass’ coordinate  $x$  and the relative coordinate  $y$ . Note that the **Wigner distribution function**  $f(x, p, t)$  is obtained from the density matrix as a Fourier transform with respect to the relative co-ordinate  $y$ ,

$$f(x, p, t) = \int_{-\infty}^{\infty} \frac{dy}{2\pi} \rho(x, y, t) e^{-ipy}. \quad (7.230)$$

Correspondingly, in the double path integral we integrate over center-of-mass-coordinate and relative-coordinate paths,

$$x_t = \frac{1}{2}(q_t + q'_t), \quad y_t = q_t - q'_t \quad (7.231)$$

The Jacobian of the corresponding discretised variable transformation is one whence one can write

$$\begin{aligned} \rho(x, y, t) &= \int dx_0 dy_0 \rho_0(x_0, y_0) J(x, y, t; x_0, y_0) \\ J(x, y, t; x_0, y_0) &= \int_{x_0}^x \mathcal{D}x \int_{y_0}^y \mathcal{D}y \exp \left[ i \int_0^t dt' (M \dot{x}_t' \dot{y}_t' - V(x + y/2) + V(x - y/2)) \right] \\ &\times \exp \{ -\Phi[x_t', y_t'] \} \end{aligned} \quad (7.232)$$

### Expansion of the Influence Phase

In order to derive a semiclassical limit from the double path integral, the central idea is to expand the influence phase in powers of the paths  $y_t'$ . The  $y_t'$ -paths describe ‘off-diagonal excursions’ from the diagonal paths  $x_t'$  in the time-evolution of  $\rho(t)$ . We write

$$\begin{aligned} \mathcal{F}[x_t', y_t'] &= \exp \{ -\Phi[x_t', y_t'] \} \quad \text{Influence Functional} \\ -\Phi[x_t', y_t'] &= - \sum_{\alpha=1}^N \int_0^t dt' \int_0^{t'} ds \{ f_\alpha[x_t' + y_t'/2] - f_\alpha[x_t' - y_t'/2] \} \\ &\times \{ S_\alpha(t' - s) f_\alpha[x_s + y_s/2] - S_\alpha^*(t' - s) f_\alpha[x_s - y_s/2] \} \\ &= - \sum_{\alpha=1}^N \int_0^t dt' \int_0^{t'} ds f'_\alpha[x_t'] y_t' \\ &\times \{ \text{Re } S_\alpha(t' - s) f'_\alpha[x_s] y_s + 2i \text{Im } S_\alpha(t' - s) f_\alpha[x_s] \} + O[y_s]^3. \end{aligned} \quad (7.233)$$

In the semiclassical approximation, we thus can write the influence as

$$\begin{aligned} \mathcal{F}_{\text{sc}}[x_t', y_t'] &\equiv \exp \{ -\Phi[x_t', y_t'] \} = \exp \{ i\phi_1 - \phi_2 \} \quad (7.234) \\ i\phi_1 &\equiv -i \int_0^t dt' \int_0^{t'} ds \varphi_1[x_s] \underline{y_t'} y_t', \quad \varphi_1[x_s] \equiv \sum_{\alpha=1}^N 2 \text{Im } S_\alpha(t' - s) f'_\alpha[x_t'] f_\alpha[x_s] \\ \phi_2 &\equiv \int_0^t dt' \int_0^{t'} ds \varphi_2[x_s] \underline{y_t'} \underline{y_s}, \quad \varphi_2[x_s] \equiv \sum_{\alpha=1}^N \text{Re } S_\alpha(t' - s) f'_\alpha[x_t'] f'_\alpha[x_s]. \end{aligned}$$

**Exercise:** Check that for the linear model (coupling linear in  $q$ ), Eq.(7.212), the influence phase becomes

$$\begin{aligned}\Phi[x_{t'}, y_{t'}] &= \int_0^t dt' \int_0^{t'} ds y_{t'} \{ \text{Re } L(t' - s) y_s + 2i \text{Im } L(t' - s) x_s \} \\ &+ i\mu \int_0^t dt' x_{t'} y_{t'}.\end{aligned}\quad (7.235)$$

For the linear model, the semiclassical expansion of the influence phase is therefore exact.

In a similar way, we expand the potential  $V(x \pm y/2)$  in the action in powers of the off-diagonal path  $y$ , thus arriving at

$$\begin{aligned}\rho_{\text{sc}}(x, y, t) &= \int dx_0 dy_0 \rho_0(x_0, y_0) J_{\text{sc}}(x, y, t; x_0, y_0) \\ J_{\text{sc}}(x, y, t; x_0, y_0) &= \int_{x_0}^x \mathcal{D}x \int_{y_0}^y \mathcal{D}y \exp \left[ i \int_0^t dt' (M \dot{x}_{t'} \dot{y}_{t'} - V'(x_{t'}) y_{t'}) \right] \\ &\times \exp \left\{ -i \int_0^t dt' \int_0^{t'} ds \varphi_1[x_s] y_{t'} - \int_0^t dt' \int_0^{t'} ds \varphi_2[x_s] y_{t'} y_s \right\}.\end{aligned}\quad (7.236)$$

The first step now is to perform an integration by parts to transform the term  $M \dot{x}_{t'} \dot{y}_{t'}$ , and to re-arrange

$$\begin{aligned}J_{\text{sc}}(x, y, t; x_0, y_0) &= \int_{x_0}^x \mathcal{D}x \int_{y_0}^y \mathcal{D}y \exp [iM(\dot{x}_t y - \dot{x}_0 y_0)] \\ &\times \exp \left[ -i \int_0^t dt' y_{t'} \{ M \ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] \} - \int_0^t dt' \int_0^{t'} ds \varphi_2[x_s] y_{t'} y_s \right] \\ F_B[x_s, t'] &\equiv \int_0^{t'} ds \varphi_1[x_s] = \int_0^{t'} ds \sum_{\alpha=1}^N 2 \text{Im } S_\alpha(t' - s) f'_\alpha[x_{t'}] f_\alpha[x_s] \\ &= - \sum_{\alpha=1}^N \int_0^{t'} ds \frac{\sin \Omega_\alpha(t' - s)}{M_\alpha \Omega_\alpha} f'_\alpha[x_{t'}] f_\alpha[x_s].\end{aligned}\quad (7.237)$$

This is an interesting expression: the term in the brackets  $\{ \}$  looks likely to lead to a classical equation of motion,

$$M \ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] = 0, \quad (7.238)$$

where  $-V'(x_{t'})$  is the force due to the potential  $V(x)$ , and  $F_B[x_s, t']$  is a retarded, position-dependent deterministic friction force due to the bath. In addition, however, there is the term quadratic in  $y$  containing the function

$$\begin{aligned}\varphi_2[x_s] &\equiv \sum_{\alpha=1}^N \text{Re } S_\alpha(t' - s) f'_\alpha[x_{t'}] f'_\alpha[x_s] \\ &= \sum_{\alpha=1}^N \frac{1}{2M_\alpha \Omega_\alpha} \coth \frac{\beta \Omega_\alpha}{2} \cos \Omega_\alpha(t' - s) f'_\alpha[x_{t'}] f'_\alpha[x_s],\end{aligned}\quad (7.239)$$

which is the only place where the bath temperature  $T = 1/\beta$  enters.

### Completing the Square

This is a useful trick when dealing with functional integrals. We start from the identity for a real symmetric, positive definite  $n \times n$  matrix  $A$ ,

$$\boxed{e^{-\frac{1}{2}\mathbf{y}A\mathbf{y}} = [2\pi \det A]^{-n/2} \int_{-\infty}^{\infty} dx_1 \dots dx_n e^{-\frac{1}{2}\mathbf{x}A^{-1}\mathbf{x} + i\mathbf{y}\mathbf{x}}} \quad (7.240)$$

**Exercise:** Prove this identity. Hint: use the standard formula for Gaussian integrals and a linear transformation that diagonalises  $A$ .

We now obtain

$$\begin{aligned} & \exp \left[ -\frac{1}{2} \int_0^t \int_0^t dt' ds A(t', s) y_{t'} y_s \right] = \lim_{N \rightarrow \infty} \exp \left[ -\frac{\varepsilon^2}{2} \sum_{j,k=0}^{N-1} A_{jk} y_j y_k \right] \\ &= \lim_{N \rightarrow \infty} [2\pi \det A]^{-N/2} \int d\xi_0 \dots d\xi_{N-1} \exp \left[ -\frac{\varepsilon^2}{2} \sum_{j,k=0}^{N-1} \xi_j \frac{A_{jk}^{-1}}{\varepsilon^2} \xi_k + i\varepsilon \sum_{j=0}^{N-1} y_j \xi_j \right] \\ &= \int \mathcal{D}\xi \exp \left[ -\int_0^t \int_0^t dt' ds \xi_{t'} A^{-1}(t', s) \xi_s + i \int_0^t dt' y_{t'} \xi_{t'} \right] \quad (7.241) \\ \mathcal{D}\xi &\equiv \lim_{N \rightarrow \infty} [2\pi \det A]^{-N/2} d\xi_0 \dots d\xi_{N-1} \\ A(t', s) &= \varphi_2[x](t', s), \quad \text{cf. Eq. (7.239).} \end{aligned}$$

Here, we have used the fact that the discrete inverse of an operator needs to be divided by  $\varepsilon^2$ ,

$$A^{-1}(t', s) \leftrightarrow \frac{1}{\varepsilon^2} A_{jk}^{-1}. \quad (7.242)$$

This can be derived by considering the discrete equivalent of the delta function and leads to the following translation table between continuous and discrete:

$$\begin{aligned} f(x) &= \int dx' \delta(x - x') f(x'), \quad f_m = \sum_n \delta_{mn} f_n = \varepsilon \sum_n \frac{\delta_{mn}}{\varepsilon} f_n \\ &\rightsquigarrow \delta(x - x') \leftrightarrow \frac{\delta_{mn}}{\varepsilon} \\ \int dx' A^{-1}(x, x') A(x', x'') &= \delta(x - x''), \quad \varepsilon \sum_{m'} \frac{A_{mm'}^{-1}}{\varepsilon^2} A_{m'm''} = \frac{\delta_{mm''}}{\varepsilon} \\ &\rightsquigarrow A^{-1}(x, x') \leftrightarrow \frac{1}{\varepsilon^2} A_{mm'}^{-1}. \quad (7.243) \end{aligned}$$

Now using the fact that  $\varphi_2$  is symmetric in  $t'$  and  $s$ , we have

$$\int_0^t dt' \int_0^{t'} ds \varphi_2[x_s] y_{t'} y_s = \frac{1}{2} \int_0^t dt \int_0^t ds \varphi_2[x_s] y_t y_s \quad (7.244)$$

and therefore

$$\begin{aligned}
J_{\text{sc}}(x, y, t; x_0, y_0) &= \int_{x_0}^x \mathcal{D}x \int_{y_0}^y \mathcal{D}y e^{iM(\dot{x}_t y - \dot{x}_0 y_0)} \\
&\times \exp \left[ -i \int_0^t dt' y_{t'} \{ M\ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] \} - \frac{1}{2} \int_0^t \int_0^t dt' ds \varphi_2[x_s] y_{t'} y_s \right] \\
&= \int_{x_0}^x \mathcal{D}x \int_{y_0}^y \mathcal{D}y e^{iM(\dot{x}_t y - \dot{x}_0 y_0)} \int \mathcal{D}\xi[x] \exp \left[ -\frac{1}{2} \int_0^t \int_0^t dt' ds \xi_{t'} \varphi_2[x_s]^{-1} \xi_s \right] \\
&\times \exp \left[ -i \int_0^t dt' y_{t'} \{ M\ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] - \xi_{t'} \} \right]. \tag{7.245}
\end{aligned}$$

Here we have explicitly indicated the dependence of the measure  $\mathcal{D}\xi[x]$  on the paths  $x_s$ , which enters through the determinant of the operator  $\varphi_2[x_s]$ . The pathintegral over  $\mathcal{D}y$  is now very easy: we find ( $\varepsilon = t/N$ )

$$\begin{aligned}
\int_{y_0}^y \mathcal{D}y \exp \left[ -i \int_0^t dt' y_{t'} b_{t'} \right] &= \lim_{N \rightarrow \infty} \int dy_1 \dots dy_{N-1} \left( \frac{M}{2\pi i \varepsilon} \right)^{\frac{N}{2}} \exp \left[ -i \varepsilon \sum_{j=0}^{N-1} y_j b_j \right] \\
&= \lim_{N \rightarrow \infty} \left( \frac{M}{2\pi i \varepsilon} \right)^{\frac{N}{2}} \frac{2\pi \delta(b_0)}{\varepsilon} \dots \frac{2\pi \delta(b_{N-1})}{\varepsilon} e^{-i \varepsilon y_0 b_0} \equiv \Delta(y_{t'} - b_{t'}), \tag{7.246}
\end{aligned}$$

Here,  $\Delta$  indicates the product of delta functions that fixes the  $y_{t'}$  path to the  $b_{t'}$  path, and for  $\varepsilon \rightarrow 0$  the  $e^{-i \varepsilon y_0 b_0}$  becomes irrelevant. Inserting yields

$$\begin{aligned}
J_{\text{sc}}(x, y, t; x_0, y_0) &= e^{iM(\dot{x}_t y - \dot{x}_0 y_0)} \int_{x_0}^x \mathcal{D}x \int \mathcal{D}\xi[x] \exp \left[ -\frac{1}{2} \int_0^t \int_0^t dt' ds \xi_{t'} \varphi_2[x_s]^{-1} \xi_s \right] \\
&\times \Delta(M\ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] - \xi_{t'}). \tag{7.247}
\end{aligned}$$

### Wigner Distribution in 'Semi-classical' Limit

Considering now the definition of the Wigner distribution function,

$$\begin{aligned}
f_{\text{sc}}(x, p, t) &= \int_{-\infty}^{\infty} \frac{dy}{2\pi} \rho(x, y, t) e^{-ipy} = \int_{-\infty}^{\infty} \frac{dy}{2\pi} e^{-ipy} \int dx_0 dy_0 \rho_0(x_0, y_0) J_{\text{sc}}(x, y, t; x_0, y_0) \\
&= \int \frac{dy}{2\pi} dx_0 dy_0 \rho_0(x_0, y_0) e^{-ipy} e^{iM(\dot{x}_t y - \dot{x}_0 y_0)} \int_{x_0}^x \mathcal{D}x \int \mathcal{D}\xi[x] e^{-\frac{1}{2} \int_0^t \int_0^t dt' ds \xi_{t'} \varphi_2[x_s]^{-1} \xi_s} \\
&\times \Delta(M\ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] - \xi_{t'}) \\
&= \int dx_0 f_0(x_0, p_0 = M\dot{x}_0) \delta(p - M\dot{x}) \int_{x_0}^x \mathcal{D}x \int \mathcal{D}\xi[x] e^{-\frac{1}{2} \int_0^t \int_0^t dt' ds \xi_{t'} \varphi_2[x_s]^{-1} \xi_s} \\
&\times \Delta(M\ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] - \xi_{t'}). \tag{7.248}
\end{aligned}$$

Here, the  $y$ -integral generated  $\delta(p - M\dot{x})$ , and the  $y_0$ -integral transformed the initial condition  $\rho_0(x_0, y_0)$  into its Wigner transform  $f_0(x_0, p_0 = M\dot{x}_0)$ . We summarise,

$$\boxed{
\begin{aligned}
f_{\text{sc}}(x, p, t) &= \int dx_0 f_0(x_0, M\dot{x}_0) \delta(p - M\dot{x}) \\
&\times \int_{x_0}^x \mathcal{D}x \int \mathcal{D}\xi[x] \exp \left[ -\frac{1}{2} \int_0^t \int_0^t dt' ds \xi_{t'} \varphi_2[x_s]^{-1} \xi_s \right] \\
&\times \Delta(M\ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] - \xi_{t'}). \tag{7.249}
\end{aligned}
}$$

## Discussion

In the semi-classical approximation, the time-evolution of the Wigner-distribution function is determined by Eq. (7.249). This equation describes a *stochastic process* for the center-of-mass co-ordinate  $x_{t'}$  of the particle, moving within a potential  $V(x)$  under the action of a deterministic friction force  $F_B[x_s, t']$ ,

$$F_B[x_s, t'] = - \sum_{\alpha=1}^N \int_0^{t'} ds \frac{\sin \Omega_{\alpha}(t' - s)}{M_{\alpha} \Omega_{\alpha}} f'_{\alpha}[x_{t'}] f_{\alpha}[x_s], \quad (7.250)$$

and a stochastic force  $\xi_{t'}$ . The motion of the particle is governed by the *stochastic integro-differential equation*

$$M \ddot{x}_{t'} + V'(x_{t'}) + F_B[x_s, t'] = \xi_{t'}, \quad (7.251)$$

where the stochastic force  $\xi_{t'}$  is a random force which itself depends on the coordinate of the particle: this can be seen by the fact that its variance,

$$\langle \xi_{t'} \xi_s \rangle = \varphi_2[x] = \sum_{\alpha=1}^N \frac{1}{2M_{\alpha} \Omega_{\alpha}} \coth \frac{\beta \Omega_{\alpha}}{2} \cos \Omega_{\alpha}(t' - s) f'_{\alpha}[x_{t'}] f'_{\alpha}[x_s], \quad (7.252)$$

depends on the particle path  $x_s$ . The Wigner distribution is obtained by integrating over all possible realisations of the stochastic force, such that Eq. (7.252) is fulfilled. Since the  $\xi$  path-integral is Gaussian, one speaks of a *Gaussian* stochastic process. This of course is due to the fact that we truncated the  $y_{t'}$  expansion in the influence phase after the term quadratic in  $y_{t'}$ .

Our results shows that the influence of the bath is two-fold: it leads to a deterministic, retarded ‘friction’ force, and to a stochastic force. The latter contains the temperature and, by means of the  $\coth(\beta \hbar \Omega / 2)$  terms in  $\varphi_2[x]$ , a fully quantum mechanical description of the bath.

For certain types of system-bath couplings, one can explicitly show that the operator  $\varphi_2$  is positive definite and therefore, the term quadratic in  $y_{t'}$  in the original double path integral exponentially suppresses strong deviations from the diagonal paths with  $y_{t'} = 0$ . In this case, the expansion of the one-particle potential  $V$ ,

$$-V(x + y/2) + V(x - y/2) \approx -V'(x)y \quad (7.253)$$

becomes more plausible. One should, however, expect that quantum mechanical effects (like particle tunneling) are destroyed by the approximation Eq. (7.253).

## Linear Dissipation (‘Ohmic Bath’)

The influence phase for the linear model, Eq.(7.212), the influence phase is (cf. Eq. (7.235,7.214,7.213))

$$\begin{aligned} \Phi[x_{t'}, y_{t'}] &= \int_0^t dt' \int_0^{t'} ds y_{t'} \{ \text{Re } L(t' - s) y_s + 2i \text{Im } L(t' - s) x_s \} \\ &+ i\mu \int_0^t dt' x_{t'} y_{t'}, \quad \mu \equiv \frac{1}{2} \sum_{\alpha} \frac{c_{\alpha}^2}{M_{\alpha} \Omega_{\alpha}^2} = \frac{2}{\pi} \int_0^{\infty} \frac{J(\omega)}{\omega} \\ L(\tau) &\equiv \frac{1}{\pi} \int_0^{\infty} d\omega J(\omega) \left( \coth \frac{\beta \omega}{2} \cos \omega \tau - i \sin \omega \tau \right), \end{aligned} \quad (7.254)$$

whence the deterministic friction force  $F_B[x_s, t']$  becomes

$$\begin{aligned}
F_B[x_s, t'] &= \mu x_{t'} + \int_0^{t'} ds 2\text{Im} L(t' - s)x_s \\
&= \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega} x_{t'} - \frac{2}{\pi} \int_0^\infty d\omega J(\omega) \int_0^{t'} ds \sin \omega(t' - s)x_s \\
&= \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega} x_{t'} - \frac{2}{\pi} \int_0^\infty d\omega J(\omega) \left[ \frac{x_{t'}}{\omega} - \frac{\cos \omega t'}{\omega} x_0 - \int_0^{t'} ds \frac{\cos \omega(t' - s)}{\omega} \dot{x}_s \right] \\
&= \frac{2}{\pi} \int_0^\infty d\omega J(\omega) \left[ \frac{\cos \omega t'}{\omega} x_0 + \int_0^{t'} ds \frac{\cos \omega(t' - s)}{\omega} \dot{x}_s \right]. \tag{7.255}
\end{aligned}$$

The term  $x_{t'}$  from the integration by parts has cancelled exactly with the counter-term  $\mu x_{t'}$ . If one now assumes a *linear* spectral function  $J(\omega)$ ,

$$J_{\text{ohmic}}(\omega) \equiv \eta\omega, \tag{7.256}$$

we recover the original Caldeira-Leggett description of quantum friction (plus the additional term  $2\eta x_0 \delta(t')$  that was missing there, cf. A. O. Caldeira, A. J. Leggett, *Physica* **121 A**, 587 (1983); *ibid.* **130 A**, 374(E), (1985); Weiss book chapter 5.1),

$$\begin{aligned}
F_{\text{ohmic}}[x_s, t'] &= \frac{2\eta}{\pi} \int_0^\infty d\omega \left[ x_0 \cos \omega t' + \int_0^{t'} ds \cos \omega(t' - s) \dot{x}_s \right] \\
&= 2\eta x_0 \delta(t') + 2\eta \int_0^{t'} ds \delta(t' - s) \dot{x}_s = 2\eta x_0 \delta(t') + \eta \dot{x}_{t'}. \tag{7.257}
\end{aligned}$$

The resulting stochastic equation of motion Eq. (7.251) is

$$M\ddot{x}_{t'} + \eta \dot{x}_{t'} + V'(x_{t'}) = \xi_{t'} - 2\eta x_0 \delta(t'). \tag{7.258}$$

Note that the ‘awkward’ term  $2\eta x_0 \delta(t')$  brings in a dependence on the ‘initial condition’  $x_0$ .

### Application: Polaron-Transport

Feynman *et al.* (R. P. Feynman, R. W. Hellwarth, C. K. Iddings, and P. M. Platzman, *Phys. Rev.* **127** 1004 (1962), K. K. Thornber, R. P. Feynman, *Phys. Rev. B* **1**, 4099 (1970)), and Janssen and Zwerger (N. Janssen and W. Zwerger, *Phys. Rev. B* **52**, 9406 (1995)) have used the influence functional theory for the *non-equilibrium polaron problem*, i.e. the motion of a single electron coupled to optical phonons in a crystal. The periodic crystal potential is considered in the form of an effective band-mass  $m^*$ , and the potential  $V$  is due to an accelerating, homogeneous force in which case the expansion Eq. (7.253) becomes exact.

## **7.9 The Spin-Boson Problem**

### **7.10 Master Equations: Some Further Remarks and Examples**

7.10.1 Lindblad Theory

7.10.2 Resonance Fluorescence (Driven Dissipative Few-Level Atom)

7.10.3 Non-Markoffian Master Equations

### **7.11 Operator Langevin Equations**



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