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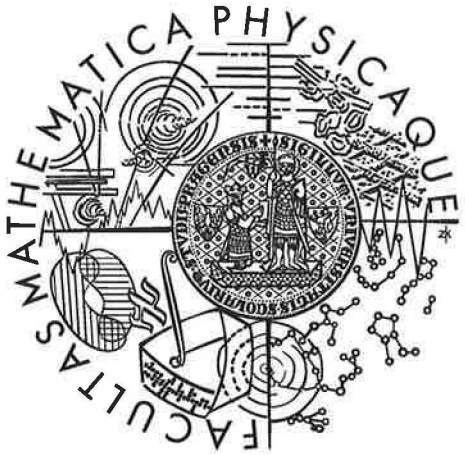

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Current noise in double quantum dots

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Study program: Physics, Physics of condensed and macromolecular matter

2008

Poděkování

Děkuji především dr. Tomášovi Novotnému za ochotu a trpělivost při vedení této práce, za cenné připomínky a postřehy k získaným výsledkům a potřebnou motivaci. Za podnětné diskuse děkuji dr. Karlovi Netočnému a profesorovi Bedřichovi Velickému.

Během celého studia i psaní práce mě neocenitelně podporovali rodiče. Děkuji jim za investice do mě vložené, které se jim snažím vracet nejen prostřednictvím jejich radosti z mých úspěchů.

Děkuji drahé Marcele za to, že při mně celou dobu stála a projevovala velikou starost o mou práci. Díky ní spatřuji ve svém konání smysl.

Prohlašuji, že jsem svou diplomovou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce a jejím zveřejňováním.

V Praze dne 28. 8. 2008 Jan Prachař

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Název práce: Proudový šum v dvojitých kvantových tečkách
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Abstrakt

V předložené práci studujeme proudový šum ve dvojité kvantové tečce, která je vázána ke dvěma vodičům v limitě nekonečného napětí mezi nimi a k tepelné disipativní lázni v limitě slabé vazby. Výpočty jsou založeny na přístupu Markovovských zobecněných řídících rovnic. Proudový šum při nulové frekvenci vypočtený pomocí kvantového regresního teorému v rámci systému (t. j. mezi tečkami) nabývá nefyzikálních záporných hodnot. Na druhou stranu proudový šum vypočtený pro proud mezi tečkami a vodiči nevykazuje žádné anomálie a zdá se být v souladu s experimenty. Hledáme původ nesouladu v přístupech, které by měly dávat shodné výsledky, jak v modelu dvojité kvantové tečky, tak i v přesně řešitelných modelech s disipativními harmonickými oscilátory. Smyslem práce je v rámci zobecněných řídících rovnic hledat náboj zachovávající schémata a pochopit dynamiku kvantových systémů vázaných na vícenásobné lázně.

Klíčová slova: zobecněné řídící rovnice, Markovovské procesy, zákon zachování náboje, disipace

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Abstract

In the presented thesis we study the current noise through a double quantum dot coupled to two leads in the high bias limit and a dissipative heat bath in the weak coupling limit. Our calculations are based on the solution of a Markovian generalized master equation. Zero-frequency component of current noise calculated within the system, i.e. between the two dots, via the quantum regression theorem exhibits unphysical negative values. On the other hand, current noise calculated for currents between the dots and the leads by the counting variable approach shows no anomalies and seems consistent with experiments. We inquire into the origin of the discrepancy between the two nominally equivalent approaches for the double dot systems as well as in exactly solvable models of dissipative harmonic oscillators. The purpose of the study is the development of charge-conserving approximation schemes within the generalized master approaches and understanding of dynamics of quantum systems coupled to multiple baths.

Keywords: generalized master equation, Markov processes, charge conservation, dissipation

Chapter 1

Introduction

Due to the advances in technology and measurement in mesoscopic semiconductor devices, the great attention have been paid to them also theoretically. One of the simplest quantum system is the double quantum dot which is a tunable two-level system for electronic energy states. The principle of operation on these devices is based on controlling energy states, for instance, by means of an external gate voltage [1]. There is also possibility to characterize the double dot as a potential quantum bit.

In a setup consisting of an array of two dots, the role of the electronic coherence is of central importance. The double quantum dot device loses coherence due to the coupling with a noisy environment (e. g. unavoidable lattice vibrations and interaction with phonons). Energy is exchanged with bosonic degrees of freedom which can give rise to transitions between states of nonequal energy by spontaneous emission of en energy quantum.

The dissipation of two level system is a subject of study for many years [2, 3]. Particularly in presence of dissipation, current noise spectrum contains additional valuable information about the quantum dynamics of the studied mesoscopic system not available in stationary current characteristics.

The topic of this thesis is a theoretical study of the current noise spectrum of electronic transport in the double quantum dot in strong Coulomb blockade regime. Method used in previous studies [4, 5] suffers from significant conceptual problems, e.g. it fails with respect to the principal physical laws such as the charge conservation. Two nominally equivalent approaches for calculation of the zero-frequency component of the current noise spectrum expose discrepancy. This fact puts under question results of these methods. Aim of this work is a detailed identification of problems connected with charge-conservation breaking in the double quantum dot device as well as in an exactly solvable model of harmonic oscillator with two heat baths and a model of two coupled dissipative harmonic oscillators and finding a general criterion for a class of approximations without these problems.

The thesis is organized as follows.

In Chapter 2 a derivation of generalized master equation for a system weakly coupled to a dissipative heat bath is given. The derivation is based on the idea of projection operators. We assume only Markovian processes.

The model of the double quantum dot device is presented in Chapter 3. The total Hamiltonian consists of the system (electronic degrees of freedom), leads and a generic heat bath. We develop theory of the zero-frequency component of the current noise spectrum where the electron transfer between the system and the leads is described by a classical Markovian process. We show that wide-band approximation together with high bias limit results in the same dynamics as the weak coupling prescription between the system and the leads.

Two methods for calculation of the zero-frequency current noise are presented in Section 3.3 – quantum regression theorem (which is applicable to the current operator between the dots and in the case of Markovian system dynamics) and MacDonald formula (which relies on the counting variable approach). The charge conservation breaking is discussed in Section 3.4.

We present results of our numerical and analytical calculations in Section 3.5. Next we study different limiting cases. The first limit is that of small tunneling rates between the leads and the system, the second limit considered is the limit of weak coupling between adjacent dots which leads to sequential tunneling. Results of the rotating wave approximation are demonstrated in Section 3.6. Pauli master equation approach is explained in Section 3.7.

The model of a harmonic oscillator coupled to two heat baths is considered in Chapter 4. Position and momentum autocorrelation functions are calculated within three methods – exact solution of Heisenberg equations of motion, the generalized master equation approach and rotating wave approximation. The positivity breaking of the autocorrelation functions and discrepancies are discussed.

Chapter 5 is about the model of two coupled dissipative harmonic oscillators. This model is interesting as a direct analog of the double quantum dot. We focus on a process of the energy exchanging between the oscillators, an operator of the energy exchange and its autocorrelation function are defined.

We state our conclusions in Chapter 6.

Chapter 2

Generalized master equation

2.1 Liouville space

In order to manipulate with an density operator, we define Liouville space. It is possible to stay in the Hilbert space, but the notation becomes very complicated. Operators in the Hilbert space can be handled as members of a linear space. The Liouville space is a linear space spanned over operators of the Hilbert space. Its basis $|n, n'\rangle\!\rangle$ is constructed from a basis $|n\rangle$ of the Hilbert space $|n, n'\rangle\!\rangle \equiv |n\rangle\langle n'|$. General operator

$$A = \sum_{n,n'} A_{nn'} |n\rangle\langle n'|$$

corresponds to the vector

$$|A\rangle\!\rangle = \sum_{n,n'} A_{nn'} |n, n'\rangle\!\rangle \,.$$

(For density operator $\varrho = \sum_{n,n'} \varrho_{nn'} |n, n'\rangle\!\rangle$.) The matrix representation of operators in the Liouville space follows from the previous.

$$\mathcal{A} = \sum_{\substack{n,n' \\ m,m'}} A_{nn',mm'} |n, n'\rangle\!\rangle\langle\!\langle m, m'| \,.$$

In order to avoid confusion, linear operators acting in the Liouville space are called superoperators. In the following, all superoperators will be denoted by calligraphic symbols, and the vectors of the Liouville space in the bra-ket notation will be distinguished by double brackets. The scalar product we define as

$$\langle\!\langle A|B\rangle\!\rangle \equiv \mathrm{Tr}\,\{A^\dagger B\} \,.$$

For example, commutator is simple superoperator

$$\mathcal{A}_{-}X \equiv AX - XA \,.$$

2.2 Reduced density operator

For the description of the dissipative model we must distinguish between the system (e. g. electronic states of the dots) and the heat bath. The task is to get an equation for a reduced density operator which is the system part of the density operator.

Let us note the quantities corresponding to the system subspace by the subscript S and the quantities corresponding to the heat bath subspace by the subscript B. The projection superoperator on the system subspace is

$$\mathcal{P} = \varrho_{\mathrm{B}} \otimes \mathrm{Tr}_{\mathrm{B}} \, .$$

The most convenient choice of ϱ_{B} is a thermal equilibrium density operator

$$\varrho_{\mathrm{B}} = \frac{\exp\left(-\beta H_{\mathrm{B}}\right)}{\mathrm{Tr}_{\mathrm{B}}\left\{\exp\left(-\beta H_{\mathrm{B}}\right)\right\}} \, .$$

We also define $\mathcal{Q} = 1 - \mathcal{P}$. These superoperators have the following properties $\mathcal{P}^2 = \mathcal{P}$, $\mathcal{Q}^2 = \mathcal{Q}$ and $\mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0$, thus we can call them projection superoperators.

Inserting the projection superoperators into the Liouville equation

$$\mathrm{i}\hbar \frac{\mathrm{d}\varrho}{\mathrm{d}t} = [H, \varrho] = \mathcal{H}_{-}\varrho$$

yields two equations

$$\mathrm{i}\hbar \frac{\mathrm{d}\mathcal{P}\varrho(t)}{\mathrm{d}t} = \mathcal{P}\mathcal{H}_{-}\mathcal{P}\varrho(t) + \mathcal{P}\mathcal{H}_{-}\mathcal{Q}\varrho(t) \, , \tag{2.1}$$

$$\mathrm{i}\hbar \frac{\mathrm{d}\mathcal{Q}\varrho(t)}{\mathrm{d}t} = \mathcal{Q}\mathcal{H}_{-}\mathcal{P}\varrho(t) + \mathcal{Q}\mathcal{H}_{-}\mathcal{Q}\varrho(t) \, , \tag{2.2}$$

which is the system of equations for $\mathcal{P}\varrho(t)$ and $\mathcal{Q}\varrho(t)$. The second one can be solved with respect to the $\mathcal{Q}\varrho(t)$

$$\mathcal{Q}\varrho(t) = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' \exp\left[-\mathrm{i}\mathcal{Q}\mathcal{H}_{-}(t-t')/\hbar\right]\mathcal{Q}\mathcal{H}_{-}\mathcal{P}\varrho(t') + \exp\left[-\mathrm{i}\mathcal{Q}\mathcal{H}_{-}t/\hbar\right]\mathcal{Q}\varrho(0) \, .$$

We assume that the system and the bath are initially independent, so that the total density operator factorizes into a direct product $\varrho(0) = \varrho_{\mathrm{S}}(0) \otimes \varrho_{\mathrm{B}}$, where ϱ_{S} is an arbitrary system density matrix. Due to this initial condition it holds $\mathcal{Q}\varrho(0) = \varrho(0) - \mathcal{P}\varrho(0) = 0$.

If we substitute $\mathcal{Q}\varrho(t)$ into the first equation (2.1), we obtain equation for the operator $\mathcal{P}\varrho(t)$ [6]

$$\frac{\mathrm{d}\mathcal{P}\varrho(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\mathcal{P}\mathcal{H}_{-}\mathcal{P}\varrho(t) - \frac{1}{\hbar^2}\int_0^t \mathrm{d}t'\mathcal{P}\mathcal{H}_{-}\exp\left[-\mathrm{i}\mathcal{Q}\mathcal{H}_{-}(t-t')/\hbar\right]\mathcal{Q}\mathcal{H}_{-}\mathcal{P}\varrho(t') \, . \tag{2.3}$$

2.3 Derivation of generalized master equation

The total Hamiltonian is the sum $H = H_{\mathrm{S}} + H_{\mathrm{BS}} + H_{\mathrm{B}}$, where H_{BS} is Hamiltonian of a interaction between the system and the heat bath. Therefore superoperator $\mathcal{H}_-$ can be written as $\mathcal{H}_- = \mathcal{H}_{\mathrm{S}-} + \mathcal{H}_{\mathrm{BS}-} + \mathcal{H}_{\mathrm{B}-}$. We then use the following properties. The relation

$$\mathcal{P}\mathcal{H}_{\mathrm{S}-} = \mathcal{H}_{\mathrm{S}-}\mathcal{P}$$

is true, because $\mathcal{P}$ and $\mathcal{H}_{\mathrm{S}-}$ operate in different subspaces. The equality

$$\mathcal{P}\mathcal{H}_{\mathrm{B}-} = \mathcal{H}_{\mathrm{B}-}\mathcal{P}$$

is true because the equation of motion given by the bath Hamiltonian must conserve probability,

$$\mathcal{H}_{\mathrm{B}-}\mathcal{P} = 0$$

is true because of $\mathcal{H}_{\mathrm{B}-}\varrho_{\mathrm{B}} = 0$. Final property says

$$\mathcal{P}\mathcal{H}_{\mathrm{BS}-}\mathcal{P} = 0\,.$$

This is equivalent to $\mathrm{Tr}_{\mathrm{B}}\{[H_{\mathrm{BS}}, \varrho_{\mathrm{B}} \otimes \mathrm{Tr}_{\mathrm{B}}\{\varrho\}]\} = 0$, which means that the interaction H_{BS} has no diagonal elements in the representation in which H_{B} is diagonal. This is true for our future choices of H_{BS}.

The equation (2.3) on the Liouville space of the system has the form

$$\frac{\mathrm{d}\varrho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\mathcal{H}_{\mathrm{S}-}\varrho_{\mathrm{S}}(t) - \\ - \frac{1}{\hbar^2}\int_0^t \mathrm{d}t'\,\mathrm{Tr}_{\mathrm{B}}\{\mathcal{H}_{\mathrm{BS}-}\exp\left[-\mathrm{i}\mathcal{Q}\mathcal{H}_-(t-t')/\hbar\right]\mathcal{Q}\mathcal{H}_{\mathrm{BS}-}\varrho_{\mathrm{S}}(t')\otimes\varrho_{\mathrm{B}}\}\,,$$

where $\varrho_{\mathrm{S}} = \mathrm{Tr}_{\mathrm{B}}\{\varrho\}$ is the reduced density operator. At this point, we assume that H_{BS} is much smaller than either H_{B} or H_{S} and that the reservoir is so large that its density operator is not significantly affected by the interaction (weak coupling assumption). Thus we neglect all terms proportional to more than the second order of interaction.

$$\frac{\mathrm{d}\varrho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\mathcal{H}_{\mathrm{S}-}\varrho_{\mathrm{S}}(t) - \\ - \frac{1}{\hbar^2}\int_0^t \mathrm{d}t'\,\mathrm{Tr}_{\mathrm{B}}\{\mathcal{H}_{\mathrm{BS}-}\exp\left[-\mathrm{i}(\mathcal{H}_{\mathrm{S}-}+\mathcal{H}_{\mathrm{B}-})(t-t')/\hbar\right]\mathcal{H}_{\mathrm{BS}-}\varrho_{\mathrm{S}}(t')\otimes\varrho_{\mathrm{B}}\}\,.$$

The reduced density operator has fast oscillating off-diagonal elements (their frequency is of order difference between electronic energy levels), so we try introduce $\varrho'(t) = \exp\left[\mathrm{i}\mathcal{H}_{\mathrm{S}-}t/\hbar\right]\varrho(t)$ (interaction picture) which has no such oscillating

elements.

$$\frac{\mathrm{d}\varrho'_{\mathrm{S}}(t)}{\mathrm{d}t} = -\frac{1}{\hbar^2}\mathrm{e}^{\mathrm{i}\mathcal{H}_{\mathrm{S}-}t/\hbar} \times \\ \times \int_0^t \mathrm{d}t' \,\mathrm{Tr}_{\mathrm{B}}\{\mathcal{H}_{\mathrm{BS}-}\mathrm{e}^{-\mathrm{i}(\mathcal{H}_{\mathrm{S}-}+\mathcal{H}_{\mathrm{B}-})(t-t')/\hbar}\mathcal{H}_{\mathrm{BS}-}\mathrm{e}^{-\mathrm{i}\mathcal{H}_{\mathrm{S}-}t'/\hbar}\varrho'_{\mathrm{S}}(t') \otimes \varrho_{\mathrm{B}}\}\,.$$

The final approximation turns this into a differential equation. Since the interaction is assumed weak, the rate of change of the system density operator ϱ'_{S} (in the interaction picture) will be quite slow compared to that of bath operators which will vary on a time scale determined by H_{B}. Thus in the integration we can replace $\varrho'_{\mathrm{S}}(t')$ by $\varrho'_{\mathrm{S}}(t)$ and we can let the lower limit of the integral go to $-\infty$. We deduce equation

$$\frac{\mathrm{d}\varrho'_{\mathrm{S}}(t)}{\mathrm{d}t} = -\frac{1}{\hbar^2}\mathrm{e}^{\mathrm{i}\mathcal{H}_{\mathrm{S}-}t/\hbar} \times \\ \times \int_0^\infty \mathrm{d}\tau \,\mathrm{Tr}_{\mathrm{B}}\{\mathcal{H}_{\mathrm{BS}-}\mathrm{e}^{-\mathrm{i}(\mathcal{H}_{\mathrm{S}-}+\mathcal{H}_{\mathrm{B}-})\tau/\hbar}\mathcal{H}_{\mathrm{BS}-}\mathrm{e}^{-\mathrm{i}\mathcal{H}_{\mathrm{S}-}(t-\tau)/\hbar}\varrho'_{\mathrm{S}}(t) \otimes \varrho_{\mathrm{B}}\}\,.$$

This procedure is known as the Markov approximation since it yields a first order differential equation for $\varrho'_{\mathrm{S}}(t)$. This means that the knowledge of $\varrho'_{\mathrm{S}}(t)$ at one point in time $t = t_0$ is sufficient to determine $\varrho'_{\mathrm{S}}(t)$ for all $t > t_0$.

If we return to the Schrödinger picture, we obtain

$$\frac{\mathrm{d}\varrho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\mathcal{H}_{\mathrm{S}-}\varrho_{\mathrm{S}}(t) - \\ - \frac{1}{\hbar^2}\int_0^\infty \mathrm{d}\tau \,\mathrm{Tr}_{\mathrm{B}}\{\mathcal{H}_{\mathrm{BS}-}\mathrm{e}^{-\mathrm{i}(\mathcal{H}_{\mathrm{S}-}+\mathcal{H}_{\mathrm{B}-})\tau/\hbar}\mathcal{H}_{\mathrm{BS}-}\mathrm{e}^{\mathrm{i}\mathcal{H}_{\mathrm{S}-}\tau/\hbar}\varrho_{\mathrm{S}}(t) \otimes \varrho_{\mathrm{B}}\}\,.$$

Inserting the definitions of the superoperators involved, we get the final generalized master equation

$$\frac{\mathrm{d}\varrho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}[H_{\mathrm{S}}, \varrho_{\mathrm{S}}(t)] - \\ - \frac{1}{\hbar^2}\int_0^\infty \mathrm{d}\tau \,\mathrm{Tr}_{\mathrm{B}}\{[H_{\mathrm{BS}}, [H_{\mathrm{BS}}(-\tau), \varrho_{\mathrm{S}}(t) \otimes \varrho_{\mathrm{B}}]]\}\,,$$

$$\frac{\mathrm{d}\varrho_{\mathrm{S}}(t)}{\mathrm{d}t} = \mathcal{L}\varrho_{\mathrm{S}}(t) = \mathcal{L}_{\mathrm{S}}\varrho_{\mathrm{S}}(t) + \mathcal{L}_{\mathrm{B}}\varrho_{\mathrm{S}}(t)\,, \tag{2.4}$$

where $H_{\mathrm{BS}}(-\tau) = \exp[-\mathrm{i}(H_{\mathrm{S}} + H_{\mathrm{B}})\tau/\hbar]H_{\mathrm{BS}}\exp[\mathrm{i}(H_{\mathrm{S}} + H_{\mathrm{B}})\tau/\hbar]$. The superoperator $\mathcal{L}$ is called Liouvillian and it contains the whole dynamics of the system.

Chapter 3

Double quantum dot

3.1 Model

In this section we are going to describe the system of our interest – the double quantum dot device [2] (see fig. 3.1). There are two electron levels (the left dot and the right dot) separated by an energy difference ε with an interdot coupling Ω. The system is in the regime of strong Coulomb blockade that only three electron states play a role: no extra electron $|0\rangle$, one extra electron on the left dot $|\mathrm{L}\rangle$ and one extra electron on the right dot $|\mathrm{R}\rangle$. This can be achieved by a suitable gating, when a very high charging energy prohibits an addition of an other electron. Also we consider spinless electrons. Hamiltonian of the double quantum dot device reads

$$H_{\mathrm{S}} = \tfrac{1}{2}\varepsilon(|\mathrm{L}\rangle\langle\mathrm{L}| - |\mathrm{R}\rangle\langle\mathrm{R}|) + \Omega\,(|\mathrm{L}\rangle\langle\mathrm{R}| + |\mathrm{R}\rangle\langle\mathrm{L}|)\,. \tag{3.1}$$

The device bias ε can be induced by a suitable gating. The term proportional to Ω enables the tunneling current through the device.

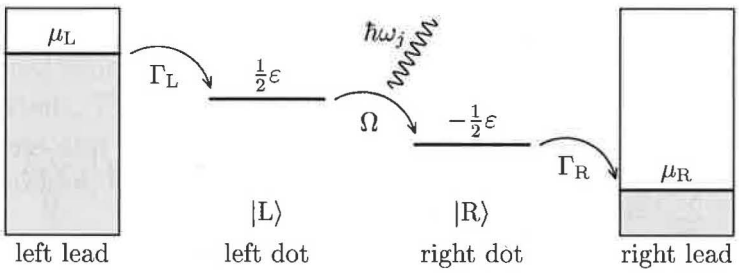

Fig. 3.1: System

The double quantum dot is coupled to two leads with a high bias applied between them. The bias is smaller than the charging energy but otherwise it is the largest energy scale in the model. We assume that the leads are coupled via standard tunneling terms

$$\begin{aligned} H_{\mathrm{C}} + H_{\mathrm{CS}} = &\sum_k E_{k\mathrm{L}} c_{k\mathrm{L}}^\dagger c_{k\mathrm{L}} + \sum_k V_{k\mathrm{L}}(c_{k\mathrm{L}}^\dagger|0\rangle\langle\mathrm{L}| + |\mathrm{L}\rangle\langle 0|c_{k\mathrm{L}}) + \\ &+ \sum_k E_{k\mathrm{R}} c_{k\mathrm{R}}^\dagger c_{k\mathrm{R}} + \sum_k V_{k\mathrm{R}}(c_{k\mathrm{R}}^\dagger|0\rangle\langle\mathrm{R}| + |\mathrm{R}\rangle\langle 0|c_{k\mathrm{R}})\,. \end{aligned} \tag{3.2}$$

The leads are held at electrochemical potentials μ_{L} and μ_{R}, their difference gives the bias. We assume that $\mu_{\mathrm{L}} \to \infty$ and $\mu_{\mathrm{R}} \to -\infty$. The tunneling densities of states

$$\Gamma_\alpha(\varepsilon) = \frac{2\pi}{\hbar} \sum_k |V_{k\alpha}|^2 \delta(\varepsilon - E_{k\alpha}) \tag{3.3}$$

are energy independent ($\alpha = \mathrm{L}, \mathrm{R}$) and equal $\Gamma_{\mathrm{L}} = \Gamma_{\mathrm{R}}$. This assumption is called the wide-band limit. Both the high bias limit and the wide-band limit are necessary for Markov approximation.

Finally, we introduce dissipative heat bath. The generic heat bath consists of an infinite set of harmonic oscillators linearly coupled to the double quantum dot

$$H_{\mathrm{B}} + H_{\mathrm{BS}} = \sum_j \hbar\omega_j (a_j^\dagger a_j + \tfrac{1}{2}) + \sum_j C_j (a_j^\dagger + a_j)(|\mathrm{L}\rangle\langle\mathrm{L}| - |\mathrm{R}\rangle\langle\mathrm{R}|)\,. \tag{3.4}$$

The heat bath is characterized by its spectral density

$$J(\omega) = 2\sum_j |C_j|^2 \delta(\omega - \omega_j)\,, \tag{3.5}$$

which is taken in the Ohmic form $J(\omega) = 2\hbar^2\gamma\omega/\pi \cdot \exp(-\omega/\omega_{\mathrm{c}})$ [7]. The parameter γ reflects the strength of the dissipation and ω_{c} is a high energy cut-off frequency.

It will be useful to write the interaction Hamiltonians in the basis of the system Hamiltonian eigenvectors $|0\rangle$, $|1\rangle$, $|2\rangle$.

$$H_{\mathrm{S}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2}\Delta & 0 \\ 0 & 0 & -\frac{1}{2}\Delta \end{pmatrix},$$

$$H_{\mathrm{BS}} = \sum_j C_j (a_j^\dagger + a_j) \frac{1}{\Delta} \begin{pmatrix} 0 & 0 & 0 \\ 0 & \varepsilon & -2\Omega \\ 0 & -2\Omega & -\varepsilon \end{pmatrix},$$

$$H_{\mathrm{CS}} = \sum_k V_{k\mathrm{L}} \frac{1}{\sqrt{2\Delta}} \begin{pmatrix} 0 & c_{k\mathrm{L}}^\dagger\sqrt{\Delta+\varepsilon} & -c_{k\mathrm{L}}^\dagger\sqrt{\Delta-\varepsilon} \\ c_{k\mathrm{L}}\sqrt{\Delta+\varepsilon} & 0 & 0 \\ -c_{k\mathrm{L}}\sqrt{\Delta-\varepsilon} & 0 & 0 \end{pmatrix}$$
$$+ \sum_k V_{k\mathrm{R}} \frac{1}{\sqrt{2\Delta}} \begin{pmatrix} 0 & c_{k\mathrm{R}}^\dagger\sqrt{\Delta-\varepsilon} & c_{k\mathrm{R}}^\dagger\sqrt{\Delta+\varepsilon} \\ c_{k\mathrm{R}}\sqrt{\Delta-\varepsilon} & 0 & 0 \\ c_{k\mathrm{R}}\sqrt{\Delta+\varepsilon} & 0 & 0 \end{pmatrix},$$

where $\Delta = \sqrt{4\Omega^2 + \varepsilon^2}$. The change-of-basis matrix elements are

$$\langle\mathrm{L}|1\rangle = \sqrt{\frac{\Delta+\varepsilon}{2\Delta}}, \qquad \langle\mathrm{L}|2\rangle = -\sqrt{\frac{\Delta-\varepsilon}{2\Delta}},$$
$$\langle\mathrm{R}|1\rangle = \sqrt{\frac{\Delta-\varepsilon}{2\Delta}}, \qquad \langle\mathrm{R}|2\rangle = \sqrt{\frac{\Delta+\varepsilon}{2\Delta}}.$$

3.2 Generalized master equation

Starting from the generalized master equation (2.4) and including also leads reservoirs, we get

$$\begin{aligned}\frac{\mathrm{d}\varrho_{\mathrm{S}}(t)}{\mathrm{d}t} &= -\frac{\mathrm{i}}{\hbar}[H_{\mathrm{S}}, \varrho_{\mathrm{S}}(t)] - \\ &\quad - \frac{1}{\hbar^2}\int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_{\mathrm{B}}\{[H_{\mathrm{BS}}, [H_{\mathrm{BS}}(-\tau), \varrho_{\mathrm{S}}(t)\otimes\varrho_{\mathrm{B}}]]\} - \\ &\quad - \frac{1}{\hbar^2}\int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_{\mathrm{C}}\{[H_{\mathrm{CS}}, [H_{\mathrm{CS}}(-\tau), \varrho_{\mathrm{S}}(t)\otimes\varrho_{\mathrm{C}}]]\} \\ \frac{\mathrm{d}\varrho_{\mathrm{S}}(t)}{\mathrm{d}t} &= \mathcal{L}\varrho_{\mathrm{S}}(t) = \mathcal{L}_{\mathrm{S}}\varrho_{\mathrm{S}}(t) + \mathcal{L}_{\mathrm{B}}\varrho_{\mathrm{S}}(t) + \mathcal{L}_{\mathrm{C}}\varrho_{\mathrm{S}}(t)\,, \end{aligned} \tag{3.6}$$

It means we have made all assumptions described in the previous chapter, in particular product initial condition, the weak coupling prescription and the Markovian dynamics.

The goal of this section is to find expression of the Liouvillian.

System Liouvillian

We begin with the simplest part $\mathcal{L}_{\mathrm{S}}$, which describes the free evolution of the system.

$$\mathcal{L}_{\mathrm{S}}\varrho_{\mathrm{S}} = -\frac{\mathrm{i}}{\hbar}[H_{\mathrm{S}}, \varrho_{\mathrm{S}}] = \frac{\mathrm{i}\Delta}{2\hbar}\begin{pmatrix} 0 & \varrho_{01} & -\varrho_{02} \\ -\varrho_{10} & 0 & -2\varrho_{12} \\ \varrho_{20} & 2\varrho_{21} & 0 \end{pmatrix},$$

The off-diagonal block elements ϱ_{0k}, ϱ_{k0} with $k = 1, 2$ are decoupled from the rest of the system. That means that they do not enter expressions for the other matrix elements and their time evolution does not depend on the other matrix elements. Therefore, they can be projected out leaving us the Liouville space with the basis

$$\{|00\rangle\!\rangle, |11\rangle\!\rangle, |22\rangle\!\rangle, |21\rangle\!\rangle, |12\rangle\!\rangle\}\,. \tag{12-basis}$$

In this basis the Liouvillian $\mathcal{L}_{\mathrm{S}}$ has the form

$$\mathcal{L}_{\mathrm{S}} = \frac{1}{\hbar}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathrm{i}\Delta & 0 \\ 0 & 0 & 0 & 0 & -\mathrm{i}\Delta \end{pmatrix}. \tag{3.7}$$

In the basis

$$\{|00\rangle\!\rangle, |\mathrm{LL}\rangle\!\rangle, |\mathrm{RR}\rangle\!\rangle, |\mathrm{RL}\rangle\!\rangle, |\mathrm{LR}\rangle\!\rangle\} \tag{LR-basis}$$

Liouvillian $\mathcal{L}_\mathrm{S}$ reads

$$\mathcal{L}_\mathrm{S} = \frac{1}{\hbar}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathrm{i}\Omega & \mathrm{i}\Omega \\ 0 & 0 & 0 & \mathrm{i}\Omega & -\mathrm{i}\Omega \\ 0 & -\mathrm{i}\Omega & \mathrm{i}\Omega & \mathrm{i}\varepsilon & 0 \\ 0 & \mathrm{i}\Omega & -\mathrm{i}\Omega & 0 & -\mathrm{i}\varepsilon \end{pmatrix}. \tag{3.8}$$

Heat bath Liouvillian

A calculation of the $\mathcal{L}_\mathrm{B}$ is straightforward. After the integration over time, the Liouvillian elements in the 12-basis are

$$\begin{aligned}(\mathcal{L}_\mathrm{B})_{kl,mn} = \\ &= \frac{\pi}{\hbar}\sum_j |C_j|^2 T_{km}T_{nl}\big(\langle a_j a_j^\dagger\rangle\delta(\varepsilon_l - \varepsilon_n + \hbar\omega_j) + \langle a_j^\dagger a_j\rangle\delta(\varepsilon_l - \varepsilon_n - \hbar\omega_j)\big) \\ &+ \frac{\pi}{\hbar}\sum_j |C_j|^2 T_{km}T_{nl}\big(\langle a_j^\dagger a_j\rangle\delta(\varepsilon_m - \varepsilon_k + \hbar\omega_j) + \langle a_j a_j^\dagger\rangle\delta(\varepsilon_m - \varepsilon_k - \hbar\omega_j)\big) \\ &- \frac{\pi}{\hbar}\sum_{j,q} |C_j|^2 T_{kq}T_{qm}\delta_{nl}\big(\langle a_j^\dagger a_j\rangle\delta(\varepsilon_m - \varepsilon_q + \hbar\omega_j) + \langle a_j a_j^\dagger\rangle\delta(\varepsilon_m - \varepsilon_q - \hbar\omega_j)\big) \\ &- \frac{\pi}{\hbar}\sum_{j,q} |C_j|^2 T_{nq}T_{ql}\delta_{km}\big(\langle a_j a_j^\dagger\rangle\delta(\varepsilon_q - \varepsilon_n + \hbar\omega_j) + \langle a_j^\dagger a_j\rangle\delta(\varepsilon_q - \varepsilon_n - \hbar\omega_j)\big),\end{aligned}$$

where T_{mn} are matrix elements of the system part of H_BS ($T_{11} = -T_{22} = \varepsilon/\Delta$, $T_{12} = T_{21} = -2\Omega/\Delta$, otherwise $T_{mn} = 0$) and ε_i are the system eigenenergies ($\varepsilon_0 = 0$, $\varepsilon_1 = \frac{1}{2}\Delta$, $\varepsilon_2 = -\frac{1}{2}\Delta$). Principal value integrals are omitted because they give rise to rather small frequency shifts, known as the Stark shift and the Lamb shift. As we know, the bath density operator is not significantly changed by an interaction, so $\langle a_j^\dagger a_j\rangle = N(\hbar\omega_j)$ represents Bose-Einstein mean occupation number

$$N(\hbar\omega) = \frac{1}{\exp(\beta\hbar\omega) - 1}.$$

Commutation relations for a_j, $a_j^\dagger$ determines $\langle a_j a_j^\dagger\rangle = N(\hbar\omega_j) + 1$.

If we consider the bath spectral density $J(\omega)$, we can perform summations over j

$$\begin{aligned}(\mathcal{L}_\mathrm{B})_{kl,mn} = \frac{\pi}{\hbar^2}T_{km}T_{nl}N(\hbar\omega_{ln})J(\omega_{ln}) + \frac{\pi}{\hbar^2}T_{km}T_{nl}N(\hbar\omega_{km})J(\omega_{km}) \\ - \frac{\pi}{\hbar^2}\sum_q T_{kq}T_{qm}\delta_{nl}N(\hbar\omega_{qm})J(\omega_{qm}) - \frac{\pi}{\hbar^2}\sum_q T_{nq}T_{ql}\delta_{km}N(\hbar\omega_{qn})J(\omega_{qn}),\end{aligned} \tag{3.9}$$

where $\omega_{mn} = (\varepsilon_m - \varepsilon_n)/\hbar$ and for purpose of shorter expression of the last formula we define $J(\omega) = -J(-\omega)$ for $\omega < 0$. After the last summation we find the matrix

form of $\mathcal{L}_{\mathrm{B}}$

$$\mathcal{L}_{\mathrm{B}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -\gamma_{\downarrow} & \gamma_{\uparrow} & 0 & 0 \\ 0 & \gamma_{\downarrow} & -\gamma_{\uparrow} & 0 & 0 \\ 0 & -\frac{\varepsilon}{2\Omega}\gamma_{\downarrow} & \frac{\varepsilon}{2\Omega}\gamma_{\uparrow} & -\frac{1}{2}\gamma_p & \frac{1}{2}\gamma_p \\ 0 & -\frac{\varepsilon}{2\Omega}\gamma_{\downarrow} & \frac{\varepsilon}{2\Omega}\gamma_{\uparrow} & \frac{1}{2}\gamma_p & -\frac{1}{2}\gamma_p \end{pmatrix}, \tag{3.10}$$

where

$$\begin{aligned} \gamma_{\downarrow} &= \frac{4\pi}{\hbar^2}\frac{\Omega^2}{\Delta^2} J(\Delta/\hbar)\frac{1}{1-\mathrm{e}^{-\beta\Delta}}, \\ \gamma_{\uparrow} &= \frac{4\pi}{\hbar^2}\frac{\Omega^2}{\Delta^2} J(\Delta/\hbar)\frac{1}{\mathrm{e}^{\beta\Delta}-1}, \\ \gamma_p &= \frac{4\pi}{\hbar^2}\frac{\Omega^2}{\Delta^2} J(\Delta/\hbar)\coth\left(\tfrac{1}{2}\beta\Delta\right). \end{aligned}$$

Other matrix elements are zero. In the LR-basis we obtain result [8, 4]

$$\mathcal{L}_{\mathrm{B}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \gamma_+ & -\gamma_- & -\gamma_p & 0 \\ 0 & \gamma_+ & -\gamma_- & 0 & -\gamma_p \end{pmatrix}, \tag{3.11}$$

where

$$\begin{aligned} \gamma_{\pm} &= -\frac{\pi}{\hbar^2}\frac{\Omega}{\Delta} J(\Delta/\hbar)\left[\frac{\varepsilon}{\Delta}\coth\left(\tfrac{1}{2}\beta\Delta\right)\pm 1\right] = -\frac{2\gamma}{\hbar}\Omega\left[\frac{\varepsilon}{\Delta}\coth\left(\tfrac{1}{2}\beta\Delta\right)\pm 1\right], \\ \gamma_p &= \frac{4\pi}{\hbar^2}\frac{\Omega^2}{\Delta^2} J(\Delta/\hbar)\coth\left(\tfrac{1}{2}\beta\Delta\right) = \frac{8\gamma}{\hbar}\frac{\Omega^2}{\Delta}\coth\left(\tfrac{1}{2}\beta\Delta\right). \end{aligned}$$

The second equality in the each equation holds only for the Ohmic bath.

Leads Liouvillian

In the case of the leads reservoir, we will proceed in a similar manner. After integration over time, the matrix elements of the Liouvillian $\mathcal{L}_{\mathrm{C}}$ have a form

$$\begin{aligned}(\mathcal{L}_{\mathrm{C}})_{kl,mn} = \frac{\pi}{\hbar}\sum_{j\alpha}|V_{j\alpha}|^2(A_{km\alpha}A^{\dagger}_{nl\alpha}\langle c_{j\alpha}c^{\dagger}_{j\alpha}\rangle\delta(\varepsilon_l-\varepsilon_n+E_{j\alpha})+\\ +A^{\dagger}_{km\alpha}A_{nl\alpha}\langle c^{\dagger}_{j\alpha}c_{j\alpha}\rangle\delta(\varepsilon_l-\varepsilon_n-E_{j\alpha}))+\\ +\frac{\pi}{\hbar}\sum_{j\alpha}|V_{j\alpha}|^2(A^{\dagger}_{km\alpha}A_{nl\alpha}\langle c^{\dagger}_{j\alpha}c_{j\alpha}\rangle\delta(\varepsilon_m-\varepsilon_k+E_{j\alpha})+\\ +A_{km\alpha}A^{\dagger}_{nl\alpha}\langle c_{j\alpha}c^{\dagger}_{j\alpha}\rangle\delta(\varepsilon_m-\varepsilon_k-E_{j\alpha}))-\\ -\frac{\pi}{\hbar}\sum_{j\alpha,q}|V_{j\alpha}|^2\delta_{nl}(A_{kq\alpha}A^{\dagger}_{qm\alpha}\langle c^{\dagger}_{j\alpha}c_{j\alpha}\rangle\delta(\varepsilon_m-\varepsilon_q+E_{j\alpha})+\\ +A^{\dagger}_{kq\alpha}A_{qm\alpha}\langle c_{j\alpha}c^{\dagger}_{j\alpha}\rangle\delta(\varepsilon_m-\varepsilon_q-E_{j\alpha}))-\\ -\frac{\pi}{\hbar}\sum_{j\alpha,q}|V_{j\alpha}|^2\delta_{km}(A^{\dagger}_{nq\alpha}A_{ql\alpha}\langle c_{j\alpha}c^{\dagger}_{j\alpha}\rangle\delta(\varepsilon_q-\varepsilon_n+E_{j\alpha})+\\ +A_{nq\alpha}A^{\dagger}_{ql\alpha}\langle c^{\dagger}_{j\alpha}c_{j\alpha}\rangle\delta(\varepsilon_q-\varepsilon_n-E_{j\alpha}))\,,\end{aligned}$$

with $\alpha = \mathrm{L},\mathrm{R}$. The $A_{mn\alpha}$ are the matrix elements of the system operator $|0\rangle\langle\alpha|$ ($A_{01\mathrm{L}} = A_{02\mathrm{R}} = \sqrt{(\Delta+\varepsilon)/2\Delta}$, $A_{01\mathrm{R}} = -A_{02\mathrm{L}} = \sqrt{(\Delta-\varepsilon)/2\Delta}$, otherwise $A_{mn\alpha} = 0$). The principal value integrals are again omitted. In this case, the mean occupation number $\langle c^{\dagger}_{j\alpha}c_{j\alpha}\rangle = f_{j\alpha}$ is given by Fermi-Dirac statistics

$$f_{j\alpha} = \frac{1}{\exp(\beta(E_{j\alpha}-\mu_\alpha))+1}\,.$$

The anticommutation relations for c_j, $c^{\dagger}_j$ determine $\langle c_{j\alpha}c^{\dagger}_{j\alpha}\rangle = 1 - f_{j\alpha}$.

The definition of the tunneling densities of states allows us to perform summation over j

$$\begin{aligned}(\mathcal{L}_{\mathrm{C}})_{kl,mn} = \sum_{\alpha}\Gamma(A_{km\alpha}A^{\dagger}_{nl\alpha}(1-f_\alpha)+A^{\dagger}_{km\alpha}A_{nl\alpha}f_\alpha)\\ -\tfrac{1}{2}\sum_{\alpha,q}\Gamma\delta_{nl}(A_{kq\alpha}A^{\dagger}_{qm\alpha}f_\alpha+A^{\dagger}_{kq\alpha}A_{qm\alpha}(1-f_\alpha))\\ -\tfrac{1}{2}\sum_{\alpha,q}\Gamma\delta_{km}(A^{\dagger}_{nq\alpha}A_{ql\alpha}(1-f_\alpha)+A_{nq\alpha}A^{\dagger}_{ql\alpha}f_\alpha)\,,\end{aligned}$$

we have also used wide-band limit and $\Gamma_{\mathrm{L}} = \Gamma_{\mathrm{R}}$ assumption. Our high bias assumption implies $f_{j\mathrm{L}} \to 1$ and $f_{j\mathrm{R}} \to 0$.

$$\begin{aligned}(\mathcal{L}_{\mathrm{C}})_{kl,mn} = \Gamma(A^{\dagger}_{km\mathrm{L}}A_{nl\mathrm{L}}+A_{km\mathrm{R}}A^{\dagger}_{nl\mathrm{R}})\\ -\tfrac{1}{2}\sum_{q}\Gamma\delta_{nl}(A_{kq\mathrm{L}}A^{\dagger}_{qm\mathrm{L}}+A^{\dagger}_{kq\mathrm{R}}A_{qm\mathrm{R}})\\ -\tfrac{1}{2}\sum_{q}\Gamma\delta_{km}(A_{nq\mathrm{L}}A^{\dagger}_{ql\mathrm{L}}+A^{\dagger}_{nq\mathrm{R}}A_{ql\mathrm{R}})\,.\end{aligned}$$

We are now ready to write the final expression for $\mathcal{L}_{\mathrm{C}}$

$$\mathcal{L}_{\mathrm{C}} = \begin{pmatrix} -\Gamma_{10}-\Gamma_{20} & \Gamma_{01} & \Gamma_{02} & \Gamma\frac{T}{\Delta} & \Gamma\frac{T}{\Delta} \\ \Gamma_{10} & -\Gamma_{01} & 0 & -\frac{1}{2}\Gamma\frac{T}{\Delta} & -\frac{1}{2}\Gamma\frac{T}{\Delta} \\ \Gamma_{20} & 0 & -\Gamma_{02} & -\frac{1}{2}\Gamma\frac{T}{\Delta} & -\frac{1}{2}\Gamma\frac{T}{\Delta} \\ -\Gamma\frac{T}{\Delta} & -\frac{1}{2}\Gamma\frac{T}{\Delta} & -\frac{1}{2}\Gamma\frac{T}{\Delta} & -\frac{1}{2}(\Gamma_{01}+\Gamma_{02}) & 0 \\ -\Gamma\frac{T}{\Delta} & -\frac{1}{2}\Gamma\frac{T}{\Delta} & -\frac{1}{2}\Gamma\frac{T}{\Delta} & 0 & -\frac{1}{2}(\Gamma_{01}+\Gamma_{02}) \end{pmatrix}, \quad (3.12)$$

where

$$\Gamma_{10} = \Gamma_{02} = \Gamma\frac{\Delta+\varepsilon}{2\Delta}, \qquad \Gamma_{01} = \Gamma_{20} = \Gamma\frac{\Delta-\varepsilon}{2\Delta}.$$

Same as in the previous case of the system Liouvillian $\mathcal{L}_{\mathrm{S}}$, it can be shown that the other matrix elements are decoupled. In the LR-basis we obtain result

$$\mathcal{L}_{\mathrm{C}} = \begin{pmatrix} -\Gamma & 0 & \Gamma & 0 & 0 \\ \Gamma & 0 & 0 & 0 & 0 \\ 0 & 0 & -\Gamma & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2}\Gamma & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2}\Gamma \end{pmatrix}. \quad (3.13)$$

Validity of our result goes beyond the weak coupling limit, because exactly the same Liouvillian was derived by Gurvitz [9] within the only high bias assumption. Nevertheless, the dynamics are still Markovian due to the energy independent tunneling density of states $\Gamma(E) \equiv \Gamma$.

As we have already mentioned, the off-diagonal block elements of the density matrix between system states containing a different number of electrons are decoupled or zero. Therefore the total Liouvillian matrix elements $\mathcal{L}_{mn,0k}$, $\mathcal{L}_{mn,k0}$, $\mathcal{L}_{0k,mn}$, $\mathcal{L}_{k0,mn}$ with $k = 1, 2$ are identically zero. The subspace $\{|0k\rangle\!\rangle, |k0\rangle\!\rangle\}$ can be projected out. Moreover, the elements which have been projected out do not enter any expression for quantities of physical interest we consider. Our choice of the LR-basis or the 12-basis is now justified.

3.3 Current noise

In this section we will show how to calculate current noise spectra for the different junctions.

Charge current operators

Let us begin with equations of motion for the operators of the occupation of the left dot $n_{\mathrm{L}} = |\mathrm{L}\rangle\langle\mathrm{L}|$ and the right dot $n_{\mathrm{R}} = |\mathrm{R}\rangle\langle\mathrm{R}|$

$$e\frac{\mathrm{d}}{\mathrm{d}t}n_{\mathrm{L}} = -\frac{\mathrm{i}e}{\hbar}[n_{\mathrm{L}}, H] = I_{\mathrm{L0}} - I_{\mathrm{RL}}, \quad (3.14)$$

$$e\frac{\mathrm{d}}{\mathrm{d}t}n_{\mathrm{R}} = -\frac{\mathrm{i}e}{\hbar}[n_{\mathrm{R}}, H] = I_{\mathrm{RL}} - I_{\mathrm{0R}}. \quad (3.15)$$

On the right side of the equations, we identify charge current operators across the different junctions (I_{L0} is the operator of the current between the left lead and the left dot, I_{RL} is the operator of the current between the dots and I_{0R} is the operator of the current between the right dot and the right lead).

$$I_{\mathrm{L0}} = -\frac{\mathrm{i}e}{\hbar}[n_{\mathrm{L}}, H_{\mathrm{CS}}] = \frac{\mathrm{i}e}{\hbar}\sum_k V_{k\mathrm{L}}(c_{k\mathrm{L}}^\dagger|0\rangle\langle \mathrm{L}| - |\mathrm{L}\rangle\langle 0|c_{k\mathrm{L}})\,, \tag{3.16}$$

$$I_{\mathrm{RL}} = \frac{\mathrm{i}e}{\hbar}[n_{\mathrm{L}}, H_{\mathrm{S}}] = -\frac{\mathrm{i}e}{\hbar}[n_{\mathrm{R}}, H_{\mathrm{S}}] = \frac{\mathrm{i}e}{\hbar}\Omega(|\mathrm{L}\rangle\langle \mathrm{R}| - |\mathrm{R}\rangle\langle \mathrm{L}|)\,, \tag{3.17}$$

$$I_{\mathrm{0R}} = \frac{\mathrm{i}e}{\hbar}[n_{\mathrm{R}}, H_{\mathrm{CS}}] = \frac{\mathrm{i}e}{\hbar}\sum_k V_{k\mathrm{R}}(|\mathrm{R}\rangle\langle 0|c_{k\mathrm{R}} - c_{k\mathrm{R}}^\dagger|0\rangle\langle \mathrm{R}|)\,. \tag{3.18}$$

Commutators with the bath operators are zero $[n_{\mathrm{L}}, H_{\mathrm{BS}}] = [n_{\mathrm{R}}, H_{\mathrm{BS}}] = 0$, therefore the heat bath gives no contribution to the current.

It will be useful to express these current operators in the 12-basis

$$\begin{aligned}
I_{\mathrm{L0}} &= \frac{\mathrm{i}e}{\hbar}\sum_k V_{k\mathrm{L}}\left[c_{k\mathrm{L}}^\dagger\left(\sqrt{\frac{\Delta+\varepsilon}{2\Delta}}|0\rangle\langle 1| - \sqrt{\frac{\Delta-\varepsilon}{2\Delta}}|0\rangle\langle 2|\right) - \right.\\
&\qquad \left. - \left(\sqrt{\frac{\Delta+\varepsilon}{2\Delta}}|1\rangle\langle 0| - \sqrt{\frac{\Delta-\varepsilon}{2\Delta}}|2\rangle\langle 0|\right)c_{k\mathrm{L}}\right]\,,\\
I_{\mathrm{RL}} &= \frac{\mathrm{i}e}{\hbar}\Omega(|1\rangle\langle 2| - |2\rangle\langle 1|)\,,\\
I_{\mathrm{0R}} &= \frac{\mathrm{i}e}{\hbar}\sum_k V_{k\mathrm{L}}\left[\left(\sqrt{\frac{\Delta-\varepsilon}{2\Delta}}|1\rangle\langle 0| + \sqrt{\frac{\Delta+\varepsilon}{2\Delta}}|2\rangle\langle 0|\right)c_{k\mathrm{R}} - \right.\\
&\qquad \left. - c_{k\mathrm{R}}^\dagger\left(\sqrt{\frac{\Delta-\varepsilon}{2\Delta}}|0\rangle\langle 1| + \sqrt{\frac{\Delta+\varepsilon}{2\Delta}}|0\rangle\langle 2|\right)\right]\,.
\end{aligned}$$

The current operator I_{RL} is obviously system operator, i. e. it acts as unity on the degrees of freedom of the leads and the heat bath. However, this is not the case of the operators of current between the dots and the leads I_{L0} and I_{0R}.

Definition of current noise

Next we define current autocorrelation function.

$$C_A(\tau) \equiv \lim_{t\to\infty}\left[\tfrac{1}{2}\langle\{I_A(t+\tau), I_A(t)\}\rangle - \langle I_A(t+\tau)\rangle\langle I_A(t)\rangle\right] \tag{3.19}$$

with $A = \mathrm{L0}, \mathrm{RL}, \mathrm{0R}$. We can note the property $C_A(\tau) = C_A(-\tau)$ since in the stationary limit

$$\lim_{t\to\infty}\langle I_A(t+\tau)I_A(t)\rangle = \lim_{t\to\infty}\langle I_A(t)I_A(t-\tau)\rangle\,.$$

We define the current noise spectrum as

$$S_A(\omega) \equiv \int_{-\infty}^{\infty} \mathrm{d}\tau C_A(\tau) \mathrm{e}^{\mathrm{i}\omega\tau} . \tag{3.20}$$

The current noise is non-negative as can be shown by using the Lehmann representation.

Formulas for the current noise will be found by projection technique [5].

Quantum regression theorem

The dynamics of the device described by the generalized master equation (2.4) is Markovian. The Liouvillian $\mathcal{L} = \mathcal{L}_\mathrm{S} + \mathcal{L}_\mathrm{B} + \mathcal{L}_\mathrm{C}$ determines the evolution superoperator $\exp(\mathcal{L}t)$, which fully characterizes the resulting quantum Markov process $\varrho(t+\tau) = \exp(\mathcal{L}\tau)\varrho(t)$. Using quantum regression theorem ([10], Sec. 5.2) we are able to calculate multitime correlation functions of *system operators*

$$\langle A(t+\tau)B(t)\rangle = \mathrm{Tr}_\mathrm{S}\{A \exp(\mathcal{L}\tau)(B\varrho_\mathrm{S}(t))\} .$$

Thus we can evaluate the correlation function $C_\mathrm{RL}(\tau)$, because I_RL is a system operator. Direct application of the quantum regression theorem yields

$$C_\mathrm{RL}(\tau) = \tfrac{1}{2}\,\mathrm{Tr}_\mathrm{S}\{I_\mathrm{RL} \exp(\mathcal{L}\tau)\{I_\mathrm{RL}, \varrho_\mathrm{stat}\}\} - \langle I_\mathrm{RL}\rangle^2 ,$$

where ϱ_stat is the stationary limit ($t \to \infty$) of $\varrho_\mathrm{S}(t)$ and $\langle I_\mathrm{RL}\rangle = \mathrm{Tr}_\mathrm{S}\{I_\mathrm{RL}\varrho_\mathrm{stat}\}$ is the stationary current.

Now we separate the expression for the current noise spectrum into two terms

$$S_\mathrm{RL}(\omega) = \int_0^\infty \mathrm{d}\tau C_\mathrm{RL}(\tau)\mathrm{e}^{\mathrm{i}\omega\tau} + \int_0^\infty \mathrm{d}\tau C_\mathrm{RL}(\tau)\mathrm{e}^{-\mathrm{i}\omega\tau} .$$

In the following we consider only the first term $S^+_\mathrm{RL}(\omega)$, result for the second one $S^-_\mathrm{RL}(\omega)$ will be analogous. Introducing a convergence factor $\omega \to \omega + \mathrm{i}0$ we get

$$S^+_\mathrm{RL}(\omega) = \frac{1}{2}\,\mathrm{Tr}_\mathrm{S}\{I_\mathrm{RL}(-\mathrm{i}\omega - \mathcal{L})^{-1}\{I_\mathrm{RL}, \varrho_\mathrm{stat}\}\} + \frac{1}{\mathrm{i}\omega}\langle I_\mathrm{RL}\rangle^2 .$$

Since we are interested in the zero-frequency noise $S_\mathrm{RL}(0)$ and therefore the limit $\omega \to 0$, we have to handle somehow the singularities associated with the resolvent $(-\mathrm{i}\omega - \mathcal{L})^{-1}$ and $1/\mathrm{i}\omega$ in that limit. The problem emerges because of non-trivial kernel of the superoperator $\mathcal{L}$. The stationary density matrix satisfies $\mathcal{L}\varrho_\mathrm{stat} = 0$, hence it is zero eigenvalue eigenstate of the Liouvillian $\varrho_\mathrm{stat} \equiv |0\rangle\!\rangle$. Since the Liouvillian is not Hermitian, left zero eigenvalue eigenstate denoted by $\langle\!\langle\tilde{0}|$ is not just the Hermitian conjugate of right zero eigenvalue eigenstate $|0\rangle\!\rangle$. But we can see that $1 = \langle\!\langle\tilde{0}|$, because for an arbitrary system operator A

$$0 = \mathrm{Tr}_\mathrm{S}\{\mathcal{L}A\} = \mathrm{Tr}_\mathrm{S}\{1\mathcal{L}A\} = \langle\!\langle\tilde{0}|\mathcal{L}|A\rangle\!\rangle .$$

We define the projector on the kernel $\mathcal{P} \equiv |0\rangle\!\rangle\langle\!\langle\tilde{0}|$ and $\mathcal{Q} \equiv 1 - \mathcal{P}$. Then $\mathcal{P}\mathcal{L} = \mathcal{L}\mathcal{P} = 0$, $\mathcal{L} = \mathcal{Q}\mathcal{L}\mathcal{Q}$ and the resolvent can be expressed as

$$(-\mathrm{i}\omega - \mathcal{L})^{-1} = (-\mathrm{i}\omega\mathcal{P} - \mathrm{i}\omega\mathcal{Q} - \mathcal{Q}\mathcal{L}\mathcal{Q})^{-1} = -\frac{1}{\mathrm{i}\omega}\mathcal{P} - \mathcal{Q}\frac{1}{\mathrm{i}\omega + \mathcal{L}}\mathcal{Q} \approx -\frac{1}{\mathrm{i}\omega}\mathcal{P} - \mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}$$

in leading order for small ω. The superoperator $\mathcal{R} \equiv \mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}$ is the pseudoinverse of the Liouvillian (inversion of the Liouvillian is now well defined, because $\mathcal{Q}$ projects out the Liouvillian kernel). Substituting the resolvent into the expression for the current noise gives

$$\begin{aligned}
S^{+}_{\mathrm{RL}}(0) &= \lim_{\omega\to 0}\left[-\frac{1}{2}\operatorname{Tr}_{\mathrm{S}}\{I_{\mathrm{RL}}\mathcal{R}\{I_{\mathrm{RL}}, \varrho_{\mathrm{stat}}\}\} - \right. \\
&\qquad \left. -\frac{1}{2\mathrm{i}\omega}\operatorname{Tr}_{\mathrm{S}}\{I_{\mathrm{RL}}\mathcal{P}\{I_{\mathrm{RL}}, \varrho_{\mathrm{stat}}\}\} + \frac{1}{\mathrm{i}\omega}\langle I_{\mathrm{RL}}\rangle^2\right] = \\
&= \lim_{\omega\to 0}\left[-e\operatorname{Tr}_{\mathrm{S}}\{I_{\mathrm{RL}}\mathcal{R}\mathcal{I}_{\mathrm{RL}}\varrho_{\mathrm{stat}}\} - \right. \\
&\qquad \left. -\frac{1}{2\mathrm{i}\omega}\operatorname{Tr}_{\mathrm{S}}\{I_{\mathrm{RL}}|0\rangle\!\rangle\langle\!\langle\tilde{0}|\{I_{\mathrm{RL}}, \varrho_{\mathrm{stat}}\}\} + \frac{1}{\mathrm{i}\omega}\langle I_{\mathrm{RL}}\rangle^2\right] = \\
&= \lim_{\omega\to 0}\left[-e^2\operatorname{Tr}_{\mathrm{S}}\{\mathcal{I}_{\mathrm{RL}}\mathcal{R}\mathcal{I}_{\mathrm{RL}}\varrho_{\mathrm{stat}}\} - \right. \\
&\qquad \left. -\frac{1}{2\mathrm{i}\omega}\operatorname{Tr}_{\mathrm{S}}\{I_{\mathrm{RL}}\varrho_{\mathrm{stat}}\}\operatorname{Tr}_{\mathrm{S}}\{\{I_{\mathrm{RL}}, \varrho_{\mathrm{stat}}\}\} + \frac{1}{\mathrm{i}\omega}\langle I_{\mathrm{RL}}\rangle^2\right] = \\
&= -e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{RL}}\mathcal{R}\mathcal{I}_{\mathrm{RL}}|0\rangle\!\rangle\,,
\end{aligned}$$

where we have introduced the current superoperator

$$\mathcal{I}_{\mathrm{RL}}\varrho \equiv \frac{1}{2e}\{I_{\mathrm{RL}}, \varrho\} \tag{3.21}$$

with the property

$$\langle I_{\mathrm{RL}}\rangle = e\operatorname{Tr}_{\mathrm{S}}\{\mathcal{I}_{\mathrm{RL}}\varrho_{\mathrm{stat}}\} = e\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{RL}}|0\rangle\!\rangle\,. \tag{3.22}$$

The divergent second and third term have cancelled. The same procedure applied on the $S^{-}_{\mathrm{RL}}(0)$ yields the same result, so

$$S_{\mathrm{RL}}(0) = -2e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{RL}}\mathcal{R}\mathcal{I}_{\mathrm{RL}}|0\rangle\!\rangle\,. \tag{3.23}$$

The matrix representation of the operator $\mathcal{I}_{\mathrm{RL}}$ is equal in both bases

$$\mathcal{I}_{\mathrm{RL}} = \frac{1}{2\hbar}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathrm{i}\Omega & -\mathrm{i}\Omega \\ 0 & 0 & 0 & \mathrm{i}\Omega & -\mathrm{i}\Omega \\ 0 & -\mathrm{i}\Omega & -\mathrm{i}\Omega & 0 & 0 \\ 0 & \mathrm{i}\Omega & \mathrm{i}\Omega & 0 & 0 \end{pmatrix}.$$

MacDonald formula

For the outer junctions (between the dots and the leads) the quantum regression theorem cannot be used, because the current operators I_{L0} and I_{0R} involve the lead operators, thereby not being system operators. However, n-resolved form of the generalized master equation and the MacDonald formula enables us to calculate the zero-frequency noise also for these junctions.

We track how many electrons have tunneled to the right lead by time t and we introduce a density matrix $\varrho_{\mathrm{S}}^{(n)}(t)$ of the system resolved with respect to that number of electrons n. The Liouvillian must be splitted into two terms and the generalized master equation has the form

$$\frac{\mathrm{d}\varrho_{\mathrm{S}}^{(n)}}{\mathrm{d}t} = (\mathcal{L} - \mathcal{I}_{\mathrm{0R}})\varrho_{\mathrm{S}}^{(n)} + \mathcal{I}_{\mathrm{0R}}\varrho_{\mathrm{S}}^{(n-1)}\,, \tag{3.24}$$

where

$$\varrho = \sum_{n=0}^{\infty} \varrho^{(n)}\,, \qquad \varrho^{(-1)} = 0$$

and

$$\mathcal{I}_{\mathrm{0R}}\varrho = \Gamma|0\rangle\langle \mathrm{R}|\varrho|\mathrm{R}\rangle\langle 0| \tag{3.25}$$

is the superoperator of the particle current between the right dot and the right lead.

Probability that n electrons have tunneled to the right lead by time t is then given by $P_n(t) = \mathrm{Tr}_{\mathrm{S}}\{\varrho_{\mathrm{S}}^{(n)}(t)\}$.

We define an operator $Q_{\mathrm{R}}(t)$ of charge transferred to the right lead $Q_{\mathrm{R}}(t) \equiv eN_{\mathrm{R}}(t) - eN_{\mathrm{R}}(0)$ with $N_{\mathrm{R}} = \sum_k c_{k\mathrm{R}}^{\dagger} c_{k\mathrm{R}}$ being the operator of the number of particles in the right lead. The current operator I_{0R} was defined as $I_{\mathrm{0R}} = e\,\mathrm{d}N_{\mathrm{R}}/\,\mathrm{d}t$, so

$$Q_{\mathrm{R}}(t) = \int_0^t \mathrm{d}t' I_{\mathrm{0R}}(t')\,.$$

Let us evaluate the following expression

$$\begin{aligned}
\lim_{t\to\infty} \frac{\mathrm{d}}{\mathrm{d}t}\left[\langle Q_{\mathrm{R}}^2(t)\rangle - \langle Q_{\mathrm{R}}(t)\rangle^2\right] &= \\
&= \lim_{t\to\infty} \frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^t \mathrm{d}t'' \int_0^t \mathrm{d}t' \langle I_{\mathrm{0R}}(t'')I_{\mathrm{0R}}(t')\rangle - \left\langle \int_0^t \mathrm{d}t' I_{\mathrm{0R}}(t')\right\rangle^2\right] \\
&= \lim_{t\to\infty}\left[\int_0^t \mathrm{d}t' \langle\{I_{\mathrm{0R}}(t'), I_{\mathrm{0R}}(t)\}\rangle - 2\int_0^t \mathrm{d}t' \langle I_{\mathrm{0R}}(t')\rangle\langle I_{\mathrm{0R}}(t)\rangle\right] \\
&= 2\int_{-\infty}^0 \mathrm{d}\tau \lim_{t\to\infty}\left[\tfrac{1}{2}\langle\{I_{\mathrm{0R}}(t+\tau), I_{\mathrm{0R}}(t)\}\rangle - \langle I_{\mathrm{0R}}(t)\rangle^2\right]\,.
\end{aligned}$$

Considering the symmetry relation $C_{0\mathrm{R}}(\tau) = C_{0\mathrm{R}}(-\tau)$, we obtain

$$S_{0\mathrm{R}}(0) = \lim_{t\to\infty} \frac{\mathrm{d}}{\mathrm{d}t} \left[\langle Q_{\mathrm{R}}^2(t)\rangle - \langle Q_{\mathrm{R}}(t)\rangle^2\right] . \tag{3.26}$$

which is known as the MacDonald formula [11].

Using the n-resolved density matrix, in principle we could find the full counting statistics of the charge transferred to the right lead. Since we are interested in the mean current and the zero-frequency current noise, we just need the mean charge and the mean square charge tunneled into the right lead by time t given by

$$\langle Q_{\mathrm{R}}(t)\rangle = e\sum_n nP_n(t)\,, \qquad \langle Q_{\mathrm{R}}^2(t)\rangle = e^2\sum_n n^2P_n(t)\,.$$

The definition of $Q_{\mathrm{R}}(t)$ and the current operator $I_{0\mathrm{R}}$ yields

$$\langle I_{0\mathrm{R}}\rangle = e\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\sum_n nP_n(t) = e\lim_{t\to\infty}\sum_n n\dot{P}_n(t)$$

and from (3.26) we have

$$\begin{aligned} S_{0\mathrm{R}}(0) &= e^2\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\Big[\sum n^2P_n(t) - \Big(\sum_n nP_n(t)\Big)^2\Big] = \\ &= e^2\lim_{t\to\infty}\Big[\sum_n n^2\dot{P}_n(t) - 2\Big(\sum_n nP_n(t)\Big)\Big(\sum_n n\dot{P}_n(t)\Big)\Big]\,. \end{aligned} \tag{3.27}$$

For time derivative of $P(n)$ from (3.24) we find

$$\dot{P}_n(t) = \mathrm{Tr}_{\mathrm{S}}\{\mathcal{I}_{0\mathrm{R}}(\varrho_{\mathrm{S}}^{(n-1)}(t) - \varrho_{\mathrm{S}}^{(n)}(t))\}$$

and consequently

$$\begin{aligned} \sum_n \dot{P}_n(t) &= 0\,, \\ \sum_n n\dot{P}_n(t) &= \mathrm{Tr}_{\mathrm{S}}\{\mathcal{I}_{0\mathrm{R}}\sum_n \varrho_{\mathrm{S}}^{(n)}(t)\} = \mathrm{Tr}_{\mathrm{S}}\{\mathcal{I}_{0\mathrm{R}}\varrho_{\mathrm{S}}(t)\}\,, \\ \sum_n n^2\dot{P}_n(t) &= \mathrm{Tr}_{\mathrm{S}}\{\mathcal{I}_{0\mathrm{R}}\sum_n[(n-1)^2\varrho_{\mathrm{S}}^{(n-1)}(t) + 2(n-1)\varrho_{\mathrm{S}}^{(n-1)}(t) + \varrho_{\mathrm{S}}^{(n-1)}(t) - \\ &\qquad - n^2\varrho_{\mathrm{S}}^{(n)}(t)]\} = \\ &= \mathrm{Tr}_{\mathrm{S}}\{\mathcal{I}_{0\mathrm{R}}\Big(\sum_n 2n\varrho_{\mathrm{S}}^{(n)}(t) + \varrho_{\mathrm{S}}(t)\Big)\}\,. \end{aligned}$$

We can immediately write the stationary mean current

$$\langle I_{0\mathrm{R}}\rangle = e\,\mathrm{Tr}_{\mathrm{S}}\{\mathcal{I}_{0\mathrm{R}}\varrho_{\mathrm{stat}}\} = e\langle\!\langle\tilde{0}|\mathcal{I}_{0\mathrm{R}}|0\rangle\!\rangle\,. \tag{3.28}$$

Now, one can employ an operator-valued generalization of the standard generating function to calculate $\sum_n n\varrho_{\mathrm{S}}^{(n)}(t)$. We introduce the object

$$F(t,z) = \sum_n \varrho_{\mathrm{S}}^{(n)}(t)z^n$$

with following properties

$$F(t,1) = \varrho_{\mathrm{S}}(t)\,, \qquad \frac{\partial}{\partial z}F(t,z)|_{z=1} = \sum_n n\varrho_{\mathrm{S}}^{(n)}(t)$$

and hence we focus on the quantity $\partial F(t,z)/\partial z|_{z=1}$. The generating function satisfies the equation of motion

$$\frac{\partial}{\partial t}F(t,z) = [\mathcal{L} + (z-1)\mathcal{I}_{0\mathrm{R}}]F(t,z)\,.$$

The Laplace transform of this equation gives

$$[s - \mathcal{L} - (z-1)\mathcal{I}_{0\mathrm{R}}]F(s,z) = \sum_n \varrho_{\mathrm{S}}^{(n)}(0)z^n\,,$$

where $\varrho_{\mathrm{S}}^{(n)}(0)$ are the initial conditions. In the Laplace picture we obtain for the quantity of interest

$$\frac{\partial}{\partial z}F(s,z)|_{z=1} = (s-\mathcal{L})^{-1}\mathcal{I}_{0\mathrm{R}}(s-\mathcal{L})^{-1}\varrho_{\mathrm{S}}(0) + (s-\mathcal{L})^{-1}\sum_n n\varrho_{\mathrm{S}}^{(n)}(0)\,.$$

Since we are interested in the $t \to \infty$ limit which is related to the $s \to 0+$ limit, we study the asymptotic behavior of the above expression for small s. The resolvent $(s-\mathcal{L})^{-1}$ has been already calculated in this limit in the previous subsection with the result $(s-\mathcal{L})^{-1} \approx \mathcal{P}/s - \mathcal{R}$. Thus, we get for the leading terms

$$\begin{aligned}\frac{\partial}{\partial z}F(s,z)|_{z=1} \approx{}& \frac{1}{s^2}\mathcal{P}\mathcal{I}_{0\mathrm{R}}\mathcal{P}\varrho_{\mathrm{S}}(0) - \\ &- \frac{1}{s}\left(\mathcal{P}\mathcal{I}_{0\mathrm{R}}\mathcal{R}\varrho_{\mathrm{S}}(0) + \mathcal{R}\mathcal{I}_{0\mathrm{R}}\mathcal{P}\varrho_{\mathrm{S}}(0) - \mathcal{P}\sum_n n\varrho_{\mathrm{S}}^{(n)}(0)\right)\,.\end{aligned}$$

In the time domain it yields

$$\frac{\partial}{\partial z}F(t,z)|_{z=1} \approx \frac{1}{e}\varrho_{\mathrm{stat}}\left(\langle I_{0\mathrm{R}}\rangle t + C_{\mathrm{init}}\right) - \mathcal{R}\mathcal{I}_{0\mathrm{R}}\varrho_{\mathrm{stat}}\,, \tag{3.29}$$

where $C_{\mathrm{init}} = e\,\mathrm{Tr}_{\mathrm{S}}\{\sum_n n\varrho_{\mathrm{S}}^{(n)}(0) - \mathcal{I}_{0\mathrm{R}}\mathcal{R}\varrho_{\mathrm{S}}(0)\}$ is an initial conditions dependent constant.

Using the generating function the current noise formula (3.27) can be rewritten as

$$S_{0\mathrm{R}}(0) = e\langle I_{0\mathrm{R}}\rangle + 2e\lim_{t\to\infty}\mathrm{Tr}\{(e\mathcal{I}_{0\mathrm{R}} - \langle I_{0\mathrm{R}}\rangle)\frac{\partial}{\partial z}F(t,z)|_{z=1}\}\,.$$

Substituting from (3.29) and considering the identity $\mathrm{Tr}_{\mathrm{S}}\{\mathcal{R}A\} = 0$ (for an arbitrary system operator A), we get

$$\begin{aligned}S_{0\mathrm{R}}(0) = e\langle I_{0\mathrm{R}}\rangle &+ 2e\,\mathrm{Tr}\{\mathcal{I}_{0\mathrm{R}}\varrho_{\mathrm{stat}}(\langle I_{0\mathrm{R}}\rangle t + C_{\mathrm{init}})\} - 2e^2\,\mathrm{Tr}\{\mathcal{I}_{0\mathrm{R}}\mathcal{R}\mathcal{I}_{0\mathrm{R}}\varrho_{\mathrm{stat}}\} - \\ &- 2e\,\mathrm{Tr}\{\langle I_{0\mathrm{R}}\rangle\varrho_{\mathrm{stat}}(\langle I_{0\mathrm{R}}\rangle t + C_{\mathrm{init}})\}\,.\end{aligned}$$

The linearly divergent terms in t and the initial condition terms cancel identically as expected and necessary. The final result for the zero-frequency current noise is

$$S_{0\mathrm{R}}(0) = e^2 \langle\!\langle \tilde{0}|\mathcal{I}_{0\mathrm{R}} - 2\mathcal{I}_{0\mathrm{R}}\mathcal{R}\mathcal{I}_{0\mathrm{R}}|0\rangle\!\rangle \,. \tag{3.30}$$

Similarly for the L0 junction one finds

$$\langle I_{\mathrm{L}0}\rangle = e\langle\!\langle \tilde{0}|\mathcal{I}_{\mathrm{L}0}|0\rangle\!\rangle \,, \qquad S_{\mathrm{L}0}(0) = e^2\langle\!\langle \tilde{0}|\mathcal{I}_{\mathrm{L}0} - 2\mathcal{I}_{\mathrm{L}0}\mathcal{R}\mathcal{I}_{\mathrm{L}0}|0\rangle\!\rangle \tag{3.31}$$

with

$$\mathcal{I}_{\mathrm{L}0}\varrho = \Gamma|\mathrm{L}\rangle\langle 0|\varrho|0\rangle\langle \mathrm{L}| \,. \tag{3.32}$$

The main results of this section are (3.23), (3.30) and (3.31), which will be the basic expressions for our further numerical calculations.

3.4 Charge conservation

In this section we are going to show, how the equations of motion (3.14) and (3.15) for the dot occupation operators (charge conservation conditions) imply that the stationary mean current and the zero frequency noise are independent of the measurement position along the circuit, i. e.

$$\langle I_{\mathrm{L}0}\rangle = \langle I_{\mathrm{RL}}\rangle = \langle I_{0\mathrm{R}}\rangle \,, \qquad S_{\mathrm{L}0}(0) = S_{\mathrm{RL}}(0) = S_{0\mathrm{R}}(0) \,.$$

Mean current conservation

The conservation of the stationary mean current can be seen immediately

$$\begin{aligned}\langle I_{\mathrm{L}0}\rangle - \langle I_{\mathrm{RL}}\rangle &= \mathrm{Tr}\{(I_{\mathrm{L}0} - I_{\mathrm{RL}})\varrho_{\mathrm{stat}}\} = -\frac{\mathrm{i}e}{\hbar}\,\mathrm{Tr}\{[n_{\mathrm{L}}, H]\varrho_{\mathrm{stat}}\} = \\ &= -\frac{\mathrm{i}e}{\hbar}\,\mathrm{Tr}\{n_{\mathrm{L}}[H, \varrho_{\mathrm{stat}}]\} = 0\end{aligned}$$

and similarly for $\langle I_{\mathrm{RL}}\rangle - \langle I_{0\mathrm{R}}\rangle = 0$.

Zero-frequency noise conservation

We insert (3.14) into the definition of the current noise $S_{\mathrm{L}0}(0)$ and also employ the mean current conservation

$$\begin{aligned}S_{\mathrm{L}0}(0) &= \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau \lim_{t\to\infty} \langle\{I_{\mathrm{L}0}(t+\tau), I_{\mathrm{L}0}(t)\}\rangle - \langle I_{\mathrm{L}0}\rangle^2 = \\ &= \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau \lim_{t\to\infty} \langle\{I_{\mathrm{RL}}(t+\tau), I_{\mathrm{L}0}(t)\}\rangle - \langle I_{\mathrm{RL}}\rangle^2 + \\ &\quad + \frac{1}{2}\lim_{\substack{t\to\infty \\ \tau\to\infty}} [\langle\{en_{\mathrm{L}}(t+\tau), I_{\mathrm{L}0}(t)\}\rangle - \langle\{en_{\mathrm{L}}(t-\tau), I_{\mathrm{L}0}(t)\}\rangle] \,,\end{aligned}$$

where the correlation functions in the stationary limit in the second term are zero for $\tau \to \infty$.

$$\begin{aligned} S_{\mathrm{L0}}(0) &= \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau \lim_{t\to\infty} \langle\{I_{\mathrm{L0}}(t-\tau), I_{\mathrm{RL}}(t)\}\rangle - \langle I_{\mathrm{RL}}\rangle^2 = \\ &= \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}\tau \lim_{t\to\infty} \langle\{I_{\mathrm{RL}}(t-\tau), I_{\mathrm{RL}}(t)\}\rangle - \langle I_{\mathrm{RL}}\rangle^2 + \\ &\quad + \frac{1}{2}\lim_{\substack{t\to\infty \\ \tau\to\infty}} [\langle\{en_{\mathrm{L}}(t+\tau), I_{\mathrm{RL}}(t)\}\rangle - \langle\{en_{\mathrm{L}}(t-\tau), I_{\mathrm{RL}}(t)\}\rangle] = \\ &= S_{\mathrm{RL}}(0) \end{aligned}$$

and similarly $S_{0\mathrm{R}}(0) = S_{\mathrm{RL}}(0)$. In general we find, that the zero-frequency noise is the same for any junction.

Charge conservation condition for superoperators

Now we try to formulate the charge conservation condition in the superoperator language. Let us evaluate the commutator $[\mathcal{N}_{\mathrm{L}}, \mathcal{L}]$ with the superoperator of occupation of the left dot $\mathcal{N}_{\mathrm{L}}\varrho = \frac{1}{2}\{n_{\mathrm{L}}, \varrho\}$.

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}]\varrho = \tfrac{1}{2}\left[n_{\mathrm{L}}(\mathcal{L}\varrho) + (\mathcal{L}\varrho)n_{\mathrm{L}} - \mathcal{L}(n_{\mathrm{L}}\varrho) - \mathcal{L}(\varrho n_{\mathrm{L}})\right] . \tag{3.33}$$

If we do not project out the reservoirs, the Liouvillian has the original form $\mathcal{L} = -\mathrm{i}[H, \varrho]/\hbar$ and it yields

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}]\varrho = -\tfrac{1}{2}\{\mathcal{L}n_{\mathrm{L}}, \varrho\} ,$$

where $\mathcal{L}n_{\mathrm{L}} = -(I_{\mathrm{L0}} - I_{\mathrm{RL}})/e$ from the equations of motions. The final formula reads

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}] = \tilde{\mathcal{I}}_{\mathrm{L0}} - \mathcal{I}_{\mathrm{RL}}$$

with $\tilde{\mathcal{I}}_{\mathrm{L0}}\varrho = \{I_{\mathrm{L0}}, \varrho\}/2e$. The superoperators $\mathcal{I}_{\mathrm{L0}}$ and $\tilde{\mathcal{I}}_{\mathrm{L0}}$ are obviously different, because $\tilde{\mathcal{I}}_{\mathrm{L0}}$ acts non-trivially in the Liouville space of the leads, while $\mathcal{I}_{\mathrm{L0}}$ is the superoperator in the system subspace only.

We return to our generalized master equation (2.4) and the corresponding Liouvillian and reexamine expression (3.33). Of course, the system part $\mathcal{L}_{\mathrm{S}}$ gives the same result

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{S}}] = -\mathcal{I}_{\mathrm{RL}} .$$

But for $\mathcal{L}_{\mathrm{C}}$ we obtain

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{C}}]\varrho_{\mathrm{S}} = \frac{1}{2\hbar^2}\int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_{\mathrm{C}}\{\{[H_{\mathrm{CS}}, n_{\mathrm{L}}], [H_{\mathrm{CS}}(-\tau), \varrho_{\mathrm{S}}\otimes\varrho_{\mathrm{C}}]\} + \\ + \{[H_{\mathrm{CS}}(-\tau), n_{\mathrm{L}}], [H_{\mathrm{CS}}, \varrho_{\mathrm{S}}\otimes\varrho_{\mathrm{C}}]\}\} + \\ + \frac{1}{2\hbar^2}\int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_{\mathrm{C}}\{\{[H_{\mathrm{CS}}, [H_{\mathrm{CS}}(-\tau), n_{\mathrm{L}}]], \varrho_{\mathrm{S}}\otimes\varrho_{\mathrm{C}}\}\}\,.$$

The operators inside the trace can be rearranged into

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{C}}]\varrho_{\mathrm{S}} = \frac{1}{2\hbar^2}\int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_{\mathrm{C}}\{\{[H_{\mathrm{CS}}, n_{\mathrm{L}}], [H_{\mathrm{CS}}(-\tau), \varrho_{\mathrm{S}}\otimes\varrho_{\mathrm{C}}]\}\} + \\ + \frac{1}{2\hbar^2}\int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_{\mathrm{C}}\{[H_{\mathrm{CS}}, \{[H_{\mathrm{CS}}(-\tau), n_{\mathrm{L}}], \varrho_{\mathrm{S}}\otimes\varrho_{\mathrm{C}}\}]\}\,.$$

These integrals can be calculated in an analogous way as when we evaluated Liouvillian $\mathcal{L}_{\mathrm{C}}$. The matrix element kl, mn of the first term reads

$$\tfrac{1}{2}\Gamma[A^\dagger_{km}A_{nl} + \tfrac{1}{2}\sum_q(\delta_{km}A_{nq}A^\dagger_{ql} + \delta_{nl}A_{kq}A^\dagger_{qm})]$$

and the matrix element kl, mn of the second term reads

$$\tfrac{1}{2}\Gamma[A^\dagger_{km}A_{nl} - \tfrac{1}{2}\sum_q(\delta_{km}A_{nq}A^\dagger_{ql} + \delta_{nl}A_{kq}A^\dagger_{qm})]\,,$$

where A_{km} are the matrix elements of the operator $|0\rangle\langle \mathrm{L}|$. Together we have

$$\sum_{mn}[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{C}}]_{kl,mn}\,(\varrho_{\mathrm{S}})_{mn} = \sum_{mn}\Gamma A^\dagger_{km}\,(\varrho_{\mathrm{S}})_{mn}\,A_{nl}$$

and hence the result is

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{C}}]\varrho_{\mathrm{S}} = |\mathrm{L}\rangle\langle 0|\varrho_S|0\rangle\langle \mathrm{L}| = \mathcal{I}_{\mathrm{L0}}\varrho_{\mathrm{S}}\,.$$

Since $[n_{\mathrm{L}}, H_{\mathrm{BS}}] = 0$, we expect that $[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{B}}]$ will be zero, therefore the final relation is

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}] = \mathcal{I}_{\mathrm{L0}} - \mathcal{I}_{\mathrm{RL}}\,. \tag{3.34}$$

This relation is the Liouvillian space analogy to the charge conservation condition (3.14). For the other outer junction (between the right dot and the right lead) we obtain similar result

$$[\mathcal{N}_{\mathrm{R}}, \mathcal{L}] = \mathcal{I}_{\mathrm{RL}} - \mathcal{I}_{\mathrm{0R}}\,. \tag{3.35}$$

Let us show the equivalence with the charge conservation conditions. Using equation (3.34)

$$\langle I_{\mathrm{L0}}\rangle = \langle\!\langle\tilde{0}|I_{\mathrm{L0}}|0\rangle\!\rangle = \langle\!\langle\tilde{0}|[\mathcal{N}_{\mathrm{L}},\mathcal{L}]|0\rangle\!\rangle + \langle\!\langle\tilde{0}|I_{\mathrm{RL}}|0\rangle\!\rangle = \langle I_{\mathrm{RL}}\rangle\,,$$

because we remember that $\mathcal{L}|0\rangle\!\rangle = \langle\!\langle\tilde{0}|\mathcal{L} = 0$. Analogously, we prove the equivalence between $S_{\mathrm{L0}}(0)$ and $S_{\mathrm{RL}}(0)$. Using the relation $\mathcal{R}\mathcal{L} = \mathcal{L}\mathcal{R} = \mathcal{Q} = 1 - |0\rangle\!\rangle\langle\!\langle\tilde{0}|$ it becomes

$$\begin{aligned}
S_{\mathrm{RL}}(0) &= -2e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{RL}}\mathcal{R}\mathcal{I}_{\mathrm{RL}}|0\rangle\!\rangle = \\
&= -e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{L0}}\mathcal{R}\mathcal{I}_{\mathrm{RL}} + \mathcal{I}_{\mathrm{RL}}\mathcal{R}\mathcal{I}_{\mathrm{L0}}|0\rangle\!\rangle + e^2\langle\!\langle\tilde{0}|\mathcal{N}_{\mathrm{L}}\mathcal{Q}\mathcal{I}_{\mathrm{RL}}|0\rangle\!\rangle - e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{RL}}\mathcal{Q}\mathcal{N}_{\mathrm{L}}|0\rangle\!\rangle \\
&= -e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{L0}}\mathcal{R}\mathcal{I}_{\mathrm{RL}} + \mathcal{I}_{\mathrm{RL}}\mathcal{R}\mathcal{I}_{\mathrm{L0}}|0\rangle\!\rangle + e^2\langle\!\langle\tilde{0}|[\mathcal{N}_{\mathrm{L}},\mathcal{I}_{\mathrm{RL}}]|0\rangle\!\rangle\,.
\end{aligned}$$

We notice

$$[\mathcal{N}_{\mathrm{L}},\mathcal{I}_{\mathrm{RL}}]\varrho = \tfrac{1}{4}\left(\{n_{\mathrm{L}},\{I_{\mathrm{RL}},\varrho\}\} - \{I_{\mathrm{RL}},\{n_{\mathrm{L}},\varrho\}\}\right) = \tfrac{1}{4}[[n_{\mathrm{L}},I_{\mathrm{RL}}],\varrho]\,,$$

thus it yields zero when traced over. Inserting the (3.34) into the last expression one more time, we obtain

$$S_{\mathrm{RL}}(0) = -2e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{L0}}\mathcal{R}\mathcal{I}_{\mathrm{L0}}|0\rangle\!\rangle + e^2\langle\!\langle\tilde{0}|[\mathcal{N}_{\mathrm{L}},\mathcal{I}_{\mathrm{L0}}]|0\rangle\!\rangle\,,$$

while

$$[\mathcal{N}_{\mathrm{L}},\mathcal{I}_{\mathrm{L0}}]\varrho = \tfrac{1}{2}\left(\{|\mathrm{L}\rangle\langle\mathrm{L}|,|\mathrm{L}\rangle\langle 0|\varrho|0\rangle\langle\mathrm{L}|\} - |\mathrm{L}\rangle\langle 0|\{|\mathrm{L}\rangle\langle\mathrm{L}|,\varrho\}|0\rangle\langle\mathrm{L}|\right) = \mathcal{I}_{\mathrm{L0}}\varrho\,.$$

We recover that zero-frequency noise must be independent of the measurement position.

$$S_{\mathrm{RL}}(0) = e^2\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{L0}} - 2\mathcal{I}_{\mathrm{L0}}\mathcal{R}\mathcal{I}_{\mathrm{L0}}|0\rangle\!\rangle = S_{\mathrm{L0}}(0)\,.$$

Charge conservation breaking

Let us return to the point where we have assumed that $[\mathcal{N}_{\mathrm{L}},\mathcal{L}_{\mathrm{B}}]$ is identically zero. This is a reasonable assumption, because the dot occupation operator n_{L} commutes with the heat bath-system interaction Hamiltonian H_{BS} and thus the bath variables do not enter explicitly the current operators. We showed that $[\mathcal{N}_{\mathrm{L}},\mathcal{L}]$ indeed do not depend on the bath variables if we operate on the whole Liouville space before projection on the system and before introducing the weak coupling and Markovian limit. However, in our approach we arrive at (equivalently to the previous lead case)

$$\begin{aligned}
[\mathcal{N}_{\mathrm{L}},\mathcal{L}_{\mathrm{B}}]\varrho_{\mathrm{S}} = \frac{1}{2\hbar^2}\int_0^\infty \mathrm{d}\tau\,\mathrm{Tr}_{\mathrm{B}}\{\{[H_{\mathrm{BS}},n_{\mathrm{L}}],[H_{\mathrm{BS}}(-\tau),\varrho_{\mathrm{S}}\otimes\varrho_{\mathrm{B}}]\}\} + \\
+ \frac{1}{2\hbar^2}\int_0^\infty \mathrm{d}\tau\,\mathrm{Tr}_{\mathrm{B}}\{[H_{\mathrm{BS}},\{[H_{\mathrm{BS}}(-\tau),n_{\mathrm{L}}],\varrho_{\mathrm{S}}\otimes\varrho_{\mathrm{B}}\}]\}\,. \qquad (3.36)
\end{aligned}$$

Apparently, the first term is equal to zero. The second one gives the anomalous current

$$-\mathcal{I}_{\mathrm{A}} \equiv -\frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \gamma_+ & \gamma_- & 0 & 0 \\ 0 & \gamma_+ & \gamma_- & 0 & 0 \end{pmatrix} \tag{3.37}$$

and hence we write

$$[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{B}}] = -\mathcal{I}_{\mathrm{A}}\,, \qquad [\mathcal{N}_{\mathrm{R}}, \mathcal{L}_{\mathrm{B}}] = \mathcal{I}_{\mathrm{A}}\,.$$

We face the fact that the charge conservation is broken. The possible consequence is that the mean current or the zero-frequency current noise are no longer equal for any pair of junctions. First, since $\langle\!\langle\tilde{0}|$ corresponds to unit operator and thus it is equal $(1,1,1,0,0)$, we see that $\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{A}}|0\rangle\!\rangle = 0$ and the mean current is conserved along the whole circuit (it is obvious from the structure of (3.36) too). Also we notice $[\mathcal{N}_{\mathrm{L}} + \mathcal{N}_{\mathrm{R}}, \mathcal{L}_{\mathrm{B}}] = 0$, therefore there is no problem with the charge conservation between the outer junctions. However, zero-frequency noise shows discrepancy between the outer junction and the inner junction, in detail

$$\begin{aligned} &S_{\mathrm{RL}}(0) - S_{\mathrm{L0}}(0) = 2e^2(\langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{A}}\mathcal{R}\mathcal{I}_{\mathrm{L0}}|0\rangle\!\rangle + \langle\!\langle\tilde{0}|\mathcal{I}_{\mathrm{L0}}\mathcal{R}\mathcal{I}_{\mathrm{A}}|0\rangle\!\rangle) = \\ &= \frac{e^2\Gamma\Omega\varepsilon\left[\hbar^2\Gamma\gamma_+(\gamma_p + \frac{1}{2}\Gamma)^2 + 2\Omega^2(\gamma_+ + \gamma_-)(\gamma_p + \frac{1}{2}\Gamma) - 2\varepsilon^2\gamma_+(\frac{2\Omega}{\varepsilon}\gamma_- - \frac{1}{2}\Gamma)\right]}{\left[\frac{1}{2}\Gamma\varepsilon^2 + 3\Omega^2(\gamma_p + \frac{1}{2}\Gamma) + \frac{1}{2}\hbar^2\Gamma(\gamma_p + \frac{1}{2}\Gamma)^2 - \Omega\varepsilon(2\gamma_+ + \gamma_-)\right]^2}\,. \end{aligned} \tag{3.38}$$

The charge conservation breaking cannot be artefact of different couplings to reservoirs (weak coupling prescription for the heat bath and the high bias limit for leads), since the identical results are obtained, as we have shown, if the both reservoirs are coupled weakly.

3.5 Results

In this section we illustrate our results, particularly where the charge conservation problems are evident.

Numerical evaluation

The evaluation of the quantities of our interest includes two steps. First, we have to find the stationary density matrix $\varrho_{\mathrm{stat}} = \varrho_{\mathrm{S}}(t \to \infty)$ independent of an initial condition and equivalently given by the equation

$$\mathcal{L}\varrho_{\mathrm{stat}} = 0\,, \quad \mathrm{Tr}_{\mathrm{S}}\,\varrho_{\mathrm{stat}} = 1\,.$$

Obtaining the stationary state from the singular value decomposition, we are able to calculate all one-time quantities such as the mean current or the dot occupation number.

To evaluate the noise, we have to find the pseudoinverse $\mathcal{R} = \mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}$ of the Liouvillian. The numerical calculation of the pseudoinverse is less computationally demanding than the eigenvalue problem.

We find the orthogonal triangular decomposition with permutations of the Liouvillian $\mathcal{L}$ (implemented in MATLAB)

$$\mathcal{U} \cdot \tilde{\mathcal{L}} = \mathcal{L} \cdot \mathcal{E} ,$$

where $\tilde{\mathcal{L}}$ is upper triangular, $\mathcal{U}$ is unitary and $\mathcal{E}$ is a permutation matrix (all have dimension 5×5). The column permutation $\mathcal{E}$ is chosen so that the numbers on the diagonal of $\tilde{\mathcal{L}}$ is decreasing in absolute value. The last row of $\tilde{\mathcal{L}}$ hence must be identically zero. Next, we find the matrix $\tilde{\mathcal{Q}}$ from the equation

$$\mathcal{U} \cdot \tilde{\mathcal{Q}} = \mathcal{Q} \cdot \mathcal{E} .$$

The last row of $\tilde{\mathcal{Q}}$ is also identically zero. The pseudoinverse of the Liouvillian is then given by the relation

$$\mathcal{R} = \mathcal{Q} \cdot \mathcal{E}\mathcal{X}\mathcal{E}^{-1} ,$$

where the matrix $\mathcal{X}$ is solution of the linear equation

$$\tilde{\mathcal{L}} \cdot \mathcal{X} = \tilde{\mathcal{Q}} .$$

Since both $\tilde{\mathcal{L}}$ and $\tilde{\mathcal{Q}}$ are not regular matrices, the above equation has an infinite number of solutions which can be written as the sum of a particular solution $\mathcal{X}_0$ and a solution of the homogenous equation

$$\mathcal{X} = \mathcal{X}_0 + \mathcal{E}^{-1} \cdot |0\rangle\rangle\langle\langle A| ,$$

where $|A\rangle\rangle$ is an arbitrary vector. Substituting to the relation for the pseudoinverse, it yields

$$\mathcal{R} = \mathcal{Q} \cdot \mathcal{E}\mathcal{X}_0\mathcal{E}^{-1} ,$$

because $\mathcal{Q}|0\rangle\rangle = 0$. The particular solution $\mathcal{X}_0$ can be chosen so that its last row is zero.

Fano factor

In purpose to represent the noise by a dimensionless quantity, we define Fano factor $F = S(0)/e\langle I\rangle$. Before presenting the results of the numerical evaluation of the Fano factor, we want to show its typical behavior for simpler models. For a system that can be treated in the Landauer-Büttiker formalism the scattering states and the transmission probabilities define the transport properties. In particular, the average current through the device is given by

$$I = \frac{2e}{\hbar} V \sum_n T_n ,$$

where T_n is the transmission probability for the n-th conducting channel and V is the bias across the system. The zero-frequency current-current correlation function reads

$$S(0) = \frac{2e}{\hbar} V \sum_n T_n(1 - T_n) .$$

For these systems the Fano factor takes the form

$$F = \frac{S(0)}{I} = \frac{\sum_n T_n(1 - T_n)}{\sum_n T_n} ,$$

which is a number between 0 and 1. For small transition probabilities (and thus very rare tunneling events) the Fano factor goes to 1. The Fano factor 1 is called Poissonian because in that regime of uncorrelated tunneling events, the random distribution of events corresponds to Poissonian process. On the other hand, transmission with no randomness $T = 1$ gives the Fano factor 0.

Landauer-Büttiker formalism can treat only sub-Poissonian noise. However, in interacting systems general theoretical prediction and numerical calculation have demonstrated the existence of super-Poissonian noise [12].

Zero dissipation

In the case without the heat bath ($\gamma = 0$), the charge conservation condition is satisfied. For the mean current and the Fano factor we obtain [13, 14]

$$\langle I \rangle = e\Gamma \frac{\Omega^2}{\varepsilon^2 + 3\Omega^2 + (\frac{1}{2}\hbar\Gamma)^2} ,$$

$$F_{\mathrm{L0}} = F_{\mathrm{RL}} = F_{\mathrm{0R}} = 1 - \frac{4\Omega^2 \left(\Omega^2 + 2(\frac{1}{2}\hbar\Gamma)^2\right)}{\left(\varepsilon^2 + 3\Omega^2 + (\frac{1}{2}\hbar\Gamma)^2\right)^2} .$$

These results are illustrated in fig. 3.2.

The mean current vs. bias ε has the Lorentzian shape with the half-width $\sqrt{3\Omega^2 + (\hbar\Gamma/2)^2}$ and maximum at $\varepsilon = 0$. The Fano factor has the dip at $\varepsilon = 0$ where quantum coherence strongly suppresses the noise. The maximum suppression $F = \frac{1}{5}$ is reached when $\hbar\Gamma = 2\sqrt{2}\,\Omega$. For large $|\varepsilon| > 0$ the mean current becomes very small and thus electrons tunnel very sparsely and consequently the tunneling events are uncorrelated which corresponds to a Poisson process with the value of the Fano factor $F \to 1$.

General case

When dissipative heat bath comes into play ($\gamma > 0$), the transport is strongly affected by the possibility of exchanging energy with the heat bath [4, 15] as it is illustrated in fig. 3.3.

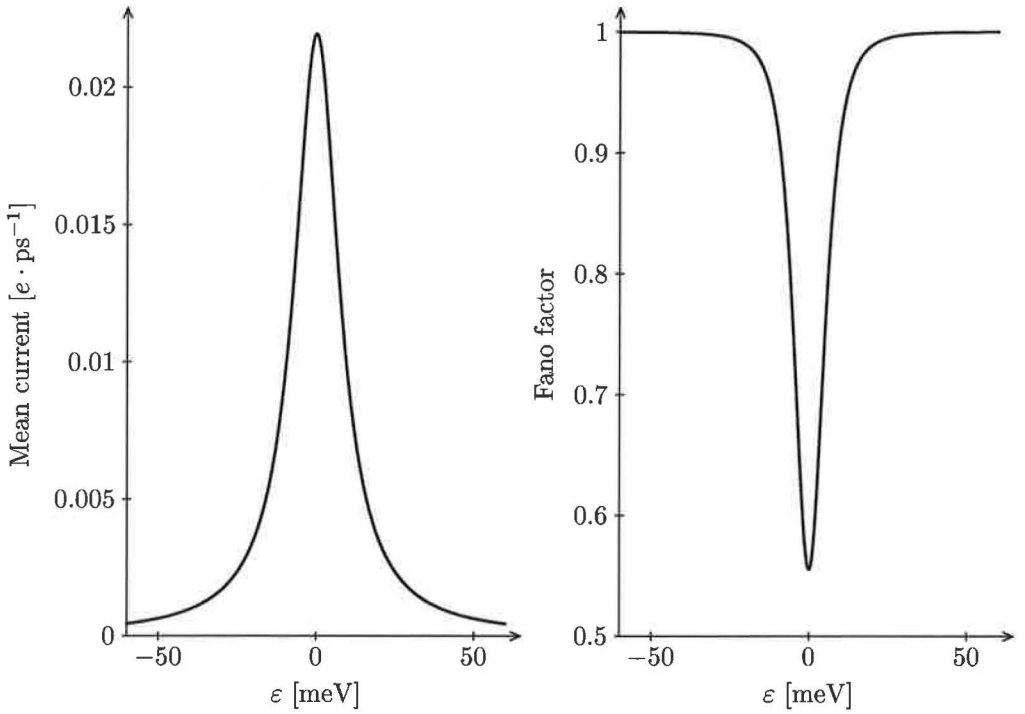

Fig. 3.2: Mean current and Fano factor vs. bias ε without the dissipative heat bath ($\gamma = 0$). Parameters: $\Omega = 5\,\mathrm{meV}$, $\Gamma = 0.1/\hbar\,\mathrm{meV}$.

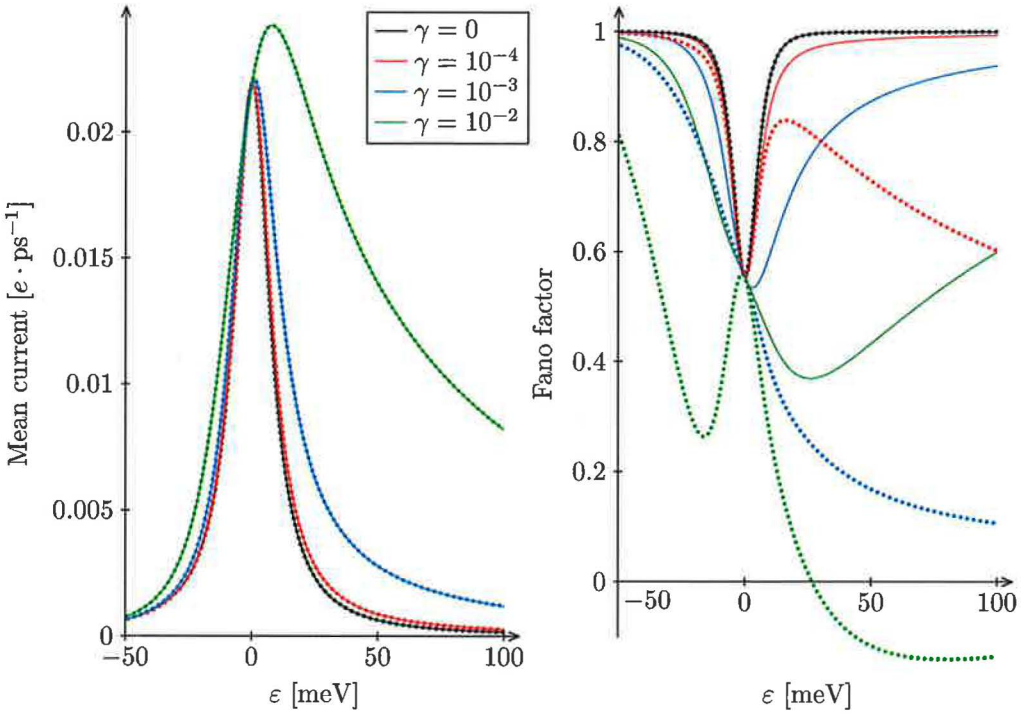

Fig. 3.3: Mean current and Fano factor vs. bias ε for different values of damping coefficient γ. Solid lines show the mean current and the Fano factor at the outer junctions L0, 0R, dotted lines at the inner junction RL. Parameters: $\Omega = 5\,\mathrm{meV}$, $\Gamma = 0.1/\hbar\,\mathrm{meV}$, $\beta = 0.1\,\mathrm{meV}^{-1}$ (temperature 120 K).

The shape of the mean current curve is no longer Lorentzian but exhibits an asymmetry. With increasing temperature the peak becomes broader and more symmetric. Analytically we obtain

$$\langle I \rangle = \frac{e\Gamma\Omega\left(\Omega(\gamma_p + \frac{1}{2}\Gamma) - \gamma_+\varepsilon\right)}{\frac{1}{2}\Gamma\varepsilon^2 + 3\Omega^2(\gamma_p + \frac{1}{2}\Gamma) + \frac{1}{2}\hbar^2\Gamma(\gamma_p + \frac{1}{2}\Gamma)^2 - \Omega\varepsilon(2\gamma_+ + \gamma_-)}. \tag{3.39}$$

In the right graph in fig. 3.3 Fano factors $F_{\mathrm{L0}} = F_{\mathrm{0R}}$ (solid lines) and F_{RL} (dotted lines) are plotted. The difference between the Fano factors obtained by different approaches is significant. Interestingly, at $\varepsilon = 0$ the Fano factors has the same value $F_{\mathrm{L0}} = F_{\mathrm{RL}}$ as follows from relation (3.38).

For $\varepsilon > 0$ spontaneous emission occurs even at very low temperatures and the noise is reduced well bellow the Poisson limit. The large couplings γ lead to very asymmetric Fano factor. At finite temperatures, absorption of energy quanta from the bath is possible and the Fano factor for $\varepsilon < 0$ is also reduced bellow the Poisson limit. With increasing temperature the effect of the emission and the absorption is growing, except the point $\varepsilon = 0$ where both the mean current and the Fano factor are temperature independent.

In the sense of the previous paragraph, it would seem that MacDonald formula yields physical results for F_{L0} and F_{RL}, whereas F_{RL} given by the Quantum regression theorem behaves pathologically – unphysical negative values and non-Poisson limit for $\varepsilon \to \infty$. For sufficiently strong coupling ($\gamma \approx 10^{-2}$) F_{RL} drops to negative values in the $\varepsilon > 0$ region and for sufficiently high temperature ($T \approx 200\,\mathrm{K}$) also in the $\varepsilon < 0$ region. Analyzing the expression (3.38) we find that for $\varepsilon \to \infty$ the noise difference $\Delta S = S_{\mathrm{RL}}(0) - S_{\mathrm{L0}}(0) \sim 1/\varepsilon$. From the relation (3.39) for the mean current in the same limit follows $\langle I \rangle \sim 1/\varepsilon$. Therefore their ratio – the difference of Fano factors $\Delta F = F_{\mathrm{RL}} - F_{\mathrm{L0}}$ does not go to zero for $\varepsilon \to \infty$ as it should.

Despite of the fact that F_{RL} behaves manifestly wrong, we cannot say whether MacDonald formula gives a better and more reliable results for F_{L0}, because our generalized master equation fails two times. First, the equations of motion for the dot occupation operators are broken, since the charge conservation condition is not satisfied. Second, the reduced density matrix should remain positive semidefinite for all time which implies that an autocorrelation function should remain also positive, however we get negative Fano factor (current autocorrelation function).

In the following sections we will investigate how both the MacDonald formula and the quantum regression theorem approach behave in several approximations or limit cases. It should answer whether MacDonald formula gives physically acceptable results indeed and should show more pathologies of the quantum regression theorem results.

Limit $\Gamma \to 0$

Now we turn to $\Gamma \to 0$ limit, which could be potentially interesting. Analogously with the limit $\gamma \to 0$ the charge conservation could be retrieved. The mean

current and the zero-frequency noise goes to zero in that limit, however the Fano factor does not.

$$F_{\mathrm{L0}} = F_{\mathrm{0R}} = 1 - \frac{4C\Delta(\varepsilon + C\Delta)}{(\varepsilon + 3C\Delta)^2},$$
$$F_{\mathrm{RL}} = 1 - \frac{-2\varepsilon^3 - 2C\varepsilon^2\Delta + 2C^2\varepsilon(4\Delta^2 + \varepsilon^2) + 2C^3\Delta(2\Delta^2 + 3\varepsilon^2)}{\varepsilon^3 + 7C\varepsilon^2\Delta + 15C^2\varepsilon\Delta^2 + 9C^3\Delta^3},$$

where $C = \coth\left(\frac{1}{2}\beta\Delta\right)$. Their difference yields

$$\Delta F = \frac{2\varepsilon^2(C^2 - 1)}{\varepsilon^2 + 4C\varepsilon\Delta + 3C^2\Delta^2}.$$

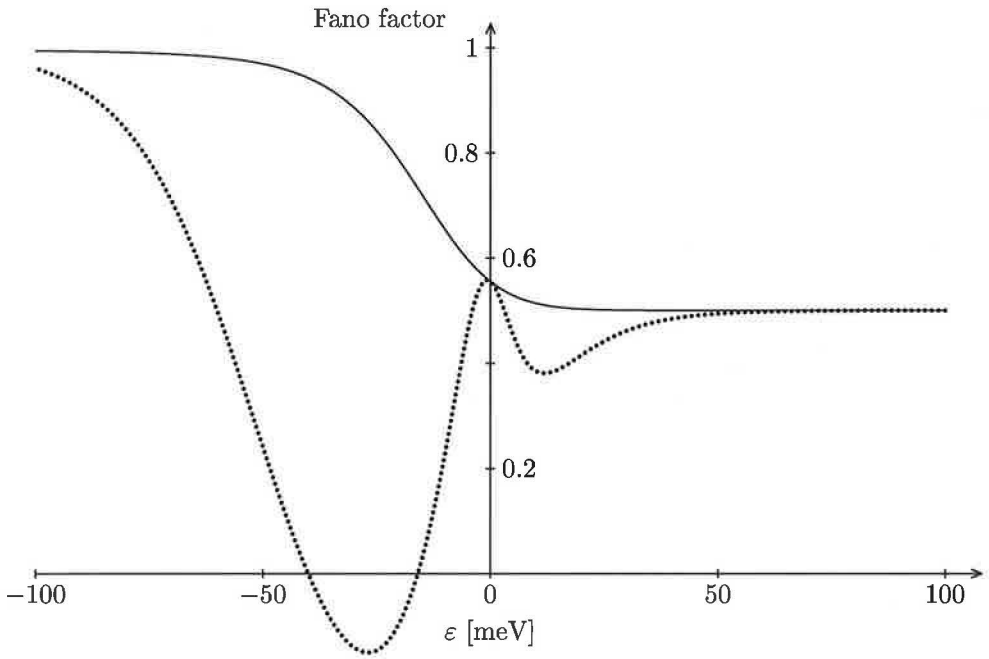

Fig. 3.4: Fano factor vs. bias ε for $\Gamma \to 0$, solid line shows $F_{\mathrm{L0}} = F_{\mathrm{0R}}$, dotted line shows F_{RL}. Parameters: $\Omega = 5\,\mathrm{meV}$, $\beta = 0.1\,\mathrm{meV}^{-1}$ (temperature 120 K).

Results are illustrated in fig. 3.4. We note quite interesting phenomenon that the Fano factor does not depend on the heat bath spectral density and thus it is not influenced by the strength γ of the dissipation. Nevertheless, all the anomalies survive. The Fano factor F_{RL} can be negative for certain ε and temperature high enough. Since the Fano factors for the three junctions are not equal, the charge conservation condition is not fulfilled. Both F_{L0} and F_{RL} become 1 for $\varepsilon \to -\infty$, 1/2 for $\varepsilon \to \infty$ and $F = 5/9$ for $\varepsilon = 0$. The striking difference between the Fano factors for inner and outer junction is that F_{0L} has no maxima or minima and just smoothly goes from 1 to 1/2, whereas F_{RL} has two minima, one for $\varepsilon < 0$ and the other for $\varepsilon > 0$.

Limit $\Omega \to 0$

Now we inquire the limit when the interdot coupling Ω goes to zero. Consequently, the mean current goes to zero. A quantum coherence in the system is disturbed, the tunneling events are very rare and thus uncorrelated, one would expect the current noise will be Poissonian $F = 1$.

Indeed, the Fano factor for the outer junctions is equal to 1. For the junction between the dots, we obtain

$$F_{\mathrm{RL}} = \frac{\hbar^2\Gamma}{\hbar^2\Gamma + 2\pi J(\varepsilon/\hbar)(1 + \coth\left(\frac{1}{2}\beta\varepsilon\right))}$$

and in the case of the Ohmic bath

$$F_{\mathrm{RL}} = \frac{\hbar\Gamma}{\hbar\Gamma + 4\gamma\varepsilon(1 + \coth\left(\frac{1}{2}\beta\Delta\right))}.$$

This expression yields 1 for $\varepsilon \to -\infty$, but goes to 0 for $\varepsilon \to \infty$. Results are also illustrated in fig. 3.5.

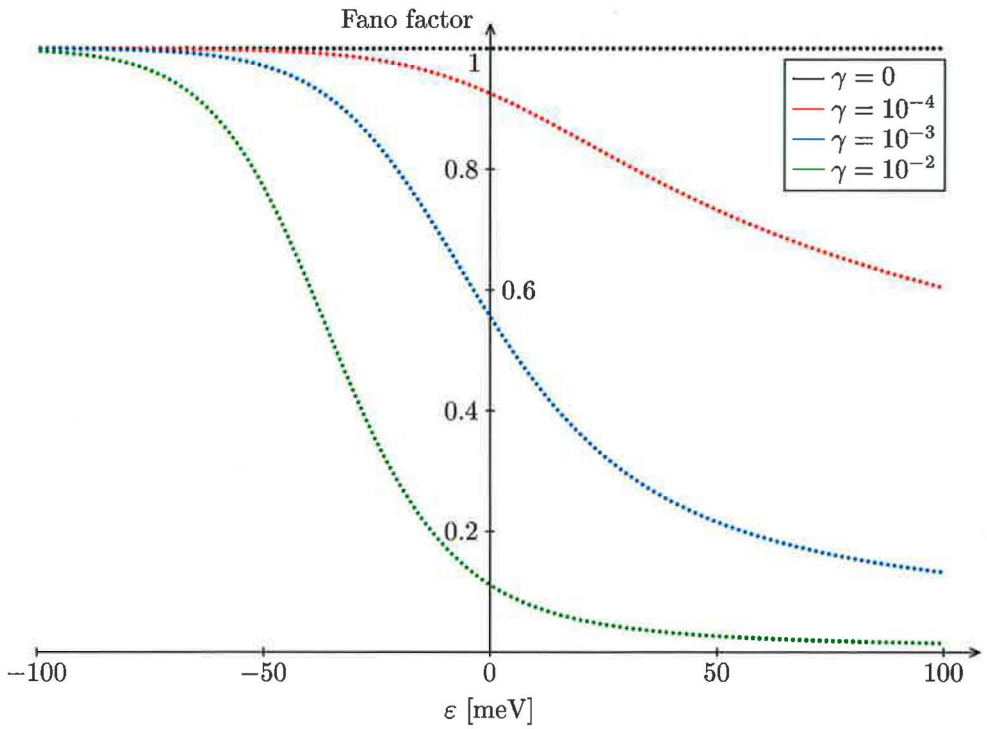

Fig. 3.5: Fano factor F_{RL} vs. bias ε for $\Omega \to 0$, $\beta = 0.1\,\mathrm{meV}^{-1}$ (temperature 120 K).

3.6 Rotating wave approximation

If a quantum dissipative system dynamics is prescribed by the generalized master equation (weak coupling prescription and Markovian limit), Heisenberg equations of motion of system operators are kept unchanged, however the reduced density matrix could violate positive semidefiniteness (i. e. negative eigenvalues can appear which would in turn imply negative probabilities).

Making a rotating wave approximation leads to violation of equations of motion, but the positivity of the reduced density matrix is retrieved. A similar discussion in a different context is in ref. [16].

It seems that in our case both characteristics are broken. First, the charge conservation problem indicates the violation of the equation of motion. Second, the negative Fano factor reveals non-positivity of the reduced density matrix. Let us see what will happen after introducing the rotating wave approximation.

Rotating wave approximation in the LR-basis

The rotating wave approximation is understood as neglecting terms of the form $a^\dagger \varrho a^\dagger$, $a\varrho a$ and keeping terms of the form $a^\dagger \varrho a$, $a\varrho a^\dagger$ in the generalized master equation $\mathrm{d}\varrho/\,\mathrm{d}t = \mathcal{L}\varrho$. In our language, we mean $a^\dagger = |\mathrm{L}\rangle\langle\mathrm{R}|$, $a = |\mathrm{R}\rangle\langle\mathrm{L}|$ and so $|\mathrm{L}\rangle\langle\mathrm{L}| = a^\dagger a$, $|\mathrm{R}\rangle\langle\mathrm{R}| = aa^\dagger$. Making the approximation on (3.11) leaves us with

$$\mathcal{L}_{\mathrm{B}}^{\mathrm{RWA1}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\gamma_p & 0 \\ 0 & 0 & 0 & 0 & -\gamma_p \end{pmatrix}.$$

As we can convince ourselves, the anomalous current (3.37) is now identically zero, thus $[\mathcal{N}_{\mathrm{L}}, \mathcal{L}_{\mathrm{B}}] = [\mathcal{N}_{\mathrm{R}}, \mathcal{L}_{\mathrm{B}}] = 0$ and therefore the charge conservation is restored. The zero-frequency noise and the Fano factor for any junction are equal.

The mean current is

$$\langle I \rangle = \frac{e\Gamma\Omega^2(\gamma_p + \frac{1}{2}\Gamma)}{\frac{1}{2}\Gamma\varepsilon^2 + 3\Omega^2(\gamma_p + \frac{1}{2}\Gamma) + \frac{1}{2}\hbar^2\Gamma(\gamma_p + \frac{1}{2}\Gamma)^2}$$

and for the Fano factor, we get

$$F = 1 - \frac{4\Omega^2\left[(\gamma_p + \frac{1}{2}\Gamma)^2\left(\Omega^2 + \frac{1}{2}\hbar^2\Gamma(\gamma_p + \Gamma)\right) + \frac{1}{2}\gamma_p\Gamma\varepsilon^2\right]}{\left[\frac{1}{2}\Gamma\varepsilon^2 + 3\Omega^2(\gamma_p + \frac{1}{2}\Gamma) + \frac{1}{2}\hbar^2\Gamma(\gamma_p + \frac{1}{2}\Gamma)^2\right]^2}.$$

These results are also illustrated in fig. 3.6.

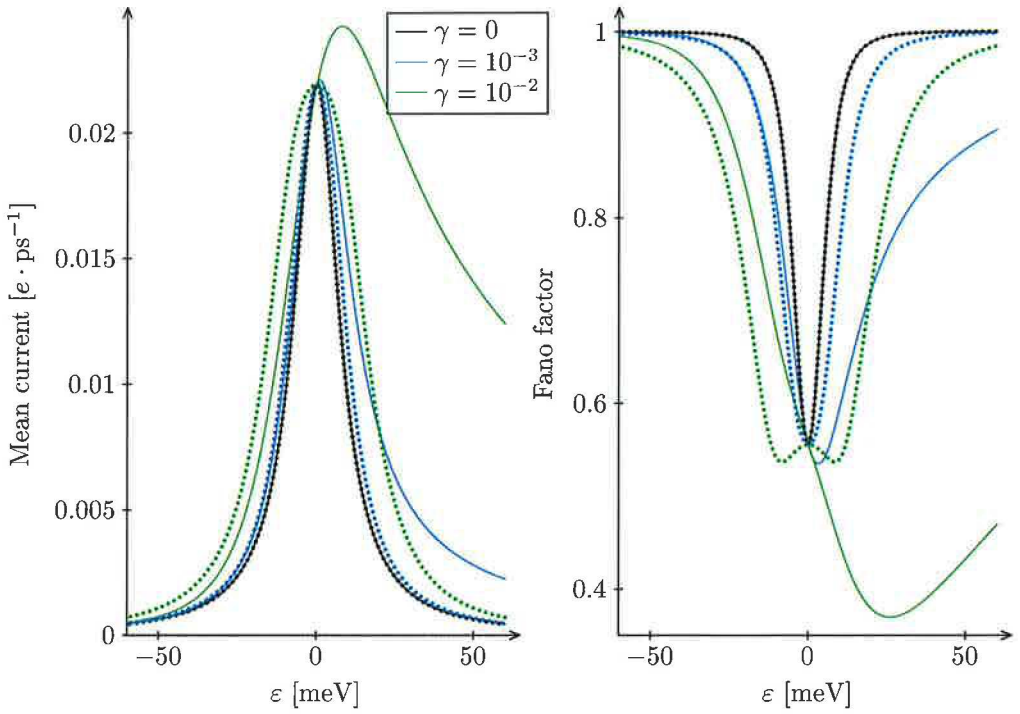

Fig. 3.6: Mean current and Fano factor vs. bias ε for different values of damping coefficient γ, solid lines correspond to the outer junctions without the rotating wave approximation (RWA), dotted lines correspond to RWA. Parameters: $\Gamma = 0.1/\hbar\,\mathrm{meV}$, $T = 5\,\mathrm{meV}$, $\beta = 0.1\,\mathrm{meV}^{-1}$ (temperature 120 K).

We can see that negative Fano factor does not appear in this approach. So it seems that all problems are fixed. However, the physical content of our results has undergone great changes. We have given reasons why the mean current and the Fano factor curves should have emission-absorption asymmetry, but we obtain absolutely symmetric curves – the mean current gained Lorentzian shape again and the Fano factor has no suppression for $\varepsilon > 0$ due to the emission process. Because of these reasons we must reject the rotating wave approximation on the physical grounds.

Rotating wave approximation in the 12-basis

In the similar way, we can introduce the rotating wave approximation in the 12-basis. Reevaluating the expression (3.9) gives

$$\mathcal{L}_{\mathrm{B}}^{\mathrm{RWA2}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -\gamma_\downarrow & \gamma_\uparrow & 0 & 0 \\ 0 & \gamma_\downarrow & -\gamma_\uparrow & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2}\gamma_p & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2}\gamma_p \end{pmatrix}$$

and the transformation into the LR-basis yields

$$\mathcal{L}_{\mathrm{B}}^{\mathrm{RWA2}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -\gamma_0^+ & \gamma_0^- & \frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) & \frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) \\ 0 & \gamma_0^+ & -\gamma_0^- & -\frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) & -\frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) \\ 0 & \tilde{\gamma}_+ & -\tilde{\gamma}_- & -\tilde{\gamma}_p & -\gamma_q \\ 0 & \tilde{\gamma}_+ & -\tilde{\gamma}_- & -\gamma_q & -\tilde{\gamma}_p \end{pmatrix},$$

where

$$\begin{aligned} \gamma_0^{\pm} &= \frac{2\pi}{\hbar^2}\frac{\Omega^2}{\Delta^4} J(\Delta/\hbar)\left((2\Omega^2+\varepsilon^2)\coth(\tfrac{1}{2}\beta\Delta) \pm \varepsilon\Delta\right), \\ \tilde{\gamma}_{\pm} &= -\frac{2\pi}{\hbar^2}\frac{\Omega^3}{\Delta^4} J(\Delta/\hbar)\left(\varepsilon\coth(\tfrac{1}{2}\beta\Delta) \pm 2\Delta\right), \\ \tilde{\gamma}_p &= \frac{2\pi}{\hbar^2}\frac{\Omega^2}{\Delta^4}(\Delta^2+2\Omega^2) J(\Delta/\hbar)\coth(\tfrac{1}{2}\beta\Delta), \\ \gamma_q &= \frac{4\pi}{\hbar^2}\frac{\Omega^4}{\Delta^4} J(\Delta/\hbar)\coth(\tfrac{1}{2}\beta\Delta). \end{aligned}$$

For the indicator of the charge conservation – the anomalous current, we obtain

$$\mathcal{I}_{\mathrm{A}} = [\mathcal{N}_{\mathrm{R}}, \mathcal{L}_{\mathrm{B}}] = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\gamma_0^- & \frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) & \frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) \\ 0 & -2\gamma_0^+ & 0 & \frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) & \frac{1}{2}(\tilde{\gamma}_+ + \tilde{\gamma}_-) \\ 0 & -\tilde{\gamma}_+ & -\tilde{\gamma}_- & 0 & 0 \\ 0 & -\tilde{\gamma}_+ & -\tilde{\gamma}_- & 0 & 0 \end{pmatrix}.$$

The direct consequences are obvious. Since $\langle\langle\tilde{0}|\mathcal{I}_{\mathrm{A}}|0\rangle\rangle \neq 0$, the mean current $\langle I_{\mathrm{L0}}\rangle$ and $\langle I_{\mathrm{RL}}\rangle$ are no longer equal to each other. Also the zero-frequency current noise and the Fano factor cannot be same for the inner and the outer junction.

The mean current and the Fano factor for the junction between the dot and the lead are illustrated in fig. 3.7. We obtain very good agreement, which means that the rotating wave approximation affected results slightly. On the other hand, results for the junctions between the dots are changed significantly, as can be seen in fig. 3.8. The emission shoulder in the mean current characteristics is missing. The Fano factor was fixed in the sense that it gives no negative values, which is the expected behavior. Similarly as in the previous, the Fano factor values do not fit the physical characteristics of the system, since we get a superpoissonian Fano factor ($F > 1$).

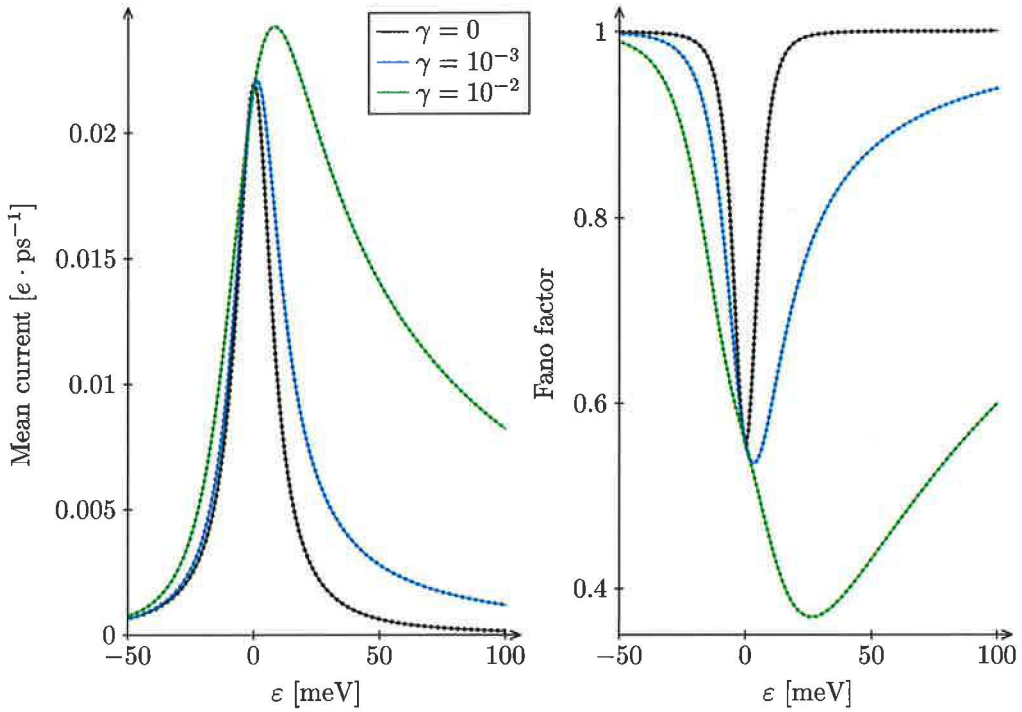

Fig. 3.7: Mean current and Fano factor vs. bias ε for different values of damping coefficient γ, solid lines correspond to the outer junction without RWA, dotted lines correspond to the outer junction with RWA. Parameters: $\Gamma = 0.1/\hbar\,\mathrm{meV}$, $T = 5\,\mathrm{meV}$, $\beta = 0.1\,\mathrm{meV}^{-1}$.

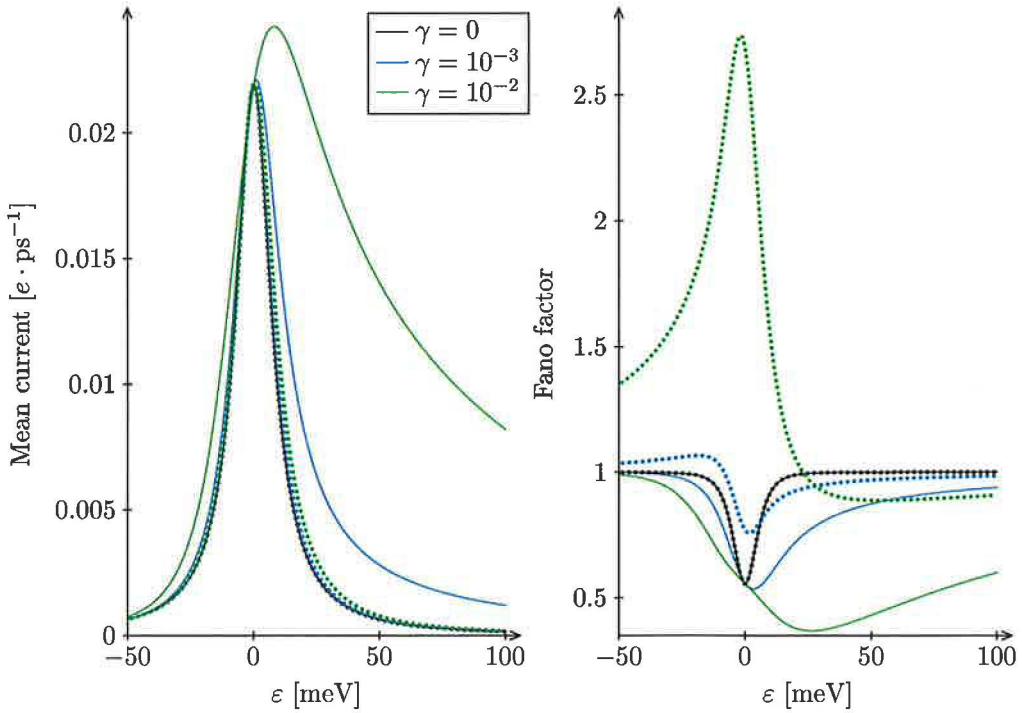

Fig. 3.8: Mean current and Fano factor vs. bias ε for different values of damping coefficient γ, solid lines corresponds to the outer junction without RWA, dotted lines corresponds to the inner junction with RWA. Parameters: $\Gamma = 0.1/\hbar\,\mathrm{meV}$, $T = 5\,\mathrm{meV}$, $\beta = 0.1\,\mathrm{meV}^{-1}$.

3.7 Pauli master equation

There is another approach which is not leading to the negative probabilities. If we do not need to keep coherences (off-diagonal elements of the density matrix), we can perform projection on the diagonal of the density matrix in the 12-basis. The dimension of the Liouville space shrinks from five to three. Its basis is $\{|00\rangle\!\rangle, |11\rangle\!\rangle, |22\rangle\!\rangle\}$. This procedure leads to Pauli master equation. As long we have a Liouvillian of the generalized master equation, we can get a Liouvillian of the Pauli master equation immediately. The projection operator has the form

$$\mathcal{P}_{\text{Pauli}} = |00\rangle\!\rangle\langle\!\langle 00| + |11\rangle\!\rangle\langle\!\langle 11| + |22\rangle\!\rangle\langle\!\langle 22| \,.$$

Projection of (3.10) and (3.12) yields

$$\mathcal{L}^{\text{Pauli}} = \begin{pmatrix} -\Gamma_{10} - \Gamma_{20} & \Gamma_{01} & \Gamma_{02} \\ \Gamma_{10} & -\Gamma_{01} & 0 \\ \Gamma_{20} & 0 & -\Gamma_{02} \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\gamma_\downarrow & \gamma_\uparrow \\ 0 & \gamma_\downarrow & -\gamma_\uparrow \end{pmatrix},$$

where

$$\Gamma_{10} = \Gamma_{02} = \Gamma\frac{\Delta+\varepsilon}{2\Delta}, \qquad \gamma_\downarrow = \frac{4\pi}{\hbar^2}\frac{\Omega^2}{\Delta^2} J(\Delta/\hbar)\frac{1}{1-\mathrm{e}^{-\beta\Delta}},$$
$$\Gamma_{01} = \Gamma_{20} = \Gamma\frac{\Delta-\varepsilon}{2\Delta}. \qquad \gamma_\uparrow = \frac{4\pi}{\hbar^2}\frac{\Omega^2}{\Delta^2} J(\Delta/\hbar)\frac{1}{\mathrm{e}^{\beta\Delta}-1}.$$

The same results can be derived from the Fermi golden rule. Transition rates between the states $|0\rangle$, $|1\rangle$ and $|2\rangle$ will be denoted $\Gamma_{0\leftarrow 1} = \Gamma_{01}$, $\Gamma_{2\leftarrow 0} = \Gamma_{20}$ etc. The Fermi golden rule says

$$\begin{aligned}\Gamma_{10} &= \frac{2\pi}{\hbar}\sum_k |\langle 1|H_{\text{CS}}|k\text{L}\rangle|^2\,\delta(E_{k\text{L}}-\Delta/2) = \\ &= \frac{2\pi}{\hbar}\sum_k |\langle 1|V_{k\text{L}}|\text{L}\rangle\langle 0|c_{k\text{L}}c_{k\text{L}}^\dagger|0\rangle|^2\,\delta(E_{k\text{L}}-\Delta/2) = \\ &= \frac{2\pi}{\hbar}\sum_k |V_{k'\text{L}}|^2|\langle 1|\text{L}\rangle|^2\,\delta(E_{k\text{L}}-\Delta/2) = \Gamma_{\text{L}}\frac{\Delta+\varepsilon}{2\Delta},\end{aligned}$$

where we have considered the wide-band limit. Analogously for the other rates

$$\Gamma_{20} = \Gamma_{\text{L}}\frac{\Delta-\varepsilon}{2\Delta}, \qquad \Gamma_{01} = \Gamma_{\text{R}}\frac{\Delta-\varepsilon}{2\Delta}, \qquad \Gamma_{02} = \Gamma_{\text{R}}\frac{\Delta+\varepsilon}{2\Delta}$$

and $\Gamma_{12} = \Gamma_{21} = 0$.

In the case of the heat bath, we obtain

$$\begin{aligned}\gamma_{21} &= \frac{2\pi}{\hbar}\sum_j |\langle 2|a_j H_{\text{BS}}|1\rangle|^2\,\delta(\Delta-\hbar\omega_j) = \\ &= \frac{2\pi}{\hbar}\sum_j |C_j|^2\left|\frac{2\Omega}{\Delta}\right|^2\delta(\Delta-\hbar\omega_j) = \frac{4\pi}{\hbar^2}\frac{\Omega^2}{\Delta^2}J(\Delta/\hbar),\end{aligned}$$

which is the zero temperature limit of $\gamma_\downarrow$.

The current superoperators in the new Liouville space are simply given by

$$\mathcal{I}_{\mathrm{L0}} = \begin{pmatrix} 0 & 0 & 0 \\ \Gamma_{10} & 0 & 0 \\ \Gamma_{20} & 0 & 0 \end{pmatrix}, \qquad \mathcal{I}_{\mathrm{0R}} = \begin{pmatrix} 0 & \Gamma_{01} & \Gamma_{02} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Since the current superoperator $\mathcal{I}_{\mathrm{RL}}$ is not defined on the given subspace, we cannot calculate the mean current and the zero-frequency noise between the dots. It means that the states occupation numbers contain no information about the current between the dots.

For the mean current and the Fano factor between the dot and the lead, we get

$$\langle I \rangle = \frac{e\Gamma\Omega\left(\Omega(\gamma_p + \frac{1}{2}\Gamma) - \gamma_+\varepsilon\right)}{\frac{1}{2}\Gamma\varepsilon^2 + 3\Omega^2(\gamma_p + \frac{1}{2}\Gamma) - \Omega\varepsilon(2\gamma_+ + \gamma_-)}$$

and

$$F = 1 - \frac{2\Omega\left[2\Omega^3(\gamma_p + \frac{1}{2}\Gamma)^2 - \Omega^2\varepsilon(\gamma_p + \frac{3}{2}\Gamma)(3\gamma_+ + \gamma_-) - \gamma_+\varepsilon^3(\gamma_p + \frac{1}{2}\Gamma)\right]}{\left[\frac{1}{2}\Gamma\varepsilon^2 + 3\Omega^2(\gamma_p + \frac{1}{2}\Gamma) - \Omega\varepsilon(2\gamma_+ + \gamma_-)\right]^2}.$$

These expressions differ from the results (3.39) for the full-space reduced density matrix in the second order of Γ. Thus we can expect, that for small values of Γ, we will obtain very good agreement between the two approaches, as it is shown in fig. 3.9.

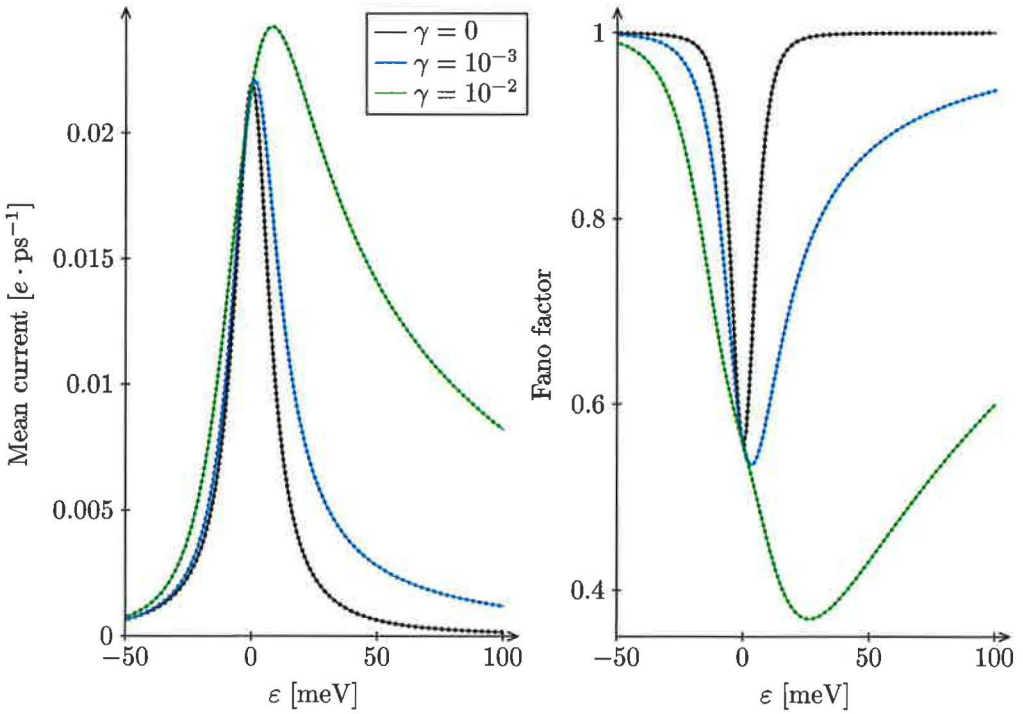

Fig. 3.9: Mean current and Fano factor at the outer junctions vs. bias ε for different values of damping coefficient γ, solid lines correspond to GME, dotted lines correspond to Pauli master equation. Parameters: $\Gamma = 0.1/\hbar\,\mathrm{meV}$, $T = 5\,\mathrm{meV}$, $\beta = 0.1\,\mathrm{meV}^{-1}$.

3.8 Summary

The mean current is conserved, so there is no problem to determine its value. Any reasonable approach gives the same results. The same can be said about the Fano factor at the outer junction (between the dot and the lead). The result given by generalized master equation and the MacDonald formula was confirmed by the rotating wave approximation in the 12-basis and the Pauli master equation. Moreover, the limit $\Gamma \to 0$ and $\Omega \to 0$ gives reasonable results only for the outer junction.

Situation within the system is troublesome. The weak coupling assumption and the Markovian limit evidently break the equation of the motion for the dot occupation operators and break positivity of the reduced density matrix. The Fano factor calculated for the system current operator I_{RL} is sheer nonsense, which cannot be fixed by the rotating wave approximation. Fundamental question, whether it is general phenomena that autocorrelation functions of the system operators of dissipative systems can be negative, will be tried to be answered in the following chapters.

Chapter 4

Harmonic oscillator coupled to two heat baths

The fact that the interaction Hamiltonians H_{BS} and H_{CS} of the double quantum dot do not commute

$$[H_{\mathrm{CS}}, H_{\mathrm{BS}}] = \sum_j C_j (a_j^\dagger + a_j) \Big[\sum_k V_{k\mathrm{L}} (c_{k\mathrm{L}}^\dagger |0\rangle\langle \mathrm{L}| - |\mathrm{L}\rangle\langle 0| c_{k\mathrm{L}}) + \\ + \sum_k V_{k\mathrm{R}} (-c_{k\mathrm{R}}^\dagger |0\rangle\langle \mathrm{R}| + |\mathrm{R}\rangle\langle 0| c_{k\mathrm{R}}) \Big]$$

deserves more attention, because we believe that this could be the main reason causing the charge conservation problem. The couplings have not a simultaneous system of eigenvectors and hence they are trying to bring system to different states. Such a contradictory activity could be possibly responsible for failing of the generalized master equation approach which still works fine in the case without the dissipation heat bath.

4.1 Model

A reasonable choice will be an exactly solvable dissipative system coupled to two baths. The harmonic oscillator provides such a system, which will be investigated in this chapter.

The harmonic oscillator is coupled separately through its position and momentum to two independent heat baths.

$$H = H_{\mathrm{S}} + H_{q\mathrm{S}} + H_q + H_{p\mathrm{S}} + H_p \,,$$

where H_{S} is the standard linear harmonic oscillator Hamiltonian

$$H_{\mathrm{S}} = \tfrac{1}{2}\omega_0 q^2 + \tfrac{1}{2}\omega_0 p^2 \,. \tag{4.1}$$

We have put $\hbar = 1$. The position q and the momentum p are dimensionless, since then Hamiltonian has a symmetry between q and p, and $[q, p] = \mathrm{i}$.

The generic heat baths consist of an infinite set of harmonic oscillators

$$H_q + H_p = \sum_j \omega_{qj} a_{qj}^\dagger a_{qj} + \sum_j \omega_{pj} a_{pj}^\dagger a_{pj} \,, \tag{4.2}$$

where a, $a^\dagger$ are phonon annihilation and creation operators. We consider a linear interaction with two Ohmic baths, via the position and the momentum

$$H_{q\mathrm{S}} + H_{p\mathrm{S}} = \sum_j C_{qj}(a_{qj}^\dagger q + q a_{qj}) + \Delta V_q(q) + \sum_j C_{pj}(a_{pj}^\dagger p + p a_{pj}) + \Delta V_p(p)\,. \quad (4.3)$$

The bath spectral densities are Ohmic

$$J_k = 2\sum_j |C_{kj}|^2 \delta(\omega - \omega_{kj}) = 2\gamma_k \omega/\pi$$

with $k = q, p$.

Since we are interested also in exact solution, we have added counter terms $\Delta V_q(q)$ and $\Delta V_p(p)$ which depend on the variables of the harmonic oscillator, but not on the dynamical variables of the reservoir. These terms are introduced in order to compensate a shift of the potential $\frac{1}{2}\omega_0 q^2$ due to the linear coupling between the baths and the harmonic oscillator. The minimum of the potential for given q is at $x_j = -C_{kj}q/\omega_{kj}$. If we wish to compensate for the shift, we put

$$\Delta V_q(q) = \sum_j \frac{|C_{qj}|^2}{\omega_{qj}} q^2\,, \qquad \Delta V_p(p) = \sum_j \frac{|C_{pj}|^2}{\omega_{pj}} p^2\,. \quad (4.4)$$

Then the bath and interaction Hamiltonians can be rewritten in a compact form [3, 17]

$$H_q + H_{q\mathrm{S}} + H_p + H_{p\mathrm{S}} = \sum_j \omega_{qj} \left| a_{qj} + \frac{C_{qj}}{\omega_{qj}} q \right|^2 + \sum_j \omega_{pj} \left| a_{pj} + \frac{C_{pj}}{\omega_{pj}} p \right|^2 , \quad (4.5)$$

where $|A|^2 \equiv A^\dagger A$.

4.2 Exact solution

Eliminating the bath variables, the Heisenberg equations of motion for q and p are obtained [17]

$$\begin{aligned} \dot{q}(t) &= \omega_0 p(t) + \gamma_p \dot{p}(t) + F_p(t)\,, \\ -\dot{p}(t) &= \omega_0 q(t) + \gamma_q \dot{q}(t) + F_q(t)\,, \end{aligned}$$

where

$$F_k(t) = \sum_j C_{kj} a_{kj} \mathrm{e}^{-\mathrm{i}\omega_{kj}t} + \sum_j C_{kj}^* a_{kj}^\dagger \mathrm{e}^{\mathrm{i}\omega_{kj}t}\,, \qquad k = q, p\,.$$

Moving time derivatives to the left side of equations, we obtain

$$\begin{aligned} (1 + \gamma_q\gamma_p)\dot{q}(t) &= \omega_0 p(t) - \gamma_p \omega_0 q(t) - \gamma_p F_q(t) + F_p(t)\,, \\ (1 + \gamma_q\gamma_p)\dot{p}(t) &= -\omega_0 q(t) - \gamma_q \omega_0 p(t) - \gamma_q F_p(t) - F_q(t)\,. \end{aligned} \quad (4.6)$$

System eigenfrequencies are

$$\omega_1 = \frac{\tilde{\omega}_0 - \frac{1}{2}\mathrm{i}\omega_0(\gamma_q + \gamma_p)}{1 + \gamma_q\gamma_p}, \qquad \omega_2 = \frac{-\tilde{\omega}_0 - \frac{1}{2}\mathrm{i}\omega_0(\gamma_q + \gamma_p)}{1 + \gamma_q\gamma_p},$$

where $\tilde{\omega}_0 = \omega_0\sqrt{1 - \frac{1}{4}(\gamma_q - \gamma_p)^2}$. Eigenvectors read

$$v_1 = \begin{pmatrix} \mathrm{i}\tilde{\omega}_0 + \frac{1}{2}\omega_0(\gamma_p - \gamma_q) \\ \omega_0 \end{pmatrix}, \qquad v_2 = \begin{pmatrix} -\mathrm{i}\tilde{\omega}_0 + \frac{1}{2}\omega_0(\gamma_p - \gamma_q) \\ \omega_0 \end{pmatrix}.$$

A solution of the equations of motion (4.6) which has the form

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = A(t)\mathrm{e}^{-\mathrm{i}\omega_1 t}v_1 + B(t)\mathrm{e}^{-\mathrm{i}\omega_2 t}v_2,$$

we find via the variation of constants. One obtains the following results

$$\begin{aligned} q(t) = {} & \frac{\mathrm{i}\tilde{\omega}_0 + \frac{1}{2}\omega_0(\gamma_p - \gamma_q)}{\omega_0} \int_{-\infty}^{t} \mathrm{d}t' \mathrm{e}^{-\mathrm{i}\omega_1(t-t')} \left(\frac{-\tilde{\omega}_0 + \frac{1}{2}\mathrm{i}\omega_0(\gamma_q + \gamma_p)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_q(t') + \right. \\ & \left. + \frac{-\gamma_q\tilde{\omega}_0 - \mathrm{i}\omega_0\left(1 - \frac{1}{2}\gamma_q(\gamma_q - \gamma_p)\right)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_p(t') \right) + \\ & + \frac{-\mathrm{i}\tilde{\omega}_0 + \frac{1}{2}\omega_0(\gamma_p - \gamma_q)}{\omega_0} \int_{-\infty}^{t} \mathrm{d}t' \mathrm{e}^{-\mathrm{i}\omega_2(t-t')} \left(\frac{-\tilde{\omega}_0 - \frac{1}{2}\mathrm{i}\omega_0(\gamma_q + \gamma_p)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_q(t') + \right. \\ & \left. + \frac{-\gamma_q\tilde{\omega}_0 + \mathrm{i}\omega_0\left(1 - \frac{1}{2}\gamma_q(\gamma_q - \gamma_p)\right)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_p(t') \right), \\ p(t) = {} & \int_{-\infty}^{t} \mathrm{d}t' \mathrm{e}^{-\mathrm{i}\omega_1(t-t')} \left(\frac{-\tilde{\omega}_0 + \frac{1}{2}\mathrm{i}\omega_0(\gamma_q + \gamma_p)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_q(t') + \right. \\ & \left. + \frac{-\gamma_q\tilde{\omega}_0 - \mathrm{i}\omega_0\left(1 - \frac{1}{2}\gamma_q(\gamma_q - \gamma_p)\right)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_p(t') \right) + \\ & + \int_{-\infty}^{t} \mathrm{d}t' \mathrm{e}^{-\mathrm{i}\omega_2(t-t')} \left(\frac{-\tilde{\omega}_0 - \frac{1}{2}\mathrm{i}\omega_0(\gamma_q + \gamma_p)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_q(t') + \right. \\ & \left. + \frac{-\gamma_q\tilde{\omega}_0 + \mathrm{i}\omega_0\left(1 - \frac{1}{2}\gamma_q(\gamma_q - \gamma_p)\right)}{2(1 + \gamma_q\gamma_p)\tilde{\omega}_0} F_p(t') \right). \end{aligned}$$

In order to calculate position autocorrelation function

$$C_{qq}(t - t') = \tfrac{1}{2} \lim_{t\to\infty} \langle \{q(t), q(t')\} \rangle,$$

we have to express the quantity

$$\tfrac{1}{2}\langle F_q(t_1)F_q(t_2) + F_q(t_2)F_q(t_1)\rangle = \frac{2\gamma_q}{\pi}\int_0^\infty \mathrm{d}\omega\,\omega\cos\left[\omega(t_1-t_2)\right]\left(N_q(\omega)+\tfrac{1}{2}\right),$$

where $N_q(\omega)$ is Bose-Einstein distribution

$$N_q(\omega_j) = \langle a_{qj}^\dagger a_{qj}\rangle = \frac{1}{\exp\left(\beta_q\omega_j\right)-1}$$

with temperature $T_q = 1/k_\mathrm{B}\beta_q$ of the heat bath coupled via the position. Analogously for the second bath

$$\tfrac{1}{2}\langle F_p(t_1)F_p(t_2) + F_p(t_2)F_p(t_1)\rangle = \frac{2\gamma_p}{\pi}\int_0^\infty \mathrm{d}\omega\,\omega\cos\left[\omega(t_1-t_2)\right]\left(N_p(\omega)+\tfrac{1}{2}\right).$$

Now we are ready to substitute the expression for $q(t)$ into the relation for autocorrelation function $C_{qq}(t-t')$. The above quantities are put to use and the double integrals over time of the following form have to be performed (the pair of frequencies ω_A and ω_B comprises various combinations of ω_1 and ω_2).

$$\int_{-\infty}^{t}\mathrm{d}t_2\int_{-\infty}^{t'}\mathrm{d}t_1\mathrm{e}^{-\mathrm{i}\omega_\mathrm{A}t_1-\mathrm{i}\omega_\mathrm{B}t_2}\cos\left[\omega(t_1-t_2)\right] =$$

$$= \mathrm{e}^{-\mathrm{i}\omega_\mathrm{A}t'-\mathrm{i}\omega_\mathrm{B}t}\frac{(\omega^2-\omega_\mathrm{A}\omega_\mathrm{B})\cos\left[\omega(t-t')\right]+\mathrm{i}\omega(\omega_\mathrm{B}-\omega_\mathrm{A})\sin\left[\omega(t-t')\right]}{(\omega^2-\omega_\mathrm{A}^2)(\omega^2-\omega_\mathrm{B}^2)}.$$

In the frequency domain

$$C_{qq}(\tau) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega C_{qq}(\omega)\cos\omega\tau$$

it gives the final results

$$\begin{aligned}
C_{qq}(\omega) &= \gamma_q(N_q(\omega)+\tfrac{1}{2})\frac{\omega_0^2\omega+\gamma_p^2\omega^3}{[(1+\gamma_q\gamma_p)\omega^2-\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2} + \\
&+ \gamma_p(N_p(\omega)+\tfrac{1}{2})\frac{\omega^3}{[(1+\gamma_q\gamma_p)\omega^2-\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}, \\
C_{pp}(\omega) &= \gamma_q(N_q(\omega)+\tfrac{1}{2})\frac{\omega^3}{[(1+\gamma_q\gamma_p)\omega^2-\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2} + \\
&+ \gamma_p(N_p(\omega)+\tfrac{1}{2})\frac{\omega_0^2\omega+\gamma_q^2\omega^3}{[(1+\gamma_q\gamma_p)\omega^2-\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}.
\end{aligned} \tag{4.7}$$

The values of these autocorrelation functions are necessarily non-negative for any real ω and will be compared with a solution of the generalized master equation in the next section. The results are also plotted in fig. 4.1 later on in Section 4.4.

Setting $\gamma_p = 0$, we restore the autocorrelation functions relations for the harmonic oscillator with a single bath [18].

4.3 Generalized master equation approach

A derivation of the generalized master equation consists of the same steps as in the Chapter 2. We assume the product initial condition, project out both baths, introduce the weak coupling prescription and the Markovian dynamics. We arrive at the following generalized master equation for the reduced density matrix ϱ of the Hilbert space of the harmonic oscillator.

$$\begin{aligned}\frac{\mathrm{d}\varrho(t)}{\mathrm{d}t} = &-\mathrm{i}[H_{\mathrm{S}}, \varrho(t)] - \\ &- \int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_q\{[H_{q\mathrm{S}}, [H_{q\mathrm{S}}(-\tau), \varrho(t) \otimes \varrho_q]]\} - \\ &- \int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_p\{[H_{p\mathrm{S}}, [H_{p\mathrm{S}}(-\tau), \varrho(t) \otimes \varrho_p]]\}\,,\end{aligned} \tag{4.8}$$

where $H_{k\mathrm{S}}(-\tau) = \exp[-\mathrm{i}(H_{\mathrm{S}} + H_k)\tau/\hbar] H_{k\mathrm{S}} \exp[\mathrm{i}(H_{\mathrm{S}} + H_k)\tau/\hbar]$ and ϱ_k is a thermal equilibrium density operator of the bath ($k = q, p$). The compensating terms (4.4) are discarded on the same grounds as the imaginary parts of the time integrals (small frequency shifts) are omitted. Resulting Liouvillian reads

$$\begin{aligned}\mathcal{L}\varrho = &-\tfrac{1}{2}\mathrm{i}\omega_0[q^2 + p^2, \varrho] \\ &- \gamma_q\omega_0\left((N_q(\omega_0) + \tfrac{1}{2})[q, [q, \varrho]] + \tfrac{1}{2}\mathrm{i}\,[q, \{p, \varrho\}]\right) \\ &- \gamma_p\omega_0\left((N_p(\omega_0) + \tfrac{1}{2})[p, [p, \varrho]] - \tfrac{1}{2}\mathrm{i}\,[p, \{q, \varrho\}]\right)\,,\end{aligned} \tag{4.9}$$

where $N_k(\omega)$ is Bose-Einstein distribution

$$N_k(\omega) = \frac{1}{\exp(\beta_k\omega) - 1}$$

with $k = q, p$, $T_k = 1/k_{\mathrm{B}}\beta_k$ is temperature of the heat bath.

Time derivatives of mean values of system operators are given by the relation $\langle \dot{A}(t)\rangle = \mathrm{Tr}\{A\mathcal{L}\varrho\}$. For the position and the momentum we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle q(t)\rangle &= \omega_0\langle p(t)\rangle - \gamma_p\omega_0\langle q(t)\rangle\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle p(t)\rangle &= -\omega_0\langle q(t)\rangle - \gamma_q\omega_0\langle p(t)\rangle\,.\end{aligned} \tag{4.10}$$

We note that these equations of motion differ from the exact ones (4.6) by the factor $1 + \gamma_q\gamma_p$ on the left-hand side and thus the difference is in the second order of the dissipation strength.

Similarly for the mean values of the q^2, p^2 and $\{q,p\}$

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle q^2(t)\rangle &= \omega_0\langle\{q,p\}(t)\rangle - 2\gamma_p\omega_0\langle q^2(t)\rangle + 2\gamma_p\omega_0(N_p(\omega_0)+\tfrac{1}{2})\,,\\
\frac{\mathrm{d}}{\mathrm{d}t}\langle p^2(t)\rangle &= -\omega_0\langle\{q,p\}(t)\rangle - 2\gamma_q\omega_0\langle p^2(t)\rangle + 2\gamma_q\omega_0(N_q(\omega_0)+\tfrac{1}{2})\,,\\
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle\{q,p\}(t)\rangle &= -\omega_0\langle q^2(t)\rangle + \omega_0\langle p^2(t)\rangle - \tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0\langle\{q,p\}(t)\rangle\,.
\end{aligned}$$

Since we inquire the stationary limit, we put the derivatives equal to zero giving the set of equations for the stationary mean values. We find

$$\begin{aligned}
\langle q^2\rangle &= (N_p+\tfrac{1}{2}) + \frac{\gamma_q}{(\gamma_q+\gamma_p)(1+\gamma_q\gamma_p)}\,(N_q-N_p)\,,\\
\langle p^2\rangle &= (N_q+\tfrac{1}{2}) + \frac{\gamma_p}{(\gamma_p+\gamma_p)(1+\gamma_q\gamma_p)}\,(N_p-N_q)\,,\\
\tfrac{1}{2}\langle\{q,p\}\rangle &= \frac{\gamma_q\gamma_p}{(\gamma_+\gamma_p)(1+\gamma_q\gamma_p)}\,(N_q-N_p)\,,
\end{aligned} \tag{4.11}$$

where the parameter by N_q and N_p has been dropped, since it is always ω_0.

Next, we define the symmetrized and non-symmetrized correlation functions

$$C_{AB}(\tau) \equiv \tfrac{1}{2}\lim_{t\to\infty}\langle A(t+\tau)B(t)+B(t)A(t+\tau)\rangle\,, \qquad J_{AB}(\tau) \equiv \lim_{t\to\infty}\langle A(t+\tau)B(t)\rangle\,.$$

Because of the stationary limit, we can proof following identity for hermitian operators A and B

$$\lim_{t\to\infty}\langle A(t+\tau)B(t)\rangle^* = \lim_{t\to\infty}\langle B(t)A(t+\tau)\rangle = \lim_{t\to\infty}\langle B(t-\tau)A(t)\rangle\,,$$

which implies following relations for the position and the momentum autocorrelation functions

$$\begin{aligned}
J^*_{qq}(\tau) &= J_{qq}(-\tau)\,, \quad J^*_{pp}(\tau) = J_{pp}(-\tau) \quad \text{and} \quad J^*_{qp}(\tau) = J_{pq}(-\tau)\,,\\
C_{qq}(\tau) &= C_{qq}(-\tau)\,, \quad C_{pp}(\tau) = C_{pp}(-\tau) \quad \text{and} \quad C_{qp}(\tau) = C_{pq}(-\tau)\,.
\end{aligned}$$

Using the general form of the quantum regression theorem ([10], Sec. 5.2.3)[1] for correlation functions, we obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}C_{qq}(\tau) &= \omega_0 C_{pq}(\tau) - \gamma_p\omega_0 C_{qq}(\tau)\,,\\
\frac{\mathrm{d}}{\mathrm{d}\tau}C_{pp}(\tau) &= -\omega_0 C_{qp}(\tau) - \gamma_q\omega_0 C_{pp}(\tau)\,,
\end{aligned} \tag{4.12}$$

[1] It says that if master equation for certain set of operators Y_i yields for any initial density operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle Y_i(t)\rangle = \sum_j G_{ij}(t)\langle Y_j(t)\rangle\,,$$

then

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\langle Y_i(t+\tau)Y_l(t)\rangle = \sum_j G_{ij}(t)\langle Y_j(t+\tau)Y_l(t)\rangle\,.$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau}C_{qp}(\tau) = \omega_0 C_{pp}(\tau) - \gamma_p\omega_0 C_{qp}(\tau)\,,$$
$$\frac{\mathrm{d}}{\mathrm{d}\tau}C_{pq}(\tau) = -\omega_0 C_{qq}(\tau) - \gamma_q\omega_0 C_{pq}(\tau)\,.$$

The same equations are valid for the non-symmetrized correlation functions.

The positive semidefiniteness of the density operator implies that the symmetrized correlation functions as well as the non-symmetrized ones in the frequency domain

$$C_{AB}(\omega) = \int_{-\infty}^{\infty} C_{AB}(t)\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t\,, \qquad J_{AB}(\omega) = \int_{-\infty}^{\infty} J_{AB}(t)\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t\,,$$

should be positive for an arbitrary ω.

Symmetrized correlation functions

Nothing more than to solve the set of differential equations (4.12) is needed to obtain expressions for the symmetrized autocorrelation functions. The initial conditions are $C_{qq}(0) = \langle q^2\rangle$, $C_{pp}(0) = \langle p^2\rangle$ and $C_{qp}(0) = C_{pq}(0) = \frac{1}{2}\langle\{q,p\}\rangle$. For $t \geq 0$ we find

$$\begin{aligned}
C_{qq}(t) &= \exp\left(-\tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0 t\right)\times \\
&\quad\times\left[\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}\langle\{q,p\}\rangle\sin(\tilde\omega_0 t) + \left(\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}(\gamma_q-\gamma_p)\sin(\tilde\omega_0 t) + \cos(\tilde\omega_0 t)\right)\langle q^2\rangle\right], \\
C_{pp}(t) &= \exp\left(-\tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0 t\right)\times \\
&\quad\times\left[-\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}\langle\{q,p\}\rangle\sin(\tilde\omega_0 t) + \left(\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}(\gamma_p-\gamma_q)\sin(\tilde\omega_0 t) + \cos(\tilde\omega_0 t)\right)\langle p^2\rangle\right],
\end{aligned} \tag{4.13}$$

where again $\tilde\omega_0 = \omega_0\sqrt{1-(\gamma_q-\gamma_p)^2/4}$.

We discover that the heat baths partially cancel each other. Most notably, oscillations may remain underdamped for arbitrarily strong coupling, if

$$|\gamma_q - \gamma_p| < 2$$

(i. e. if the two baths couple with comparable strength). This effect of decrease of the strength of the effective coupling (judging by the frequency of oscillations) is called quantum frustration and it is a direct consequence of the non-compatibility of position and momentum [17].

We perform the Fourier transform of the symmetrized autocorrelation functions

$$C(\omega) = \int_{-\infty}^{\infty} C(t)\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t = \int_{0}^{\infty} C(-t)\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t + \int_{0}^{\infty} C(t)\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t = 2\int_{0}^{\infty} C(t)\cos\omega t\,\mathrm{d}t$$

and it yields

$$\begin{aligned} C_{qq}(\omega) &= \gamma_q(N_q(\omega_0)+\tfrac{1}{2})\,\frac{\omega_0^3}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}+ \\ &+\gamma_p(N_p(\omega_0)+\tfrac{1}{2})\,\frac{\omega_0\omega^2+\gamma_q^2\omega_0^3}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}\,. \\ C_{pp}(\omega) &= \gamma_q(N_q(\omega_0)+\tfrac{1}{2})\,\frac{\omega_0\omega^2+\gamma_p^2\omega_0^3}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}+ \\ &+\gamma_p(N_p(\omega_0)+\tfrac{1}{2})\,\frac{\omega_0^3}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}\,. \end{aligned} \tag{4.14}$$

Apparently, the position and momentum autocorrelation functions are positive for arbitrary ω and thus, unfortunately for us, non-positivity of the density matrix is not exhibited on this level of correlation functions.

Comparing with the exact results (4.7) we can notice that they correspond for small damping coefficients γ_q and γ_p and around peak maximum ($\omega \to \omega_0$) as it is also visible in the plots in figs 4.1 in Section 4.4. In particular, the significant differences are in the numerators, the denominators are the same to the first order in γ. Notably, the statistical distribution depends on the frequency in the exact solution, however, it is evaluated at the point ω_0 in this approach.

The frequency curves have the Lorentzian-like shape, whose width is proportional to the sum of the damping coefficients $\gamma_q + \gamma_p$.

Non-symmetrized correlation functions

We will also show results for non-symmetrized correlation functions. We solve the set of equations (4.12) same as in the previous case of the symmetrized correlation functions, but the initial condition are different $J_{qq}(0) = \langle q^2\rangle$, $J_{pp}(0) = \langle p^2\rangle$ and

$$J_{qp}(0) = \tfrac{1}{2}\langle\{q,p\}\rangle + \tfrac{1}{2}\mathrm{i}\,, \qquad J_{pq}(0) = \tfrac{1}{2}\langle\{q,p\}\rangle - \tfrac{1}{2}\mathrm{i}\,.$$

The results read (for $t \geq 0$)

$$\begin{aligned} J_{qq}(t) &= \exp\left(-\tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0 t\right)\times \\ &\times\left[\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}\left(\langle\{q,p\}\rangle-\mathrm{i}\right)\sin(\tilde\omega_0 t)+\left(\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}(\gamma_q-\gamma_p)\sin(\tilde\omega_0 t)+\cos(\tilde\omega_0 t)\right)\langle q^2\rangle\right], \\ J_{pp}(t) &= \exp\left(-\tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0 t\right)\times \\ &\times\left[-\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}\left(\langle\{q,p\}\rangle+\mathrm{i}\right)\sin(\tilde\omega_0 t)+\left(\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}(\gamma_p-\gamma_q)\sin(\tilde\omega_0 t)+\cos(\tilde\omega_0 t)\right)\langle p^2\rangle\right], \\ J_{pq}(t) &= \exp\left(-\tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0 t\right)\times \\ &\times\left[-\frac{\omega_0}{\tilde\omega_0}\langle q^2\rangle\sin(\tilde\omega_0 t)+\frac{1}{2}\left(\frac{1}{2}\frac{\omega_0}{\tilde\omega_0}(\gamma_p-\gamma_q)\sin(\tilde\omega_0 t)+\cos(\tilde\omega_0 t)\right)\left(\langle\{q,p\}\rangle-\mathrm{i}\right)\right], \end{aligned}$$

$$J_{qp}(t) = \exp\left(-\tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0 t\right)\times$$
$$\times\left[\frac{\omega_0}{\tilde{\omega}_0}\langle p^2\rangle\sin(\tilde{\omega}_0 t)+\frac{1}{2}\left(\frac{1}{2}\frac{\omega_0}{\tilde{\omega}_0}(\gamma_q-\gamma_p)\sin(\tilde{\omega}_0 t)+\cos(\tilde{\omega}_0 t)\right)(\langle\{q,p\}\rangle+\mathrm{i})\right].$$

The spectral functions for the autocorrelation functions are expressed by

$$J_{AA}(\omega)=\int_{-\infty}^{\infty}J_{AA}(t)\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t=2\int_0^{\infty}[\mathrm{Re}\{J_{AA}(t)\}\cos\omega t+\mathrm{Im}\{J_{AA}(t)\}\sin\omega t]\,\mathrm{d}t,$$

hence

$$\begin{aligned}J_{qq}(\omega)&=C_{qq}(\omega)-\frac{1}{2}\frac{(\gamma_q+\gamma_p)\omega_0^2\omega}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2},\\ J_{pp}(\omega)&=C_{pp}(\omega)-\frac{1}{2}\frac{(\gamma_q+\gamma_p)\omega_0^2\omega}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}.\end{aligned}\tag{4.15}$$

Contrary to the symmetrized autocorrelation functions, our results for non-symmetrized ones can be negative at low temperatures around $\omega=\omega_0$ as it is shown in fig. 4.2. This reflects the fact, that the density operator could break positivity.

For the other correlation functions we obtain relations

$$J_{pq}(\omega)=\int_0^{\infty}\left(J_{qp}^*(t)\mathrm{e}^{\mathrm{i}\omega t}+J_{pq}(t)\mathrm{e}^{-\mathrm{i}\omega t}\right)\mathrm{d}t,$$
$$J_{qp}(\omega)=\int_0^{\infty}\left(J_{pq}^*(t)\mathrm{e}^{\mathrm{i}\omega t}+J_{qp}(t)\mathrm{e}^{-\mathrm{i}\omega t}\right)\mathrm{d}t=J_{pq}^*(\omega)$$

which yield

$$\begin{aligned}J_{pq}(\omega)=\gamma_q(N_q(\omega_0)+\tfrac{1}{2})&\frac{\omega_0^2(\gamma_p\omega_0+\mathrm{i}\omega)}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}+\\ +\gamma_p(N_p(\omega_0)+\tfrac{1}{2})&\frac{\omega_0^2(-\gamma_q\omega_0+\mathrm{i}\omega)}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}+\\ +\frac{1}{4}&\frac{(\gamma_q^2-\gamma_p^2)\omega_0^2\omega-\mathrm{i}\left[(\gamma_q+\gamma_p)\omega_0\left(\omega^2+(1+\gamma_q\gamma_p)\omega_0^2\right)\right]}{[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}.\end{aligned}\tag{4.16}$$

4.4 Rotating wave approximation

Making the rotating wave approximation, which is understood as neglecting terms proportional to aa or $a^\dagger a^\dagger$ and leaving only terms proportional to $a^\dagger a$ or $aa^\dagger$, turn the Liouvillian (4.9) into

$$\begin{aligned}
\mathcal{L}\varrho &= -\tfrac{1}{2}\mathrm{i}\omega_0[a^\dagger a,\varrho] \\
&\quad -\tfrac{1}{2}\gamma_q\omega_0\left((N_q(\omega_0)+\tfrac{1}{2})([a,[a^\dagger,\varrho]]+[a^\dagger,[a,\varrho]])+\right. \\
&\qquad\qquad \left.+\tfrac{1}{2}([a,\{a^\dagger,\varrho\}]-[a^\dagger,\{a,\varrho\}])\right) \\
&\quad -\tfrac{1}{2}\gamma_p\omega_0\left((N_p(\omega_0)+\tfrac{1}{2})([a,[a^\dagger,\varrho]]+[a^\dagger,[a,\varrho]])+\right. \\
&\qquad\qquad \left.+\tfrac{1}{2}([a,\{a^\dagger,\varrho\}]-[a^\dagger,\{a,\varrho\}])\right) \\
&= -\tfrac{1}{2}\mathrm{i}\omega_0[a^\dagger a,\varrho] \\
&\quad -\tfrac{1}{2}\omega_0\left[\gamma_q\left(N_q(\omega_0)+\tfrac{1}{2}\right)+\gamma_p\left(N_p(\omega_0)+\tfrac{1}{2}\right)\right]([a,[a^\dagger,\varrho]]+[a^\dagger,[a,\varrho]]) \\
&\quad -\tfrac{1}{4}\omega_0(\gamma_q+\gamma_p)([a,\{a^\dagger,\varrho\}]-[a^\dagger,\{a,\varrho\}])\,.
\end{aligned} \tag{4.17}$$

In other words, both heat baths generate Liouvillian in the exactly same form and it does not matter if the heat bath is coupled via position or momentum within the rotating wave approximation. Surprisingly, exactly the same Liouvillian without any neglecting can by reproduced from Liouvillian (4.9) by formal putting $\gamma = \gamma_q = \gamma_p$, $N = N_q = N_p$ and replacement

$$\gamma \equiv \tfrac{1}{2}(\gamma_q+\gamma_p)\,, \qquad N \equiv \frac{\gamma_q N_q+\gamma_p N_p}{\gamma_q+\gamma_p}\,.$$

This give us great help with a derivation of autocorrelation functions.

First, we notice that stationary limit of mean values $\langle q^2\rangle$ and $\langle p^2\rangle$ goes to the canonical quantum mechanical equilibrium values

$$\langle q^2\rangle = \langle p^2\rangle = \frac{\gamma_q(N_q+\frac{1}{2})+\gamma_p(N_p+\frac{1}{2})}{\gamma_q+\gamma_p}\,, \qquad \tfrac{1}{2}\langle\{q,p\}\rangle = 0\,,$$

where the role of canonical distribution plays the weighted average of the statistical distribution of the particular heat baths. For the position autocorrelation function in the time domain, we obtain

$$C_{qq}(t) = \exp\left(-\tfrac{1}{2}(\gamma_q+\gamma_p)\omega_0 t\right)\cos(\omega_0 t)\langle q^2\rangle$$

and analogously for $C_{pp}(t)$, moreover $C_{qq}(t) = C_{pp}(t)$. Interestingly, the oscillations remain underdamped for arbitrary values of damping coefficients γ_q and γ_p.

In the frequency domain it yields

$$\begin{aligned}
C_{qq}(\omega) = C_{pp}(\omega) &= \frac{1}{2}\left[\gamma_q(N_q(\omega_0)+\tfrac{1}{2})+\gamma_p(N_p(\omega_0)+\tfrac{1}{2})\right]\times \\
&\quad\times\frac{\omega_0\omega^2+\omega_0^3\left(1+\frac{1}{4}(\gamma_q+\gamma_p)^2\right)}{\left[\omega^2-\left(1+\frac{1}{4}(\gamma_q+\gamma_p)^2\right)\omega_0^2\right]^2+(\gamma_q+\gamma_p)^2\omega_0^2\omega^2}\,.
\end{aligned} \tag{4.18}$$

In a certain sense, this result is similar to (4.14) because the rotating wave approximation does not change a structure of the Liouvillian.

The non-symmetrized autocorrelation functions within the rotating wave approximation read

$$J_{qq}(\omega) = J_{pp}(\omega) = C_{qq}(\omega) - \frac{\frac{1}{2}(\gamma_q + \gamma_p)\omega_0^2\omega}{\left[\omega^2 - \left(1 + \frac{1}{4}(\gamma_q + \gamma_p)^2\right)\omega_0^2\right]^2 + (\gamma_q + \gamma_p)^2\omega_0^2\omega^2}.$$

Let us show that this autocorrelation function is always positive. In the zero temperature limit it yields (its dependence on the temperature is increasing)

$$J_{qq}(\omega)|_{T\to 0} = \frac{1}{2}\frac{\omega_0\omega^2 - (\gamma_q + \gamma_p)\omega_0^2\omega + \omega_0^3\left(1 + \frac{1}{4}(\gamma_q + \gamma_p)^2\right)}{\left[\omega^2 - \left(1 + \frac{1}{4}(\gamma_q + \gamma_p)^2\right)\omega_0^2\right]^2 + (\gamma_q + \gamma_p)^2\omega_0^2\omega^2}.$$

The zero points of the numerator are given by the solution of the quadratic equation. Its discriminant is equal to -4 and thus the numerator is always positive.

As a consequence of introducing the rotating wave approximation, the positivity of the autocorrelation functions is restored. This behavior is analogous to the model of the harmonic oscillator with a single bath, where the density operator within the rotating wave approximation satisfies positivity, whereas the positivity is broken in the generalized master equation approach [16].

Results for the position symmetrized autocorrelation function for different approaches are plotted in fig. 4.1. We notice very good agreement around peak maximum $\omega = \omega_0$ for smaller damping. The results of the generalized master equation are identical to the results of the rotating wave approximation for $\gamma_q = \gamma_p$ as follows from our analytical formulas. The damping coefficients are chosen relatively quite big so that the differences between the curves can be recognized.

Results for the position non-symmetrized autocorrelation function for the generalized master equation approach and the rotating wave approximation are plotted in fig. 4.2. We can convince ourselves that the rotating wave approximation curves remain positive.

Finally, we present equations of motion for the mean values of the momentum and the position

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle q(t)\rangle &= \omega_0\langle p(t)\rangle - \tfrac{1}{2}(\gamma_q + \gamma_p)\omega_0\langle q(t)\rangle\,, \\
\frac{\mathrm{d}}{\mathrm{d}t}\langle p(t)\rangle &= -\omega_0\langle q(t)\rangle - \tfrac{1}{2}(\gamma_q + \gamma_p)\omega_0\langle p(t)\rangle\,.
\end{aligned} \tag{4.19}$$

As we know, the rotating wave approximation violates the equations of motion of harmonic oscillator for q and p (do not fulfill requirement of translation invariance). In our model of harmonic oscillator with the baths coupled via position and momentum the equations of motion are changed only slightly (cf. (4.10)), the damping coefficients are mixed together.

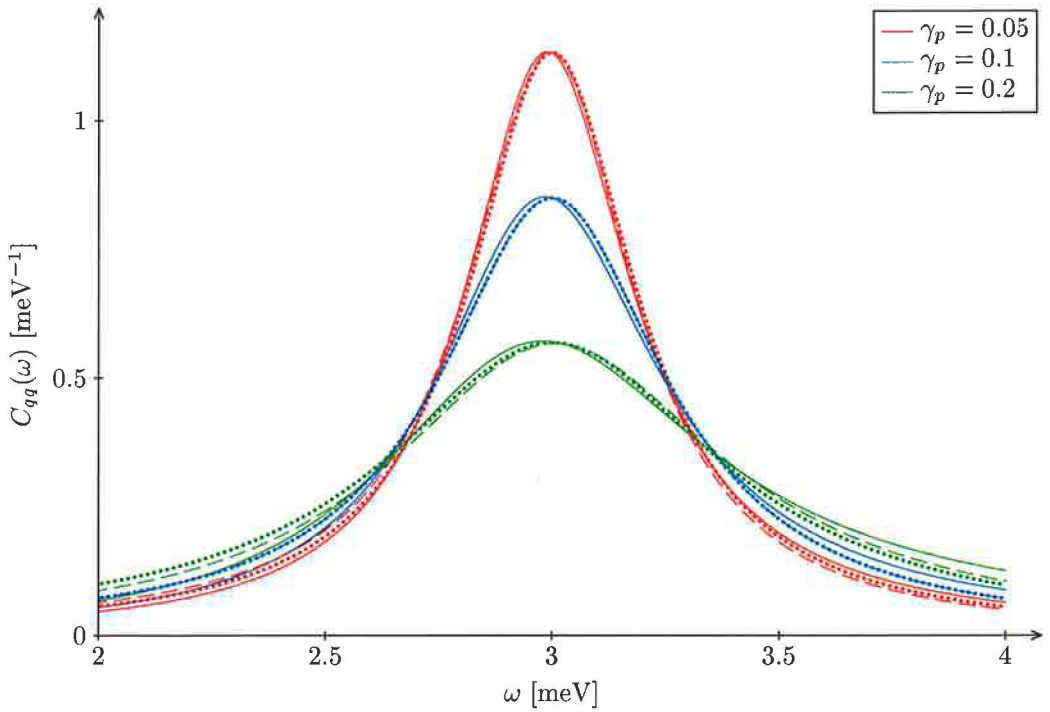

Fig. 4.1: Position symmetrized autocorrelation function C_{qq} vs. frequency ω for exact solution (solid lines), generalized master equation (dashed lines) and rotating wave approximation (dots). Parameters: $\omega_0 = 3\,\mathrm{meV}$, $\gamma_q = 0.1$, $\beta_q = 1.6\,\mathrm{meV}^{-1}$, $\beta_p = 1.6\,\mathrm{meV}^{-1}$.

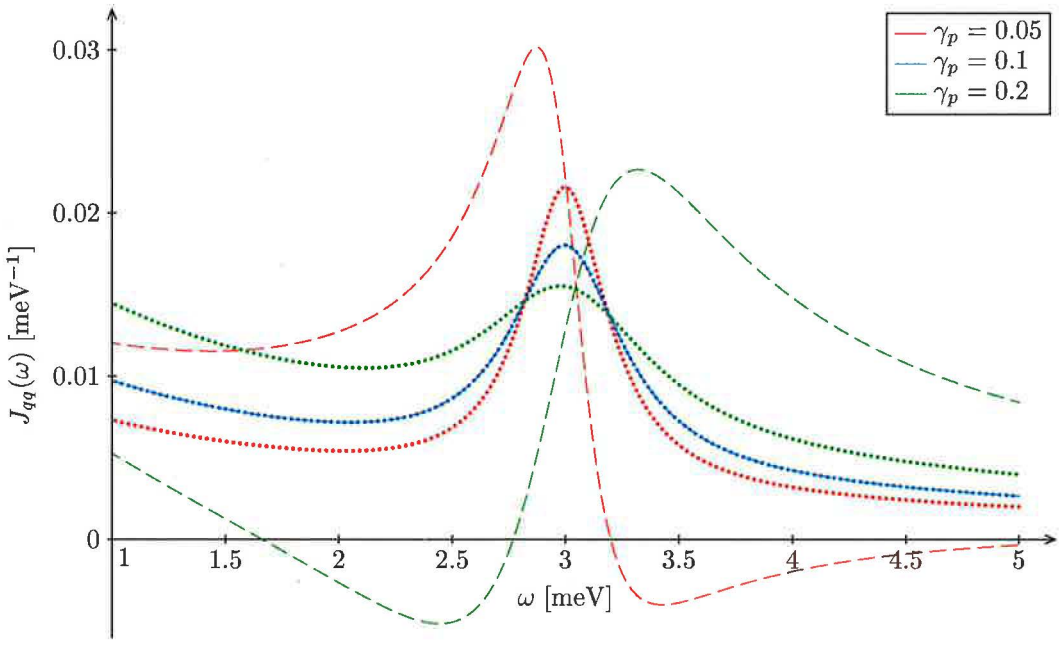

Fig. 4.2: Position non-symmetrized autocorrelation function J_{qq} vs. frequency ω for generalized master equation (dashed lines) and rotating wave approximation (dots). Parameters: $\omega_0 = 3\,\mathrm{meV}$, $\gamma_q = 0.1$, $\beta_q = 1.6\,\mathrm{meV}^{-1}$, $\beta_p = 1.6\,\mathrm{meV}^{-1}$.

4.5 Higher order correlation functions

In principle one could look at higher order correlation functions of the position and the momentum operator, for instance oscillator energy autocorrelation functions or qp autocorrelation function. Using the Wick formula which is valid for Gaussian processes, we arrive at

$$\begin{aligned} J_{qp,qp}(\tau) &= \lim_{t\to\infty}\langle q(t+\tau)p(t+\tau)q(t)p(t)\rangle - \lim_{t\to\infty}\langle q(t)p(t)\rangle^2 = \\ &= \lim_{t\to\infty}\langle q(t+\tau)q(t)\rangle\langle p(t+\tau)p(t)\rangle \\ &\quad + \lim_{t\to\infty}\langle q(t+\tau)p(t)\rangle\langle p(t+\tau)q(t)\rangle \\ &= J_{qq}(\tau)J_{pp}(\tau) + J_{qp}(\tau)J_{pq}(\tau)\,, \end{aligned}$$

Applying the property of a correlation function $J_{qp}(\omega) = J^*_{pq}(\omega)$ at the second term, in the Fourier domain at the zero frequency we obtain

$$\begin{aligned} J_{qp,qp}(\omega{=}0) &= \int_{-\infty}^{\infty} \mathrm{d}\omega J_{qq}(\omega)J_{pp}(-\omega) + \int_{-\infty}^{\infty} \mathrm{d}\omega J_{qp}(\omega)J_{pq}(-\omega) = \\ &= \int_{-\infty}^{\infty} \mathrm{d}\omega J_{qq}(\omega)J_{pp}(-\omega) + \int_{-\infty}^{\infty} \mathrm{d}\omega J^*_{pq}(\omega)J_{pq}(-\omega)\,. \end{aligned}$$

Using (4.15) and (4.16) it gives

$$\begin{aligned} J_{qp,qp}(\omega{=}0) = &\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{2\gamma_q^2\gamma_p^2\left((N_q(\omega_0)+\frac{1}{2})^2 + (N_p(\omega_0)+\frac{1}{2})^2\right)\omega_0^6}{\left([\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} + \\ &+ \int_{-\infty}^{\infty} \mathrm{d}\omega\, \gamma_q\gamma_p\left(N_q(\omega_0)+\tfrac{1}{2}\right)\left(N_p(\omega_0)+\tfrac{1}{2}\right) \times \\ &\qquad \times \frac{\omega_0^2\left([\omega^2-(1-\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q-\gamma_p)^2\omega_0^2\omega^2\right)}{\left([\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} + \\ &+ \int_{-\infty}^{\infty} \mathrm{d}\omega \left(\frac{(\gamma_q+\gamma_p)^2\omega_0^2[\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2}{16\left([\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} + \right. \\ &\qquad \left. + \frac{(\gamma_q+\gamma_p)^2\omega_0^2[4\gamma_q\gamma_p-(\gamma_q-\gamma_p)^2]\omega_0^2\omega^2}{16\left([\omega^2-(1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} \right)\,. \end{aligned} \tag{4.20}$$

The integrand is plotted in fig. 4.3. We can show that the integrand is non-negative only if $\gamma_q \geq (5-2\sqrt{6})\gamma_p$ and $\gamma_p \geq (5-2\sqrt{6})\gamma_q$, where $5-2\sqrt{6} \doteq 0.10$.

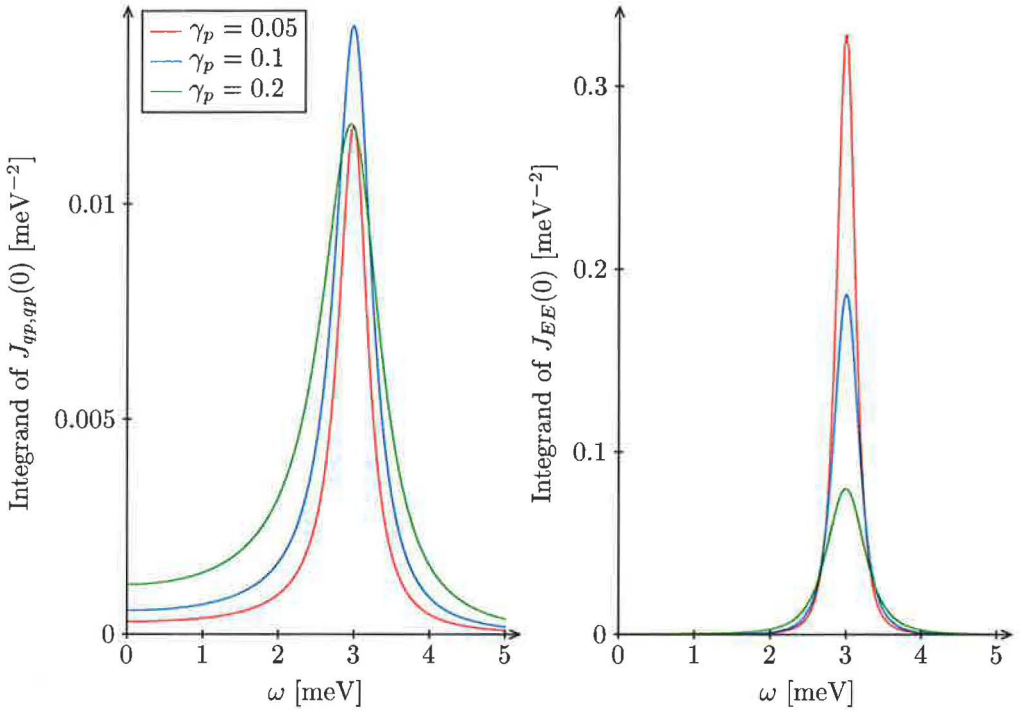

Fig. 4.3: Integrand of the integral (4.20) for the autocorrelation function $J_{qp,qp}$ at zero frequency (left panel) and integrand of the integral (4.21) for the autocorrelation function J_{EE} at zero frequency (right panel). Parameters: $\omega_0 = 3\,\mathrm{meV}$, $\gamma_q = 0.1$, $\beta_q = 1.6\,\mathrm{meV}^{-1}$, $\beta_p = 1.6\,\mathrm{meV}^{-1}$.

Analogously, we can proceed in the case of the energy autocorrelation function, where we define the energy simply as $E = q^2 + p^2$

$$\begin{aligned} J_{EE}(\tau) &= \lim_{t\to\infty} \langle [q^2(t+\tau) + p^2(t+\tau)][q^2(t) + p^2(t)] \rangle - \langle q^2 + p^2 \rangle^2 = \\ &= 2\left(J_{qq}^2(\tau) + J_{pp}^2(\tau) + J_{pq}^2(\tau) + J_{qp}^2(\tau)\right) . \end{aligned}$$

Transforming to the Fourier domain, it yields at the zero frequency

$$J_{EE}(\omega{=}0) = 2\int_{-\infty}^{\infty} \mathrm{d}\omega \left[J_{qq}(\omega)J_{qq}(-\omega) + J_{pp}(\omega)J_{pp}(-\omega) + 2\,\mathrm{Re}\left\{J_{pq}(\omega)J_{pq}(-\omega)\right\}\right] .$$

Substituting from (4.14) and (4.16) we obtain

$$
\begin{aligned}
J_{EE}(\omega{=}0) = \\
&= \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{2\gamma_q^2 \left(N_q(\omega_0) + \frac{1}{2}\right)^2 \omega_0^2 \left(\omega^2 + (1+\gamma_p^2)\omega_0^2\right)^2}{\left([\omega^2 - (1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} + \\
&+ \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{2\gamma_p^2 \left(N_p(\omega_0) + \frac{1}{2}\right)^2 \omega_0^2 \left(\omega^2 + (1+\gamma_q^2)\omega_0^2\right)^2}{\left([\omega^2 - (1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} + \\
&+ \int_{-\infty}^{\infty} \mathrm{d}\omega \, \left(N_q(\omega_0) + \tfrac{1}{2}\right)\left(N_p(\omega_0) + \tfrac{1}{2}\right) \times \\
&\qquad \times \frac{4\gamma_q\gamma_p\omega_0^4 \left(4\omega^2 + (\gamma_q-\gamma_p)^2\omega_0^2\right)}{\left([\omega^2 - (1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} - \\
&- \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{(\gamma_q+\gamma_p)^2\omega_0^2 \left([\omega^2 + (1+\gamma_q\gamma_p)\omega_0^2]^2 + [4 + (\gamma_q-\gamma_p)^2]\omega_0^2\omega^2\right)}{4\left([\omega^2 - (1+\gamma_q\gamma_p)\omega_0^2]^2 + (\gamma_q+\gamma_p)^2\omega_0^2\omega^2\right)^2} .
\end{aligned}
\tag{4.21}
$$

The integrand is plotted in fig. 4.3.

Chapter 5

Two coupled harmonic oscillators

In this chapter we will be concerned with a model of two coupled harmonic oscillators coupled to two dissipative heat baths. This model should be a direct analogue of the double quantum dot device because the harmonic oscillators can exchange energy much like the dots exchange charge. We will focus on a quantity which represents the oscillator energy change and calculate its autocorrelation function.

5.1 Model

A system Hamiltonian consists of two linear harmonic oscillator Hamiltonians and an interaction term proportional to the coordinates of both oscillators

$$H_{\mathrm{S}} = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}\omega_1^2 q_1^2 + \tfrac{1}{2}p_2^2 + \tfrac{1}{2}\omega_2^2 q_2^2 - \omega_0^2 q_1 q_2 \,, \tag{5.1}$$

where we have put $\hbar = 1$ and chosen $m_1 = m_2 = 1$. We suppose $\omega_2 \geq \omega_1$. The position and the momentum fulfill the following commutation relations

$$[q_1, p_1] = [q_2, p_2] = \mathrm{i}\,, \qquad [q_1, q_2] = [p_1, p_2] = [q_1, p_2] = [q_2, p_1] = 0\,.$$

Then we consider two generic heat baths (infinite set of harmonic oscillators) coupled through position of the oscillators

$$\begin{aligned} H_{\mathrm{B1}} + H_{\mathrm{BS1}} &= \sum_j \omega_{j1} a_{j1}^\dagger a_{j1} + \sum_j C_{j1}(a_{j1}^\dagger q_1 + q_1 a_{j1})\,, \\ H_{\mathrm{B2}} + H_{\mathrm{BS2}} &= \sum_j \omega_{j2} a_{j2}^\dagger a_{j2} + \sum_j C_{j2}(a_{j2}^\dagger q_2 + q_2 a_{j2})\,. \end{aligned} \tag{5.2}$$

The bath spectral densities are Ohmic

$$\begin{aligned} J_1(\omega) &= 2\sum_j |C_{j1}|^2 \delta(\omega - \omega_{j1}) = 2\gamma_1 \omega/\pi\,, \\ J_2(\omega) &= 2\sum_j |C_{j2}|^2 \delta(\omega - \omega_{j2}) = 2\gamma_2 \omega/\pi\,. \end{aligned}$$

Foremost, we find such coordinates that the system Hamiltonian has the diagonal form. System eigenfrequencies are

$$\Omega_1^2 = \tfrac{1}{2}(\omega_1^2 + \omega_2^2 - \omega_{\mathrm{X}}^2)\,, \qquad \Omega_2^2 = \tfrac{1}{2}(\omega_1^2 + \omega_2^2 + \omega_{\mathrm{X}}^2)$$

with

$$\omega_{\mathrm{X}}^2 \equiv \sqrt{(\omega_1^2 - \omega_2^2)^2 + 4\omega_0^4}\,.$$

The new coordinates are given by

$$Q_1 = \frac{R_1 q_1 + R_2 q_2}{\sqrt{2}}\,, \qquad Q_2 = \frac{-R_2 q_1 + R_1 q_2}{\sqrt{2}}\,,$$
$$P_1 = \frac{R_1 p_1 + R_2 p_2}{\sqrt{2}}\,, \qquad P_2 = \frac{-R_2 p_1 + R_1 p_2}{\sqrt{2}}\,,$$

where

$$R_1 = \frac{\sqrt{-\omega_1^2 + \omega_2^2 + \omega_{\mathrm{X}}^2}}{\omega_{\mathrm{X}}}\,, \qquad R_2 = \frac{\sqrt{\omega_1^2 - \omega_2^2 + \omega_{\mathrm{X}}^2}}{\omega_{\mathrm{X}}}\,.$$

In these coordinates the system Hamiltonian has the form

$$H_{\mathrm{S}} = \tfrac{1}{2}P_1^2 + \tfrac{1}{2}\Omega_1^2 Q_1^2 + \tfrac{1}{2}P_2^2 + \tfrac{1}{2}\Omega_2^2 Q_2^2\,.$$

Finally, we state the inverse transformation

$$q_1 = \frac{R_1 Q_1 - R_2 Q_2}{\sqrt{2}}\,, \qquad q_2 = \frac{R_2 Q_1 + R_1 Q_2}{\sqrt{2}}\,,$$
$$p_1 = \frac{R_1 P_1 - R_2 P_2}{\sqrt{2}}\,, \qquad p_2 = \frac{R_2 P_1 + R_1 P_2}{\sqrt{2}}\,.$$

5.2 Generalized master equation

To obtain the generalized master equation we employ results (2.4) of the second chapter. There are two heat baths – one coupled through q_1 and the second coupled through q_2. Both q_1 and q_2 are linear combinations of the new coordinates Q_1 and Q_2, thus one can arrive at the expression

$$\begin{aligned}
\mathcal{L}\varrho = {} & -\mathrm{i}[H_{\mathrm{S}}, \varrho] \\
& - \tfrac{1}{2}\left[\gamma_1\omega_1\left(N_1(\Omega_1) + \tfrac{1}{2}\right)R_1^2 + \gamma_2\omega_2\left(N_2(\Omega_1) + \tfrac{1}{2}\right)R_2^2\right]\Omega_1[Q_1,[Q_1,\varrho]] - \\
& \qquad - \tfrac{1}{4}\mathrm{i}(\gamma_1\omega_1 R_1^2 + \gamma_2\omega_2 R_2^2)[Q_1,\{P_1,\varrho\}] \\
& - \tfrac{1}{2}\left[\gamma_1\omega_1\left(N_1(\Omega_2) + \tfrac{1}{2}\right)R_2^2 + \gamma_2\omega_2\left(N_2(\Omega_2) + \tfrac{1}{2}\right)R_1^2\right]\Omega_2[Q_2,[Q_2,\varrho]] - \\
& \qquad - \tfrac{1}{4}\mathrm{i}(\gamma_1\omega_1 R_2^2 + \gamma_2\omega_2 R_1^2)[Q_2,\{P_2,\varrho\}] \\
& - \tfrac{1}{2}\left[\gamma_2\omega_2\left(N_2(\Omega_1) + \tfrac{1}{2}\right) - \gamma_1\omega_1\left(N_1(\Omega_1) + \tfrac{1}{2}\right)\right]\Omega_1 R_1 R_2[Q_2,[Q_1,\varrho]] - \\
& \qquad - \tfrac{1}{4}\mathrm{i}(\gamma_2\omega_2 - \gamma_1\omega_1)R_1 R_2[Q_2,\{P_1,\varrho\}] \\
& - \tfrac{1}{2}\left[\gamma_2\omega_2\left(N_2(\Omega_2) + \tfrac{1}{2}\right) - \gamma_1\omega_1\left(N_1(\Omega_2) + \tfrac{1}{2}\right)\right]\Omega_2 R_1 R_2[Q_1,[Q_2,\varrho]] - \\
& \qquad - \tfrac{1}{4}\mathrm{i}(\gamma_2\omega_2 - \gamma_1\omega_1)R_1 R_2[Q_1,\{P_2,\varrho\}]\,.
\end{aligned}$$

Substituting the new coordinates by the original ones, we obtain Liouvillian

$$\begin{aligned}\mathcal{L}\varrho = &-\tfrac{1}{2}\mathrm{i}\,[p_1^2 + p_2^2 + \omega_1^2 q_1^2 + \omega_2^2 q_2^2 - 2\omega_0^2 q_1 q_2, \varrho] \\ &- \tfrac{1}{2}\gamma_1\omega_1\big((N_1(\Omega_1) + \tfrac{1}{2})\Omega_1(R_1^2[q_1,[q_1,\varrho]] + R_1R_2[q_1,[q_2,\varrho]]) + \\ &\quad + (N_1(\Omega_2) + \tfrac{1}{2})\Omega_2(R_2^2[q_1,[q_1,\varrho]] - R_1R_2[q_1,[q_2,\varrho]]) + \\ &\quad + \mathrm{i}\,[q_1,\{p_1,\varrho\}]\big) \\ &- \tfrac{1}{2}\gamma_2\omega_2\big((N_2(\Omega_2) + \tfrac{1}{2})\Omega_2(R_1^2[q_2,[q_2,\varrho]] - R_1R_2[q_1,[q_2,\varrho]]) + \\ &\quad + (N_2(\Omega_1) + \tfrac{1}{2})\Omega_1(R_2^2[q_2,[q_2,\varrho]] + R_1R_2[q_1,[q_2,\varrho]]) + \\ &\quad + \mathrm{i}\,[q_2,\{p_2,\varrho\}]\big)\,.\end{aligned} \tag{5.3}$$

If we put $\omega_0 = 0$, then $R_1 = 2$, $R_2 = 0$, $\Omega_1 = \omega_1$ and $\Omega_2 = \omega_2$ and the Liouvillian of the two independent dissipative harmonic oscillators is recovered.

Having the Liouvillian, the dynamics of the system is fully prescribed and thus we can arrange equations for mean values of system operators. For the operators q_1, p_1, q_2 and p_2 we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle q_1(t)\rangle &= \langle p_1(t)\rangle\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle q_2(t)\rangle &= \langle p_2(t)\rangle\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle p_1(t)\rangle &= -\omega_1^2\langle q_1(t)\rangle - \gamma_1\omega_1\langle p_1(t)\rangle + \omega_0^2\langle q_2(t)\rangle\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle p_2(t)\rangle &= -\omega_2^2\langle q_2(t)\rangle - \gamma_2\omega_2\langle p_2(t)\rangle + \omega_0^2\langle q_1(t)\rangle\,.\end{aligned} \tag{5.4}$$

It follows from the quantum regression theorem that the correlation functions

$$J_{AB}(\tau) = \lim_{t\to\infty}\langle A(t+\tau)B(t)\rangle$$

of the position and the momentum operators (q_1, p_1, q_2 and p_2) obey the same set of equation (5.4) as their mean values which we gave reasons for in the previous chapter. The initial conditions $J_{AB}(0) = \lim_{t\to\infty}\langle A(t)B(t)\rangle$ can be obtained from the equations for the second order correlation functions. The equations read

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle q_1^2\rangle &= 2\langle q_1p_1\rangle - \mathrm{i}\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle q_2^2\rangle &= 2\langle q_2p_2\rangle - \mathrm{i}\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle p_1^2\rangle &= -2\omega_1^2\langle q_1p_1\rangle - 2\gamma_1\omega_1\langle p_1^2\rangle + 2\omega_0^2\langle p_1q_2\rangle + \mathrm{i}\omega_1^2 + \nu_1^2\,, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle p_2^2\rangle &= -2\omega_2^2\langle q_2p_2\rangle - 2\gamma_2\omega_2\langle p_2^2\rangle + 2\omega_0^2\langle q_1p_2\rangle + \mathrm{i}\omega_2^2 + \nu_2^2\,,\end{aligned}$$

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle q_1 p_1\rangle &= -\omega_1^2\langle q_1^2\rangle - \gamma_1\omega_1\langle q_1 p_1\rangle + \langle p_1^2\rangle + \omega_0^2\langle q_1 q_2\rangle + \tfrac{1}{2}\mathrm{i}\gamma_1\omega_1\,,\\
\frac{\mathrm{d}}{\mathrm{d}t}\langle q_2 p_2\rangle &= -\omega_2^2\langle q_2^2\rangle - \gamma_2\omega_2\langle q_2 p_2\rangle + \langle p_2^2\rangle + \omega_0^2\langle q_1 q_2\rangle + \tfrac{1}{2}\mathrm{i}\gamma_2\omega_2\,,\\
\frac{\mathrm{d}}{\mathrm{d}t}\langle q_1 q_2\rangle &= \langle q_1 p_2\rangle + \langle p_1 q_2\rangle\,,\\
\frac{\mathrm{d}}{\mathrm{d}t}\langle q_1 p_2\rangle &= \omega_0^2\langle q_1^2\rangle - \omega_2^2\langle q_1 q_2\rangle - \gamma_2\omega_2\langle q_1 p_2\rangle + \langle p_1 p_2\rangle\,,\\
\frac{\mathrm{d}}{\mathrm{d}t}\langle p_1 q_2\rangle &= \omega_0^2\langle q_2^2\rangle - \omega_1^2\langle q_1 q_2\rangle - \gamma_1\omega_1\langle p_1 q_2\rangle + \langle p_1 p_2\rangle\,,\\
\frac{\mathrm{d}}{\mathrm{d}t}\langle p_1 p_2\rangle &= \omega_0^2\langle q_1 p_1\rangle + \omega_0^2\langle q_2 p_2\rangle - \omega_1^2\langle q_1 p_2\rangle - \omega_2^2\langle p_1 q_2\rangle -\\
&\quad - 2(\gamma_1\omega_1 + \gamma_2\omega_2)\langle p_1 p_2\rangle - \mathrm{i}\omega_0^2 + \nu^2\,,
\end{aligned}
$$

where

$$
\begin{aligned}
\nu_1^2 &= \gamma_1\omega_1\left[\left(N_1(\Omega_1) + \tfrac{1}{2}\right)\Omega_1 R_1^2 + \left(N_1(\Omega_2) + \tfrac{1}{2}\right)\Omega_2 R_2^2\right]\,,\\
\nu_2^2 &= \gamma_2\omega_2\left[\left(N_2(\Omega_2) + \tfrac{1}{2}\right)\Omega_2 R_1^2 + \left(N_2(\Omega_1) + \tfrac{1}{2}\right)\Omega_1 R_2^2\right]\,,\\
\nu^2 &= \tfrac{1}{2}R_1 R_2\left(\gamma_1\omega_1\left[\left(N_1(\Omega_1) + \tfrac{1}{2}\right)\Omega_1 - \left(N_1(\Omega_2) + \tfrac{1}{2}\right)\Omega_2\right] -\right.\\
&\quad \left. -\gamma_2\omega_2\left[\left(N_2(\Omega_2 + \tfrac{1}{2}\right)\Omega_2 - \left(N_2(\omega_1) + \tfrac{1}{2}\right)\Omega_1\right]\right)\,.
\end{aligned}
$$

In the limit $t \to \infty$ the derivatives on the left hand sides go to zero and we arrive at the system of the algebraic equations.

Now, everything is set up to calculate any correlation function. Due to the extent of final expressions, the results are not explicitly shown here.

5.3 Operator of energy exchange

In order to define an energy flux between the oscillators, the system Hamiltonian must be divided into the two parts like

$$
\left(\tfrac{1}{2}p_1^2 + \tfrac{1}{2}\omega_1^2 q_1^2 - \alpha\omega_0^2 q_1 q_2\right) + \left(\tfrac{1}{2}p_2^2 + \tfrac{1}{2}\omega_2^2 q_2^2 - (1-\alpha)\omega_0^2 q_1 q_2\right)\,.
$$

The interaction term must be also divided between the two parts, but we cannot simply say whether it belongs to the first or to the second oscillator. Therefore we have introduced parameter $0 < \alpha < 1$ which determines how big portion of the interaction energy belongs to the first oscillator.

Operators of the energy exchange are defined in the Heisenberg picture in the following way

$$
\begin{aligned}
I_{21} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\tfrac{1}{2}p_1^2 + \tfrac{1}{2}\omega_1^2 q_1^2 - \alpha\omega_0^2 q_1 q_2\right) =\\
&= -\mathrm{i}\left[\tfrac{1}{2}p_1^2 + \tfrac{1}{2}\omega_1^2 q_1^2 - \alpha\omega_0^2 q_1 q_2, H_\mathrm{S}\right]\,,\\
I_{12} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\tfrac{1}{2}p_2^2 + \tfrac{1}{2}\omega_2^2 q_2^2 - (1-\alpha)\omega_0^2 q_1 q_2\right) =\\
&= -\mathrm{i}\left[\tfrac{1}{2}p_2^2 + \tfrac{1}{2}\omega_2^2 q_2^2 - (1-\alpha)\omega_0^2 q_1 q_2, H_\mathrm{S}\right]\,,
\end{aligned}
$$

which yields

$$I_{12} = -I_{21} = \alpha\omega_0^2 q_1 p_2 - (1-\alpha)\omega_0^2 p_1 q_2 \,. \tag{5.5}$$

We define the autocorrelation function of this operator in the standard way

$$\begin{aligned} J_{II}(\tau) = {} & \alpha^2\omega_0^4 \lim_{t\to\infty}\left[\langle q_1(t+\tau)p_2(t+\tau)q_1(t)p_2(t)\rangle - \langle q_1(t)p_2(t)\rangle^2\right] \\ & + (1-\alpha)^2\omega_0^4 \lim_{t\to\infty}\left[\langle p_1(t+\tau)q_2(t+\tau)p_1(t)q_2(t)\rangle - \langle p_1(t)q_2(t)\rangle^2\right] \\ & - \alpha(1-\alpha)\omega_0^4 \lim_{t\to\infty}\left[\langle p_1(t+\tau)q_2(t+\tau)q_1(t)p_2(t)\rangle - \right. \\ & \qquad \left. - \langle p_1(t)q_2(t)\rangle\langle q_1(t)p_2(t)\rangle\right] \\ & - \alpha(1-\alpha)\omega_0^4 \lim_{t\to\infty}\left[\langle q_1(t+\tau)p_2(t+\tau)p_1(t)q_2(t)\rangle - \right. \\ & \qquad \left. - \langle p_1(t)q_2(t)\rangle\langle q_1(t)p_2(t)\rangle\right] . \end{aligned}$$

Using the Wick formula, we arrive at

$$\begin{aligned} J_{II}(t) = {} & \alpha^2\omega_0^4[J_{q_1q_1}(t)J_{p_2p_2}(t) + J_{q_1p_2}(t)J_{p_2q_1}(t)] \\ & + (1-\alpha)^2\omega_0^4[J_{q_2q_2}(t)J_{p_1p_1}(t) + J_{q_2p_1}(t)J_{p_1q_2}(t)] \\ & - \alpha(1-\alpha)\omega_0^4[J_{p_1q_1}(t)J_{q_2p_2}(t) + J_{p_1p_2}(t)J_{q_2q_1}(t)] \\ & - \alpha(1-\alpha)\omega_0^4[J_{q_1p_1}(t)J_{p_2q_2}(t) + J_{p_2p_1}(t)J_{q_1q_2}(t)] , \end{aligned}$$

which yields in the Fourier domain at the zero frequency

$$\begin{aligned} J_{II}(\omega=0) = {} & \alpha^2\omega_0^4 \int_{-\infty}^{\infty} \mathrm{d}\omega[J_{q_1q_1}(\omega)J_{p_2p_2}(-\omega) + J_{q_1p_2}(\omega)J^*_{q_1p_2}(-\omega)] \\ & + (1-\alpha)^2\omega_0^4 \int_{-\infty}^{\infty} \mathrm{d}\omega[J_{q_2q_2}(\omega)J_{p_1p_1}(-\omega) + J_{q_2p_1}(\omega)J^*_{q_2p_1}(-\omega)] \\ & - 2\alpha(1-\alpha)\omega_0^4 \int_{-\infty}^{\infty} \mathrm{d}\omega\,\mathrm{Re}\left\{J_{q_1p_1}(\omega)J^*_{q_2p_2}(-\omega) + J_{q_1q_2}(\omega)J^*_{p_1p_2}(-\omega)\right\} . \end{aligned}$$

The next task is to investigate sign of the expression for $J_{II}(\omega = 0)$ for different values of the oscillator frequencies ω_1, ω_2, the coupling constant ω_0 and the damping coefficients γ_1, γ_2. This job is left temporarily unfinished, but first calculations for the particular choice ($\omega_1 = 1\,\mathrm{meV}$, $\omega_2 = 2\,\mathrm{meV}$, $\omega_0 = 0.5\,\mathrm{meV}$, $\gamma_1 = 0.1$, $\gamma_2 = 0.02$ and $\alpha = \frac{1}{2}$) give positive values of $J_{II}(\omega=0)$.

Chapter 6

Conclusions

We showed that the equations of motion for the dot occupation operators imply charge conservation, i. e. the mean current and the zero-frequency current noise must be the same along the whole circuit. The mean current and the zero-frequency current noise were evaluated at all junctions – between the dots (inner junction) using the quantum regression theorem and between the dots and the leads (outer junctions) using counting variable approach. Obtained results for the mean current are identical, whereas the zero-frequency noise current results exhibit discrepancy and unphysical negative values appear between the dots.

We disproved a possibility that the problem is caused by the assumption of additivity of two kinds of bath couplings – the Fermi seas of the leads via singular coupling (the high bias limit and the wide-band limit) and the heat bath via the weak coupling. The leads can be coupled also weakly which leads to the same dynamics, the same Liouvillian.

We found the criterion (3.34) for the charge conserving Liouvillians.

In the case without the heat bath the charge conservation condition is fully satisfied.

In the limit of small tunneling rates between the dots and the leads $\Gamma \to 0$ as well as in the limit of small interdot coupling $\Omega \to 0$ the Fano factor for the outer junctions gives meaningful results while the Fano factor for the inner junction reveals some pathological behavior – negative values or wrong $\varepsilon \to \infty$ limit.

The Liouvillian obtained from the rotating wave approximation in the LR-basis satisfy charge conservation condition and gives no negative values for the zero-frequency current noise. However, we gave reasons why the results must be rejected on the physical grounds.

The problem with negative values of the zero-frequency current noise is also fixed within the rotating wave approximation in the 12-basis. This approach and the generalized master equation give corresponding results at the outer junctions. However, completely different values are obtained at the inner junction and therefore the charge conservation condition remains broken.

In Pauli master equation approach the mean current and the zero-frequency current noise can be evaluated at the outer junctions. The results correspond to generalized master equation approach for small values of Γ.

It seems that the weak coupling prescription together with the Markovian approximation breaks positivity of the reduced density matrix of the double quantum dot. Consequently, the charge conservation condition is broken and negative values for the current noise (current autocorrelation function) are obtained. Nevertheless, we believe that results obtained for the outer junctions have good physical meaning.

Autocorrelation functions were also studied for the system of the harmonic oscillator coupled to two heat baths. The heat baths are coupled via incompatible operators – position and momentum. The exact results for the position and the momentum autocorrelation function were showed to be necessarily non-negative. In the generalized master equation approach we calculated symmetrized and non-symmetrized autocorrelation functions. The symmetrized ones are proved to be non-negative, but the non-symmetrized ones can be negative for certain values of frequency. Therefore positivity of density matrix is broken also in this system and it has the same consequence as in the case of the double quantum dot.

It seems that the rotating wave approximation restores positivity of the reduced density matrix because the non-symmetrized autocorrelation functions are non-negative at this time. The equations of motion for mean values of position and momentum are not broken within the rotating wave approximation.

The model of coupled dissipative harmonic oscillators is proposed as another illustration of the problem.

There is open question of finding a general criterion for "charge conserving" approximations, e. g. method for calculating the zero-frequency current noise between the dots of the double quantum dot device. It would be also important to study the same problem for non-Markovian generalized master equation.

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