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# 單量子點在與電極之耦合強度隨時間變化下的非馬可夫量子傳輸研究

# Non-Markovian Quantum Transport of a Quantum Dot with Time-Dependent Coupling Strength

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# 國立臺灣大學碩士學位論文
# 口試委員會審定書

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本論文係**楊智偉**君（R01222068）在國立臺灣大學物理學系、所完成之碩士學位論文，於民國 104 年 7 月 13 日承下列考試委員審查通過及口試及格，特此證明

口試委員：

管希聖（簽名）

（指導教授）

林俊達

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# 中文摘要

在此篇論文中，我們討論通過兩個電極之間的單量子點 (single quantum dot) 的電子傳輸行為，亦即特別在考慮電極對量子點上電子的非馬可夫效應情況下通過單量子點的電流。傳統上研究通過單量子點的電流，大部分使用馬可夫近似，馬可夫近似是指電子的傳輸行為不會受到環境過去的資訊影響，只和當下的環境產生交互作用，而得到近似後的馬可夫約化密度矩陣主方程式 (reduced density matrix master equation )。而在研究非馬可夫環境下，通過量子點的電流，主要有Feynman Vernon influence functional theory、Non-equilibrium Green function method、Quantum state diffusion equation幾種方法。此篇論文中，我們使用非馬可夫量子態擴散方程式 (non-Markovian quantum state diffusion equation , NMQSD) 去推導出在外加時變偏壓與時變閘極電壓，且單量子點和電極之間耦合常數亦為時變下精確的約化密度矩陣主方程式。然後用約化密度算出量子點的平均粒子數，再經由海森堡方程式，進而得到通過量子點的電流。

關鍵字: 非馬可夫動力學、 量子點、 隨時變耦合強度

# Abstract

In this thesis, we discuss the electron transport behavior of the single quantum dot between two electrodes, that is, the current flowing into the single quantum dot, especially under the non-Markovian effect of the electrodes. Traditionally, the study on the current flowing into the quantum dot is under Markovian approximation. Markovian approximation means that the electron transport behavior will not be affected by the past information of the environment, which we call it the bath in this thesis. It is affected only by the environment at the present time. The main research method on transient current flowing into the quantum dot are Feynman- Vernon influence functional theory, non-equilibrium Green function method, quantum state diffusion equation. In this thesis, we use non-Markovian quantum state diffusion equation (NMQSD) to derive the master equation under time-dependent bias voltage, time-dependent gate voltage and time-dependent transmission coefficient controlled by the left and the right gate voltage. Finally, by Heisenberg equation, we get the transient current flowing into the single quantum dot.

Keywords: Non-Markovian Dynamics, Quantum Dot, Time-Dependent Coupling Strength

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# 1 Introduction

Recent progress in the fabrication technology of nanostructure has made the size of the transistor from micrometer ($10^{-6}\,m$) toeard nanometer ($10^{(-9)}\,m$). The traditional transistor devices with channel length below 10 nanometers may be no longer operated very well due to the large statistical fluctuation of the threshold voltage caused by its small size. A single electron transistor (SET) is considered as one of the alternatives for the traditional transistor.

In this thesis, we use quantum dot with only single energy level under Coulomb blockade as our physical model to study the electron transport property of a SET. We controll our single-energy-level quantum dot with the time-dependent bias voltage on the left and right leads, the time-dependent gate voltage on the quantum dot, and the time-dependent left and right gate voltage to create potential barrier controlling the coupling strength as in Fig. 1.0.1. By controlling these three parameter, we hope to model and control the electron transport through the SET.

Because the interaction between the quantum dot and the leads are in general Non-Markovian, that is, the system would be affected by the correlation of the leads at an earlier time, we use Non-Markovian quantum- state-diffusion (NMQSD) method to derive the master equation and the transient current tunneling from the left and the right leads.

In chapter 2, we briefly present the formalism of the NMQSD. To describe the fermionic NMQSD, we introduce the Grassman variable and fermionic coherent state. We then represent our NMQSD in fermionic coherent state. In NMQSD, one most important point is that we make an Ansatz that the functional derivatives of the state with respect to the Grassman variables can be expressed as an operator acting on the state. That is,

$$\frac{\delta}{\delta z^*_\lambda(s)}\left|\phi(t,z^*,w^*)\right\rangle = O_1(t,s,z^*,w^*)\left|\phi(t,z^*,w^*)\right\rangle,$$

$$\frac{\delta}{\delta w^*_\lambda(s)}\left|\phi(t,z^*,w^*)\right\rangle = O_2(t,s,z^*,w^*)\left|\phi(t,z^*,w^*)\right\rangle,$$

where $O_{1,2}(t,s,z^*,w^*)$ are operators. In chapter 3, we use the method of NMQSD to derive the exact master equation. In chapter 4, we use the master equation in chapter 3 to derive our current formula. We take various calculations to simplify the current formula, including using Novikov theorem to transform Grassman average of random Grassman variable into Grassman average of $O_1$ , $O_2$ operators. In this chapter, we also use the Heisenberg approach to derive the time evolution equations of $O_1$ , $O_2$. In chapter 5, we construct a physical model of time-dependent tunneling barrier to calculate the time-dependent effective transmission coefficients in our model.

All the detailed calculations can be found in the appendix.

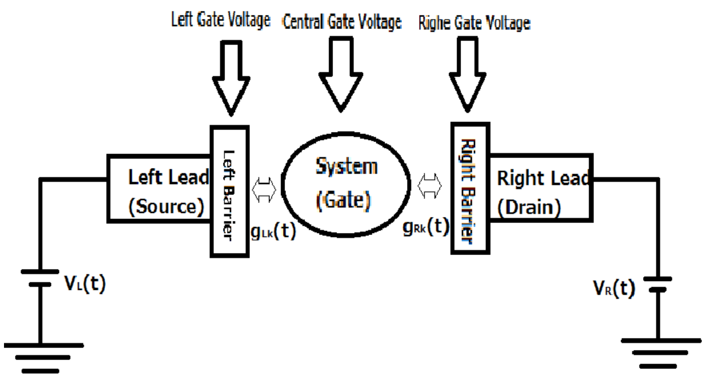


Figure 1.0.1: The symbolic figure o f the model setup.

# 2 Non-Markovian Quantum State Diffusion

## 2.1 Introduction

In real situations, due to the fact that the system of our interest unavoidablely couples to its surroundings, the closed quantum system is hard to be found and to be relaized . This means that there are lots of irreversable dymanical properties, such as relaxation, decoherence, noise...etc. that need to be taken into account for description of such a coupled system. Obviously, the traditional qauntum mechanics formalism (Scheodinger eqaution approach) is not adequate for tackling these difficulties. Hence, the so-called "theory of open quantum systems" was developed. Traditionally, the dynamic of the open quantum systems is mainly investigated under two important approximations:

1. Born approximation: Suppose that the interaction between system and its surroundings are so weak [1].

2. Markov approximation. (We brief introduce the Markov approximation in Appendix 1.)

These two approximations can lead to a simpler evolution equation for the reduced density operator of the open system called a Markovian master equation of Lindblad form. This kind of equation can neglect the memory effect of the environment and can help us understand the main physics of the open quantum systems. There, however, are many cases that the Markovian master equation fails to demonstrate the real physics. For example, if the coupling strength between the environment and the open quantum system is too strong such that the memory effect of the environment on the open quantum systems can't be neglected. Therefore, we must consider the non-Markovian master equation for the reduced density operator of the open system by counting the memory effect in.

There are many techniques to tackle the non-Markovian dynamics. For example, the non-equilibrium Green's function (NEGF) method is used especially in transport problem such as electron transport or thermal transport [2, 3, 4]. The Feynman Vernon influence functional method [5, 6, 7, 8, 9] puts the environmental non-Markovian memory effect into the influence functional. The the non-Markovian quantum state diffusion (NMQSD) is a recently developed method [10, 11, 12]. In this approach, the non-Markovian environmental memory effect is represented by an O-operator, and the main purpose of this method is to properly guess the form of the O-operator. If we obtain the O-operator, the time evolution of the reduced density operator of the open system is determined by taking the ensemble average of NMQSD equation.

The NMQSD is orginally used to solve bosonic non-Markovian problems. Recently, fermionic NMQSD has come up to solve many problems in solid state physics such as quantum transport [13, 14, 15]. The structure of fermionic NMQSD is similar to the bosonic one. But fermionic particles obey Pauli exclusion principle so we need to introduce a new kind of number, Grassman number. By utilizing the fermionic creation and annihilation operators and Grassman variable, we can modify the bosonic NMQSD to fit the fermionic system.

## 2.2 Non-Markovian Dynamics of a Single Energy Level Quantum Dot (SEQD):

### 2.2.1 Experiment Setup and the Theoretical Model of SEQD:

In this thesis, we consider the experimental setup of SEQD that only one electron can occupy the one single energy level of the QD by the assumption of Coulomb blockade here.

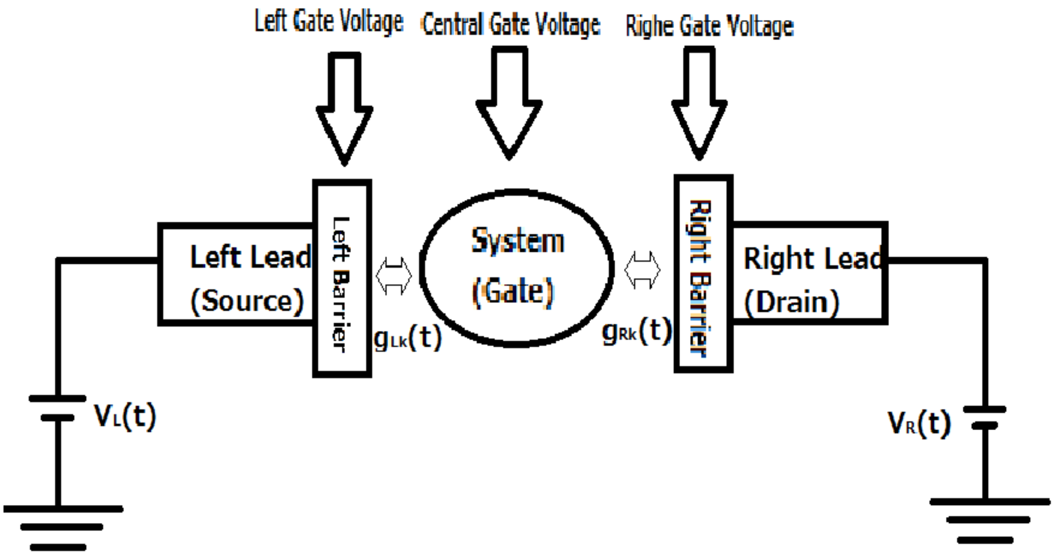


Figure 2.2.1: The symbolic figure of the SEQD setup.

The total Hamiltonian of the composite system (the environment and the open quantum system) is as follows:

$$H = H_S + H_R + H_{SR}, \tag{2.2.1}$$

$$H_S = \hbar\omega_S(t)c^+c, \tag{2.2.2}$$

$$H_R = \sum_{\lambda k} \hbar\omega_{\lambda k}(t) a^+_{\lambda k} a_{\lambda k}, \tag{2.2.3}$$

$$H_{SR} = \sum_{\lambda k} (g_{\lambda k}(t) c^+ a_{\lambda k} + H.c.). \tag{2.2.4}$$

Here $\lambda$ represent the left and the right leads, $H_S$is the system Hamiltonian and the $\hbar\omega_S(t)$ is the time-dependent single energy level controlld by an external voltage $V_S(t)$ such that $\hbar\omega_S(t) = \hbar\omega_S + eV_S(t)$, $H_R$ is the non-interacting Hamiltonian of the environment (if there are interactions, we need to add the transition terms $\sum_{\lambda ij} \epsilon_{\lambda ij}(t) a^+_{\lambda i} a_{\lambda j}$) controlled by external bias voltage $V_L(t)$ and $V_R(t)$ such that $\hbar\omega_{\lambda k}(t) = \hbar\omega_{\lambda k} + eV_\lambda(t)$ and $H_{SR}$ is the interaction term between the system and the environment. $g_{\lambda k}(t)$ is the coupling strength between the $\lambda k - mode$ energy level of the environment and the system. The effect of all $g_{\lambda k}(t)$ in different modes $k$ is related to the effective transmission coefficient of the elctron from $\lambda$ lead. The transmission coefficient $\overline{V}_\lambda(t)$ is determined by the external gate voltage $eV_{G\lambda}(t)$ applied on the $\lambda$ barrier, the gate voltage $eV_S(t)$ applied on the system, and the bias voltage applied on the $\lambda$ lead by the theory of tunneling throught a time-dependent barrier [16, 17].

The NMQSD can be used only when the environment oscillators are originally in their ground state ($T = 0$). But in real situations, it's not the case (i.e. $T \neq 0$). So we need to modify the $T \neq 0$ case to satisfy the NMQSD. Fortunately, there's a mathematical trick widely used in field theory that can canonically transform the environment of temperature $T \neq 0$ into another effective environment with $T = 0$. This trick is called Bogoliubov transformation that is first used in a superconducting theory by Nikolai Bogoliubov [18]. We now introduce Bogoliubov transformation and how it is used in transforming the non-zero temperature environment into another effectively zero temperature environment.

### 2.2.2 Bogoliubov Transformation

In order to deal with finite-temperature case, we introduce another virtual environment with another kind of operators $b_{\lambda k}(b^{+}_{\lambda k})$. We need to add $b_{\lambda k}(b^{+}_{\lambda k})$ into our original Hamiltonian $H_R(t)$ carefully so that we don't change the interaction between the environment and the system. We simply add a term $\sum_{\lambda k}\hbar\omega_{\lambda k}(t)b_{\lambda k}b^{+}_{\lambda k}$ into $H_R(t)$. Because operators $b_{\lambda k}(b^{+}_{\lambda k})$ don't couple to the system operators $c(c^{+})$, so it won't change the interaction between the system and the environment. The action of the virtual environment $\sum_{\lambda k}\hbar\omega_{\lambda k}(t)b_{\lambda k}b^{+}_{\lambda k}$ is a bit like the shift of the energy reference. So it won't change the physics. Now we have two sets of operator $\{a_{\lambda k}(a^{+}_{\lambda k})\,,\,b_{\lambda k}(b^{+}_{\lambda k})\}$, we can use Bogoliubov transformation. Bogoliubov transformation is a linear transformation between two sets of operator. Thus, we make the Bogoliubov transformation as follows:

$$a_{\lambda k}=\sqrt{1-n_{\lambda k}}d_{\lambda k}-\sqrt{n_{\lambda k}}e^{+}_{\lambda k}, \tag{2.2.5}$$

$$b_{\lambda k}=\sqrt{1-n_{\lambda k}}e_{\lambda k}+\sqrt{n_{\lambda k}}d^{+}_{\lambda k}, \tag{2.2.6}$$

where $n_{\lambda k}=\frac{1}{1+e^{[\hbar\omega_{\lambda k}/(k_BT)]}}$ is the initial equilibrium average particle number and $\{d_{\lambda k}(d^{+}_{\lambda k})\,,\,e_{\lambda k}(e^{+}_{\lambda k})\}$ are the new sets of operators. We then get the new Hamiltonian:

$$H^{'}(t)=\hbar\omega_S(t)c^{+}c+\sum_{\lambda k}[\hbar\omega_{\lambda k}(t)(d^{+}_{\lambda k}d_{\lambda k}+e_{\lambda k}e^{+}_{\lambda k})]+\sum_{\lambda k}(\sqrt{n_{\lambda k}}g^{*}_{\lambda k}(t)ce_{\lambda k}+\sqrt{1-n_{\lambda k}}g_{\lambda k}(t)c^{+}_{\lambda}d_{\lambda k}+H.c). \tag{2.2.7}$$

Here $H.c.$ means Hermitian conjugate. We now recognize $\sum_{\lambda k}[\hbar\omega_{\lambda k}(t)(d^{+}_{\lambda k}d_{\lambda k}+e_{\lambda k}e^{+}_{\lambda k})]$ as the new virtual environment Hamiltonian $H^{'}_R(t)$ and $H^{'}_{SR}(t)=\sum_{\lambda k}(\sqrt{n_{\lambda k}}g^{*}_{\lambda k}(t)ce_{\lambda k}+\sqrt{1-n_{\lambda k}}g_{\lambda k}(t)c^{+}_{\lambda}d_{\lambda k}+H.c)$. Because we are interested only in the part $H_S(t)+H^{'}_{SR}(t)$(the interaction part and the non-interaction part of the system), we take the interaction picture with repect to $H^{'}_R(t)$ to obtain:

$$H_T = e^{\frac{i}{\hbar}\int_0^t dt' H_R'(t')}(H_S(t) + H_{SR}'(t))e^{-\frac{i}{\hbar}\int_0^t dt' H_R'(t')}, \tag{2.2.8}$$

where $H_T$ is the total Hamiltonian with respect to the environment interaction picture.

## 2.3 Fermionic Non-Markovian Quantum State Diffusion

### 2.3.1 Fermionic Coherent State:

In order to simplify the total Hamiltonian in the environment interaction picture, we first jump to introduce the fermionic operator and then introduce the fermionic coherent state for later calculation.

Unlike the bosonic creation and annihilation operator satisfying commutation relation:

$$[b_i, b_j^+] = \delta_{ij}, \tag{2.3.1}$$

$$[b_i, b_j] = [b_i^+, b_j^+] = 0. \tag{2.3.2}$$

The fermionic creation and annihilation operator satisfy anti-commutation:

$$\{a_i, a_j^+\} = \delta_{ij}, \tag{2.3.3}$$

$$\{a_i, a_j\} = \{a_i^+, a_j^+\} = 0 \tag{2.3.4}$$

in order to satisfy Fermi-Dirac distribution or more fundamentally, Pauli exclusion principle. After we know the fermionic operator, we can pave our way to the fermionic coherent state just like the bosonic case. Recall the definition of bosonic coherent state in quantum optics. There are kinds of definitions of the bosonic coherent state [19]:

1. the state that has the minimum uncertainty $\Delta x \Delta p = \frac{\hbar}{2}$

2. the eigenstate of the $k$-mode bosonic annihilation operator: $|\alpha_k\rangle = e^{\alpha_k a_k^+ - \alpha_k^* a_k} |0\rangle_k$,

where $\alpha_k$ is a complex constant and $|0\rangle_k$ is the vaccum state of $k$-mode. Since there's no classical correspondence of $\Delta x$ and $\Delta p$ in a fermionic harmonic oscillator [20], we choose the second definition as our building block to the fermionic coherent state. In [21], we have the fermionic coherent state as: $|\xi\rangle = e^{-\xi a^+} |0\rangle$, which $|0\rangle$ is the vaccum state whcih is assumed to be normalized $\langle 0 \mid 0 \rangle$=1 and $a|0\rangle = 0$. (And $\xi$ is a new kind of number called Grassman variable corresponding to $a^+$ and is a variable used to describe the fermion particle like the general number used to describe the boson particle). For a comprehensive introduction of the fermionic coherent state, one can refer to [21, 22]. Now, we introduce the Grassman variables. The Grassman variables satisfy the following properties:

$$\{\xi_i, \xi_j\} = 0, \tag{2.3.5}$$

$$\{\xi_i^*, \xi_j\} = 0, \tag{2.3.6}$$

$$\{\xi_i^*, \xi_j^*\} = 0, \tag{2.3.7}$$

$$(\xi_i \xi_j)^* = \xi_j^* \xi_i^*, \tag{2.3.8}$$

$$\{a_i, \xi_j\} = 0. \tag{2.3.9}$$

From the above anti-commutation relation of the Grassman variables, one can verify that $\xi_i^2 = (\xi_i^*)^2 = 0$ easily. This relation can greatly simplify the calculation in the fermionic system. For example:

$$e^{-\xi a^+} = \sum_n \frac{1}{n!}(-\xi a^+)^n$$

$$= 1 - \xi a^+ + \frac{1}{2}\xi a^+ \xi a^+ - \frac{1}{6}\xi a^+ \xi a^+ \xi a^+ + ...$$

Because we know that $\xi^n = 0$ for $n \geq 2$,

$$e^{-\xi a^+} = 1 - \xi a^+. \tag{2.3.10}$$

The above formula is profitable to simplfy the later calculation. We then introduce the rules of differentiation and integration of the Grassman variables that are also important in later calculation of fermionic coherent state and the derivation of NMQSD for fermion.

*Differentiation:*

Because $\frac{\partial}{\partial \xi_i}$is also a Grassman variable (the partial differentiation of the Grassman variable ), we know that

$$\{\frac{\partial}{\partial \xi_i}, \xi_j\} = 0, \tag{2.3.11}$$

$$\{\frac{\partial}{\partial \xi_i}, a_j\} = 0, \tag{2.3.12}$$

$$\{\frac{\partial}{\partial \xi_i}, a_j^+\} = 0. \tag{2.3.13}$$

The same is hold for $\frac{\partial}{\partial \xi_i^*}$.

*Integration:*

Integration is very important in obtaining the Grassman average (we will define this later) over an operator. The integration over Grassman variables is defined as follows:

$$\int d\xi_i = 0, \tag{2.3.14}$$

$$\int \xi_j d\xi_i = \delta_{ji}. \tag{2.3.15}$$

Now that we have defined the important properties of the Grassman variable and fermionic operator, we can discuss more about the fermionic coherent state. We first examine that $|\xi\rangle = e^{-\xi a^+}|0\rangle$ is truly the eigenstate of the fermionic annihilation operator $a$.

$Proof$ :

$$a|\xi\rangle = ae^{-\xi a^+}|0\rangle$$

$$= a(1 - \xi a^+)|0\rangle$$

$$= -a\xi a^+|0\rangle$$

$$= \xi(1 - a^+ a)|0\rangle$$

$$= \xi|0\rangle . \ qed$$

Except for the examination of the fact that $|\xi\rangle$ is the eigenstate of the fermionic annihilation operator, it's also interesting to look at how the creation operator act on the coherent state $|\xi\rangle$ .We find that the effect of the creation operator on the coherent state is:

$$a^+|\xi\rangle = -\frac{\partial |\xi\rangle}{\partial \xi}. \tag{2.3.16}$$

*Proof* :

$$a^{+}\left|\xi\right\rangle = a^{+}(1-\xi a^{+})\left|0\right\rangle$$

$$= a^{+}\left|0\right\rangle$$

And

$$-\frac{\partial\left|\xi\right\rangle}{\partial\xi} = -\frac{\partial}{\partial\xi}[(1-\xi a^{+})\left|0\right\rangle]$$

$$= a^{+}\left|0\right\rangle = a^{+}\left|\xi\right\rangle . \ qed$$

We also have the completeness relation: $\int e^{-\xi^{*}\xi}\left|\xi\right\rangle\left\langle\xi\right| d\xi^{*}d\xi = I$ in the coherent state representation here. We can examine that as follows:

*Proof* :

$$\int e^{-\xi^{*}\xi}\left|\xi\right\rangle\left\langle\xi\right| d\xi^{*}d\xi\left|0\right\rangle$$

$$= \int e^{-\xi^{*}\xi}d\xi^{*}d\xi\left|\xi\right\rangle\left\langle\xi\right| 0\rangle$$

And,

$$\left\langle\xi\right| 0\rangle$$

$$= \left\langle 0\right|(1-a\xi^{*})\left|0\right\rangle$$

$$= \langle 0|\, 0\rangle = 1$$

Hence,

$$\int e^{-\xi^*\xi} d\xi^* d\xi \,|\xi\rangle \langle \xi|\, 0\rangle$$

$$= \int (1-\xi^*\xi) d\xi^* d\xi (1-\xi a^+)\,|0\rangle$$

$$= \int (1-\xi a^+ - \xi^*\xi) d\xi^* d\xi \,|0\rangle = |0\rangle \;\; qed$$

Similarly, one can easily prove that $\int e^{-\xi^*\xi} d\xi^* d\xi \,|\xi\rangle \langle \xi|\, 1\rangle = |1\rangle$ as well. Here, $|1\rangle = a^+\,|0\rangle$.Consequently, $\int e^{-\xi^*\xi}\,|\xi\rangle \langle \xi|\, d\xi^* d\xi = I$ for the reason that $|0\rangle$ , $|1\rangle$ is the basis of the fermion state.

For there are multi-mode fermionic operator; $\{a_k\}_{k=1}^{N}$ , $\{a_k^+\}_{k=1}^{N}$, the completeness relation is generalized to:

$$\int e^{-\sum_k \xi_k^*\xi_k}\,|\xi\rangle \langle \xi| \prod_k d\xi_k^* d\xi_k = 1, \tag{2.3.17}$$

where $|\xi\rangle = \prod_k (1-\xi_k a_k^+)\,|0\rangle$ After we introduce the necessary algebra of fermionic state, we can proceed our derivation of fermionic NMQSD without difficulty.

### 2.3.2 The Derivation of Fermionic Non-Markovian Quantum State Diffusion

In the begining of this section, we name the virtual environment as bath. The left environment that can be an electrode or other object interacting with the system is the left bath, and the right environment is the right bath. The bath has a large degrees of freedom in general. We continue from equation:

$$H_T = e^{\frac{i}{\hbar}\int_0^t dt' H_R'(t')}(H_S(t) + H_{SR}'(t))e^{-\frac{i}{\hbar}\int_0^t dt' H_R'(t')}. \tag{2.3.18}$$

In generally, there should be a time ordering operation $T$ before$e^{-\frac{i}{\hbar}\int_0^t dt' H_R'(t')}$: $Te^{-\frac{i}{\hbar}\int_0^t dt' H_R'(t')}$. But one can prove it easily that:

$$[d^+_{\lambda' k'} d_{\lambda' k'}\, , \, e_{\lambda k} e^+_{\lambda k}] = 0, \tag{2.3.19}$$

$$[d^+_{\lambda k} d_{\lambda k}\, , \, d^+_{\lambda' k'} d_{\lambda' k'}] = 0, \tag{2.3.20}$$

$$[e_{\lambda' k'} e^+_{\lambda' k'}\, , \, e_{\lambda k} e^+_{\lambda k}] = 0. \tag{2.3.21}$$

for any $\lambda$, $k$, $\lambda'$, $k'$.

Hence,

$$[H_R'(t')\, , \, H_R'(t)]$$

$$= [\sum_{\lambda' k'} \hbar\omega_{\lambda' k'}(t')(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'})\, , \, \sum_{\lambda k} \hbar\omega_{\lambda k}(t)(d^+_{\lambda k} d_{\lambda k} + e_{\lambda k} e^+_{\lambda k})]$$

$$= \sum_{\lambda, k, \lambda', k'} \hbar^2 \omega_{\lambda' k'}(t')\omega_{\lambda k}(t)([d^+_{\lambda' k'} d_{\lambda' k'}\, , \, d^+_{\lambda k} d_{\lambda k}] + [d^+_{\lambda' k'} d_{\lambda' k'}\, , \, e_{\lambda k} e^+_{\lambda k}]$$

$$+[e_{\lambda' k'} e^+_{\lambda' k'}\, , \, d^+_{\lambda k} d_{\lambda k}] + [e_{\lambda' k'} e^+_{\lambda' k'}\, , \, e_{\lambda k} e^+_{\lambda k}]) = 0. \tag{2.3.22}$$

The Hamiltonians of different times are commute. The order of Hamiltonian at different times are thus not so important. We can final simplify $H_T(t)$ to get :

$$H_T(t) = H_S(t) + \sum_{\lambda k}(g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+ d_{\lambda k}e^{-i\varpi_{\lambda k}(t)} + g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\varpi_{\lambda k}(t)}e^+_{\lambda k}c^+ + H.c.). \tag{2.3.23}$$

Here, $\varpi_{\lambda k}(t) \equiv \int_0^t \omega_{\lambda k}(t^{'})dt^{'}$ and the detailed calculation will be shown in Appendix 2. Since we have the total Hamiltonian in the interaction picture, we can now determine the time evolution of the quantum state of the total system,which includes the system and the bath by the equation: $\frac{\partial\left|\Psi_t^I(t)\right\rangle}{\partial t} = -i\frac{1}{\hbar}H_T(t)\left|\Psi_t^I(t)\right\rangle$. The superscript $I$ means that the state $\left|\Psi_t^I(t)\right\rangle$ is in the interaction picture and the time evolution equation of the quantum state of the total system can be easily proved by taking partial derivative of time of $\left|\Psi_t^I(t)\right\rangle = e^{-i\frac{1}{\hbar}\int_0^t H_T(t^{'})dt^{'}}\left|\Psi_t^I(0)\right\rangle$. We assume that we tune the interaction between the system and the bath at the initial time $t=0$ so that the initial quantum state of the total state can be asssumed to be factorized at the initial time, in other words, $|\Psi_t(0)\rangle = |\psi_0\rangle \otimes |0\rangle$, where$|0\rangle$ is the vaccum state of the bath. In the following content, we are in the interaction picture and we ignore the $I$ in the superscript for simplicity.

Just as the fact that the state is a wave function in the corrdinate representation in quantum mechanics, we choose the coherent state representation and project the quantum state of the total system into the coherent state of the bath. This projection can eliminate the degrees of freedom of the bath and take the effect of the bath on the system into account by the Grassmann variable of the bath. Inasmuch as that there are two kinds of particles $d_{\lambda k}(d^+_{\lambda k})$ , $e_{\lambda k}(e^+_{\lambda k})$ in the bath, we need to introduce the coherent state of the bath as:

$$|zw\rangle \equiv \prod_{\lambda k}(1 - z_{\lambda k}d^+_{\lambda k})(1 - w_{\lambda k}e^+_{\lambda k})\,|0\rangle\,. \tag{2.3.24}$$

$z_{\lambda k}$ , $w_{\lambda k}$ are the Grassman random variables that have the statistical mean over the random Grassmann variables as follows:

$$M[z_{\lambda k}(\ w_{\lambda k})] = \int (\prod_{\lambda' k'} dz^*_{\lambda' k'} dz_{\lambda' k'} dw^*_{\lambda' k'} dw_{\lambda' k'} e^{-z^*_{\lambda' k'} z_{\lambda' k'}} e^{-w^*_{\lambda' k'} w_{\lambda' k'}}) z_{\lambda k} (or\ w_{\lambda k}) = 0, \tag{2.3.25}$$

$$M[z_{\lambda k} z^*_{\lambda k}] = \int (\prod_{\lambda' k'} dz^*_{\lambda' k'} dz_{\lambda' k'} dw^*_{\lambda' k'} dw_{\lambda' k'} e^{-z^*_{\lambda' k'} z_{\lambda' k'}} e^{-w^*_{\lambda' k'} w_{\lambda' k'}}) z_{\lambda k} z^*_{\lambda k} = 1, \tag{2.3.26}$$

where

$$M[\bullet] \equiv \int (\prod_{\lambda' k'} dz^*_{\lambda' k'} dz_{\lambda' k'} dw^*_{\lambda' k'} dw_{\lambda' k'} e^{-z^*_{\lambda' k'} z_{\lambda' k'}} e^{-w^*_{\lambda' k'} w_{\lambda' k'}})[\bullet] \tag{2.3.27}$$

is defined as the statistical mean over the random Grassmann variables. The random variables satisfying the above average is called a Grassmann Gaussian process due to the zero average of $z_{\lambda k}$ $or$ $w_{\lambda k}$. We now project the time evolution equation: $\frac{\partial |\Psi_t(t)\rangle}{\partial t} = -i\frac{1}{\hbar} H_T(t) |\Psi_t(t)\rangle$ into the coherent state: $|zw\rangle$ and get the time evolution equation of the quantum state of the total system in the coherent state representtion as follow:

$$\langle zw| \frac{\partial}{\partial t} |\Psi_t(t)\rangle = -i\frac{1}{\hbar} \langle zw| H_T(t) |\Psi_t(t)\rangle$$

$$= -i\frac{1}{\hbar} \langle zw| H_S(t) + \sum_{\lambda k} (g_{\lambda k}(t)\sqrt{1-n_{\lambda k}} c^+ d_{\lambda k} e^{-i\varpi_{\lambda k}(t)} + g_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{-i\varpi_{\lambda k}(t)} e^+_{\lambda k} c^+ + H.c.) |\Psi_t(t)\rangle . \tag{2.3.28}$$

After simplifying the above equation, we eventually arrive at the result (the detailed derivation will be demonstrated in Appendix 3):

$$\frac{\partial}{\partial t}\left|\phi(t,z^*,w^*)\right\rangle = -\frac{i}{\hbar}H_S(t)\left|\phi(t,z^*,w^*)\right\rangle - \frac{1}{\hbar}\sum_{\lambda} c^{+}\int_0^t \alpha_{\lambda 1}(t,s)\frac{\delta\left|\phi(t,z^*,w^*)\right\rangle}{\delta z^*_{\lambda}(s)}ds$$

$$-\frac{1}{\hbar}\sum_{\lambda} c\int_0^t \alpha_{\lambda 2}(t,s)\frac{\delta\left|\phi(t,z^*,w^*)\right\rangle}{\delta w^*_{\lambda}(s)}ds - \frac{1}{\hbar}\sum_{\lambda} c^{+}w^*_{\lambda}(t)\left|\phi(t,z^*,w^*)\right\rangle - \frac{1}{\hbar}\sum_{\lambda} c z^*_{\lambda}(t)\left|\phi(t,z^*,w^*)\right\rangle, \tag{2.3.29}$$

with the following definitions of the parameters:

$$\left|\phi(t,z^*,w^*)\right\rangle \equiv \left\langle zw\right|\left.\Psi_t(t)\right\rangle, \tag{2.3.30}$$

$$z^*_{\lambda}(t) \equiv -i\sum_k \sqrt{1-n_{\lambda k}}\,g^*_{\lambda k}(t)z^*_{\lambda k}e^{i\overline{\omega}_{\lambda k}(t)}, \tag{2.3.31}$$

$$w^*_{\lambda}(t) \equiv -i\sum_k \sqrt{n_{\lambda k}}\,g_{\lambda k}(t)w^*_{\lambda k}e^{-i\overline{\omega}_{\lambda k}(t)}, \tag{2.3.32}$$

$$\alpha_{\lambda 1}(t,s) = \sum_k (1-n_{\lambda k})g_{\lambda k}(t)g^*_{\lambda k}(s)e^{-i\overline{\omega}_{\lambda k}(t-s)}, \tag{2.3.33}$$

$$\alpha_{\lambda 2}(t,s) = \sum_k n_{\lambda k}g_{\lambda k}(s)g^*_{\lambda k}(t)e^{i\overline{\omega}_{\lambda k}(t-s)}, \tag{2.3.34}$$

$$\overline{\omega}_{\lambda k}(t-s) \equiv \overline{\omega}_{\lambda k}(t) - \overline{\omega}_{\lambda k}(s)$$

$$= \int_s^t \omega_{\lambda k}(\tau)d\tau, \tag{2.3.35}$$

where $\left|\phi(t,z^*,w^*)\right\rangle$ is the reduced quantum state of the total system by projecting the total state into the bath coherent state, and $(z^*, w^*)$ represent the set of all $(z^*_{\lambda k}, w^*_{\lambda k})$ variables. The time evolution equation of that state $|\phi(t, z^*, w^*)\rangle$ is the NMQSD. The function $\alpha_{\lambda n}(t, s)$ is the bath correlation function of two times $t$, $s$ and will be discussed later.

## 2.4 The O Operator and Its Time Evolution Equation

After we derive the fermionic NMQSD, it seems that we can determine the behavior of the system as we wish. It is, however, not the case. Owing to the fact that we don't know what $\frac{\delta|\phi(t,z^*,w^*)\rangle}{\delta z^*_\lambda(s)}$ $(or\ \frac{\delta|\phi(t,z^*,w^*)\rangle}{\delta w^*_\lambda(s)})$ is, how to deal with the functional derivative $\frac{\delta|\phi(t,z^*,w^*)\rangle}{\delta z^*_\lambda(s)}$ $(or\ \frac{\delta|\phi(t,z^*,w^*)\rangle}{\delta w^*_\lambda(s)})$ becomes a troublesome task. In this section, we will introduce an Ansatz to simplify this problem.

For the reason that $\frac{\delta|\phi(t,z^*,w^*)\rangle}{\delta z^*_\lambda(s)}$ $(or\ \frac{\delta|\phi(t,z^*,w^*)\rangle}{\delta w^*_\lambda(s)})$ is dependent on variable $t, s, z^*_{\lambda k}, w^*_{\lambda k}$, we introduce the Ansatz in such a way:

$$\frac{\delta}{\delta z^*_\lambda(s)} |\phi(t, z^*, w^*)\rangle = O_{\lambda 1}(t, s, z^*, w^*) \, |\phi(t, z^*, w^*)\rangle \, , \tag{2.4.1}$$

$$\frac{\delta}{\delta w^*_\lambda(s)} |\phi(t, z^*, w^*)\rangle = O_{\lambda 2}(t, s, z^*, w^*) \, |\phi(t, z^*, w^*)\rangle \, . \tag{2.4.2}$$

We now transfer the functional derivatives into the operators. Afterwards, we need to determine the time evolution equation of $O_{\lambda 1}(t, s, z^*, w^*)$ and $O_{\lambda 2}(t, s, z^*, w^*)$. We only give the derivation of the time evolution equation of $O_{\lambda 1}(t, s, z^*, w^*)$. It's the same for $O_{\lambda 2}(t, s, z^*, w^*)$.

The equation can be determined by the consistency condition:

$$\frac{\partial}{\partial t} \frac{\delta \, |\phi(t, z^*, w^*)\rangle}{\delta z^*_\lambda(s)} = \frac{\delta}{\delta z^*_\lambda(s)} \frac{\partial \, |\phi(t, z^*, w^*)\rangle}{\partial t}, \tag{2.4.3}$$

and the time evolution equation of the reduced quantum state $|\phi(t, z^*, w^*)\rangle$:

$$\frac{\partial}{\partial t}|\phi\rangle = -\frac{i}{\hbar}H_S(t)|\phi\rangle - \frac{1}{\hbar}\sum_\lambda c^+ \int_0^t \alpha_{\lambda 1}(t,s)\frac{\delta|\phi\rangle}{\delta z_\lambda^*(s)}ds - \frac{1}{\hbar}\sum_\lambda c \int_0^t \alpha_{\lambda 2}(t,s)\frac{\delta|\phi\rangle}{\delta w_\lambda^*(s)}ds$$

$$-\frac{1}{\hbar}\sum_\lambda c^+ w_\lambda^*(t)|\phi\rangle - \frac{1}{\hbar}\sum_\lambda c z_\lambda^*(t)|\phi\rangle . \tag{2.4.4}$$

n

We now derive the equation briefly. First, we deal with the left hand side of Eq. (2.4.3):

$$\frac{\partial}{\partial t}\frac{\delta|\phi\rangle}{\delta z_\lambda^*(s)} = \frac{\partial}{\partial t}(O_{\lambda 1})|\phi\rangle)$$

$$= \frac{\partial O_{\lambda 1}}{\partial t}|\phi\rangle + O_{\lambda 1}\frac{\partial|\phi\rangle}{\partial t} \tag{2.4.5}$$

Then, we deal with the right hand side of Eq. (2.4.3) by Eq. (2.4.4):

$$\frac{\delta}{\delta z_\lambda^*(s)}\frac{\partial|\phi\rangle}{\partial t}$$

$$= \frac{\delta}{\delta z_\lambda^*(s)}(-\frac{i}{\hbar}H_S(t)|\phi\rangle - \frac{1}{\hbar}\sum_\lambda c^+ \int_0^t \alpha_{\lambda 1}(t,s)\frac{\delta|\phi\rangle}{\delta z_\lambda^*(s)}ds$$

$$-\frac{1}{\hbar}\sum_\lambda c \int_0^t \alpha_{\lambda 2}(t,s)\frac{\delta|\phi\rangle}{\delta w_\lambda^*(s)}ds - \frac{1}{\hbar}\sum_\lambda c^+ w_\lambda^*(t)|\phi\rangle - \frac{1}{\hbar}\sum_\lambda c z_\lambda^*(t)|\phi\rangle). \tag{2.4.6}$$

By equating the left and the right hand sides, we can finally get the equation of $O_{\lambda 1}(t,s,z^*,w^*)$ and the same is for $O_{\lambda 2}(t,s,z^*,w^*)$:

$$\frac{\partial O_{\lambda 1}}{\partial t} = -\frac{i}{\hbar}[H_S, O_{\lambda 1}] - \frac{1}{\hbar}[\sum_{\lambda'}(c^+\overline{O}_{\lambda' 1} + c\overline{O}_{\lambda' 2}), O_{\lambda 1}] + \frac{1}{\hbar}[O_{\lambda 1}, \sum_{\lambda'} c^+ w^*_{\lambda'}(t)]$$

$$+\frac{1}{\hbar}[O_{\lambda 1}, cz^*_{\lambda'}(t)] + \frac{1}{\hbar}\sum_{\lambda'} c^+ \frac{\delta \overline{O}_{\lambda' 1}}{\delta z^*_{\lambda}(s)} + \frac{1}{\hbar}\sum_{\lambda'} c \frac{\delta \overline{O}_{\lambda' 2}}{\delta z^*_{\lambda}(s)}, \tag{2.4.7}$$

$$\frac{\partial O_{\lambda 2}}{\partial t} = -\frac{i}{\hbar}[H_S, O_{\lambda 2}] - \frac{1}{\hbar}[\sum_{\lambda'}(c^+\overline{O}_{\lambda' 1} + c\overline{O}_{\lambda' 2}), O_{\lambda 2}] + \frac{1}{\hbar}[O_{\lambda 2}, \sum_{\lambda'} c^+ w^*_{\lambda'}] + \frac{1}{\hbar}[O_{\lambda 2}, cz^*_{\lambda'}]$$

$$+\frac{1}{\hbar}\sum_{\lambda'} c^+ \frac{\delta \overline{O}_{\lambda' 1}}{\delta w^*_{\lambda}(s)} + \frac{1}{\hbar}\sum_{\lambda'} c \frac{\delta \overline{O}_{\lambda' 2}}{\delta w^*_{\lambda}(s)}, \tag{2.4.8}$$

where $\overline{O}_{\lambda' n}(t, z^*, w^*) \equiv \int_0^t \alpha_{\lambda' n}(t,s) O_{\lambda' n}(t, s, z^*, w^*) ds$ is the average of $O_{\lambda' n}(t, s, z^*, w^*)$ with the bath correlation function.

After we substitute the Ansatz Eq. (2.4.1) and Eq. (2.4.2) into Eq. (2.4.4), the time non-local linear NMQSD equation becomes the time-local or time-convolutionless equation:

$$\frac{\partial}{\partial t}|\phi\rangle = -\frac{i}{\hbar}H_S|\phi\rangle - \frac{1}{\hbar}\sum_{\lambda} c^+\overline{O}_{\lambda 1}(t, z^*, w^*)|\phi\rangle - \frac{1}{\hbar}\sum_{\lambda} c\overline{O}_{\lambda 2}(t, z^*, w^*)|\phi\rangle$$

$$-\frac{1}{\hbar}\sum_{\lambda} c^+ w^*_{\lambda}(t)|\phi\rangle - \frac{1}{\hbar}\sum_{\lambda} cz^*_{\lambda}(t)|\phi\rangle. \tag{2.4.9}$$

The time evolution of the reduced quantum state $|\phi(t, z^*, w^*)\rangle$ seems not to be influenced by the past history at the earlier time $s$ by virtue of the substitution of $\overline{O}_{\lambda' n}(t, z^*, w^*)$. All the past memories in the time integral over the past time are assumed to be $\overline{O}_{\lambda' n}(t, z^*, w^*)$. $\overline{O}_{\lambda' n}(t, z^*, w^*)$ is extremely crucial for NMQSD for the reason that it contain all the information of the past history. If we can solve it exactly, we can then directly determine the time evolution behavior of $|\phi\rangle$, in other words, the system behavior under the interaction of the bath.

## 2.5 Summary

In the beginning, we briefly introduce our physical model and write down the Hamiltonian of the total system. The bias voltage between the source and the drain electrodes, gate voltage applied to control the system energy and the barrier between source ( or drain ) are all time-dependent. At the beginning, all the fermionic environment oscillators are not in the ground strate at finite temperature. We introduce Bogoliubov transformation to canonically map the environment onto another effective zero temperature environment so that we can use NMQSD at the finite temperature bath. The effect of temperature is now in the coefficients of the Bogoliubov transformation.Then, we project the NMQSD into the bath coherent states. Because the coherent state is the eigenstate of annihilation operator, this projection can simplify the NMQSD significantly.

Althought now we derive the fermionic NMQSD in the coherent state representation, it is usually a difficult task to exactly get the time evolution information from it for the sake of the functional derivative terms inside the time integral. Instead of evaluating the functional derivative terms directly which is very troublesome, we introduce the $O$ operator Ansatz. In $O$ operator Ansatz, we introduce $\overline{O}$ operator to include the past history trajectory so that the time evolution of the system at time $t$ seems not to be affected by the past history trajectory of the whole system at the earlier time $s$.

Finally, we derive the time evolution equation of $O$ operator by the consistency condition of Eq. (2.4.3) and the time evolution equation (2.4.4) with the appropriate initial condition of $O$ operator. If we can exactly solve the $O$ operator, we can determine the time evolution of the system. Nonetheless, it is usually not the case that $O$ operator can be solved exactly. In many cases, $O$ operator can only be solved perturbatively.

# 3 Exact Master Equation

## 3.1 Introduction

In quantum statistical mechanis, we have learned a very important concept, which is density operator $\chi(t)$. It can express the expectation value of physical quantity of an ensemble in a more compact way by taking the trace of the density operator and the physical observable:

$$\langle O \rangle = Tr(O\chi(t)). \tag{3.1.1}$$

So, it is very important to determine the time evolution equation of the density operator of the total system in order to determine the expectation value of the physical quantity we are concerned. One can find a more detailed introduction in [23]. However, we are seeking information about the system $S$ without requiring detailed information about the total system $S \otimes R$ in generl. Thus, we neglect the degrees of the part we don't care by tracing them out. In other words, we take the statistical average of the bath part (the part we are not concern) in advance as follows [24]:

$$\langle O(t) \rangle = Tr_{S\otimes R}[O(t)\chi(t)] = Tr_S[O(t)Tr_R(\chi(t))] = Tr_S[O(t)\rho(t)]. \tag{3.1.2}$$

We are in the bath interaction picture as the previous chapter and define the reduced density operator by tracing over the bath degrees of freedom :

$$\rho(t) \equiv Tr_R(\chi(t)). \tag{3.1.3}$$

We achieve our goal that we can only care about the specific part of the total system. The time evolution equation of the reduced density operator is called a master equation. In general, the bavior of the open quantum system is investigated by the master equation. Traditionally, we use the quantum Markovian master equation in Lindblad form to investigate the system we are concerned with. If the coupling strength between the bath and the system is strong, then we need to use a non-Markovian master equation.

In this chapter, we derive the non-Markovian master equation by NMQSD. We will introduce Novikov theorem in the process of the derivation. It is a profitable theorem to transform the troublesome Grassman average into the average of the $O$ operator. The $O$ operator is just what we want and can simplify the problem.

## 3.2 Exact Master Equation from Fermionic Non-Markovian Quantum State Diffusion

In this section, we derive the exact master equation from fermionic NMQSD. By definition, the reduced density operator can be obtained by taking the statistical mean for the density operator related to the total system state $|\Psi_t(t)\rangle$: $\rho(t) = Tr_R(\chi(t)) = Tr_R(|\Psi_t(t)\rangle \langle\Psi_t(t)|)$. We now do some mathematical trick on $\rho(t)$ and get (the detailed calculation is presented in Appendix 4):

$$\rho(t) = M[\langle zw| \Psi_t(t)\rangle \langle\Psi_t(t)| -z-w\rangle]. \tag{3.2.1}$$

Here $M$ represent the statistical mean over the random Grassmann variables as defined in Eq. (2.3.27). The ket $|-z-w\rangle$ is defined as the stochastic density operator as follows:

$$|-z-w\rangle \equiv \prod_k (1+z_{\lambda k}d^+_{\lambda k}) \prod_l (1+w_{\lambda k}e^+_{\lambda k})\,|0\rangle\,. \tag{3.2.2}$$

For simplicity, we use the definition in Eq. (2.3.30):

$$|\phi(t,z^*,w^*)\rangle \equiv \langle zw|\;\Psi_t(t)\rangle\,,$$

$$\langle\phi(t,-z,-w)| \equiv \langle\Psi_t(t)|\,-z-w\rangle\,. \tag{3.2.3}$$

The master equation is then:

$$\frac{\partial\rho(t)}{\partial t} = \frac{\partial M[|\phi(t,z^*,w^*)\rangle\,\langle\phi(t,-z,-w)|]}{\partial t}$$

$$= M[\frac{\partial\,|\phi(t,z^*,w^*)\rangle}{\partial t}\,\langle\phi(t,-z,-w)| + |\phi(t,z^*,w^*)\rangle\,\frac{\partial\,\langle\phi(t,-z,-w)|}{\partial t}]. \tag{3.2.4}$$

From Eq. (3.2.1), we say that the reduced density operator can be unraveled by quantum trajectories: $|\phi\rangle = |\phi(t,z^*,w^*)\rangle$ following Eq. (2.4.9), and $\langle\phi| = \langle\phi(t,-z,-w)| \equiv \langle\Psi_t(t)|\,-z-w\rangle$ satisfies the following equation:

$$\frac{\partial\,\langle\phi|}{\partial t} = \frac{i}{\hbar}\,\langle\phi|\,H_S - \frac{1}{\hbar}\sum_\lambda \langle\phi|\,\overline{O}^+_{\lambda 1}(t,-z,-w)c - \frac{1}{\hbar}\sum_\lambda \langle\phi|\,\overline{O}^+_{\lambda 2}(t,-z,-w)c^+$$

$$+\frac{1}{\hbar}\sum_\lambda \langle\phi|\,w_\lambda(t)c + \frac{1}{\hbar}\sum_\lambda \langle\phi|\,z_\lambda(t)c^+. \tag{3.2.5}$$

The above equation can be readily obtained by first taking the Hermitian conjugate of Eq. (2.4.9) and then change variables: $z_{\lambda k} \to -z_{\lambda k}$, $w_{\lambda k} \to -w_{\lambda k}$. Consequently, by Eq. (2.4.9) and Eq. (3.2.5), we finally derive the exact non-Markovian fermionic master equation by Novikov theorem:

$$\frac{\partial\rho(t)}{\partial t} = \frac{-i}{\hbar}[H_S(t), \rho(t)] + \frac{1}{\hbar}\sum_{\lambda}([c, M[P_t\overline{O}^{+}_{\lambda 1}(t, -z, -w)]] - [c^{+}, M[\overline{O}_{\lambda 1}(t, z^{*}, w^{*})P_t]]$$

$$-[c, M[\overline{O}_{\lambda 2}(t, z^{*}, w^{*})P_t]] + [c^{+}, M[P_t\overline{O}^{+}_{\lambda 2}(t, -z, -w)]]). \qquad (3.2.6)$$

Here we define the stochastic density operator $P_t \equiv \langle zw|\, \Psi_t(t)\rangle \langle\Psi_t(t)|\, -z-w\rangle = |\phi\rangle\langle\phi|$. The detailed calculation is given in Appendix 5. The exact master equation is derived without perturbation, hence it can be applied to the case of strong coupling strength between the system and the environments.

The solution $\rho(t)$ of the exact master equation Eq. (3.2.6) satisfies the following equation:

$$Tr_S(\rho(t)) = 1, \qquad (3.2.7)$$

$$\rho(t) = \rho^{+}(t), \qquad (3.2.8)$$

$$\langle S|\, \rho(t)\, |S\rangle \geq 0 \; for\ any\ system\ state \qquad (3.2.9)$$

which can be apparently proved. That is, the reduced density operator preserves the Hermicity, the positivity and the trace.

## 3.3 Two-Time Correlation Function of the Bath

Correlation function is a very important physical quantiy that measures the correlation between noises of different modes in different timings. Thus, the correlation function of

$z_{\lambda k}(t)$ and $z^*_{\lambda k}(s)$ is defined as:

$$M[z_{\lambda k}(t) z^*_{\lambda k}(s)]. \tag{3.3.1}$$

In section 2.3.2, we have introduced the bath correlation function:

$$M[z_{\lambda k}(t) z^*_{\lambda k}(s)] \equiv \alpha_{\lambda 1}(t,s) = \sum_k (1-n_{\lambda k}) g_{\lambda k}(t) g^*_{\lambda k}(s) e^{-i\overline{\omega}_{\lambda k}(t-s)}, \tag{3.3.2}$$

$$M[w_{\lambda k}(t) w^*_{\lambda k}(s)] \equiv \alpha_{\lambda 2}(t,s) = \sum_k n_{\lambda k} g_{\lambda k}(s) g^*_{\lambda k}(t) e^{i\overline{\omega}_{\lambda k}(t-s)}, \tag{3.3.3}$$

for discrete mode. Equations (3.3.2) and (3.3.3) can be proved easily by the definition of $M[\bullet]$.

If the distribution of the coupling strength $g_{\lambda k}(t)$ is continuous rather than discrete, we need to introduce the density of state $\rho_\lambda(\omega)$ to describe the distribution of $g_\lambda(\omega,t) g_\lambda(\omega,s)$. The spectral density $J_\lambda(\omega,t,s)$ is defined as $\rho_\lambda(\omega) g_\lambda(\omega,t) g_\lambda(\omega,s)$. We consider in this thesis the spectral density of Lorentzian form:

$$J_\lambda(\omega,t,s) = \frac{1}{2\pi} \frac{\overline{V}_\lambda(t) \overline{V}^*_\lambda(s) \Gamma_\lambda W_\lambda^2}{(\hbar\omega - \mu_\lambda)^2 + W_\lambda^2}. \tag{3.3.4}$$

Here $W_\lambda$ is the bandwidth of the spectral density. It can be thought of as the width of the peak of $J_\lambda$ and $\Gamma_\lambda$ is a constant of unit $Joule^2$. When $W_\lambda \to \infty$, $J_\lambda \to \frac{1}{2\pi} \overline{V}_\lambda(t) \overline{V}^*_\lambda(s) \Gamma_\lambda$, and $J_\lambda$ is independent of $\omega$. This is called the wide-band limit. After we take the wide-band limit, $J_\lambda = \frac{1}{2\pi} \overline{V}_\lambda(t) \overline{V}^*_\lambda(s) \Gamma_\lambda$ becomes a constant independent of $\omega$. By introducing the continuous spectral density $J_\lambda(\omega,t,s)$, the bath correlation functions $\alpha_{\lambda 1}(t,s)$ and $\alpha_{\lambda 2}(t,s)$ become:

$$\alpha_{\lambda 1}(t,s) = e^{-ie\int_s^t d\tau V_\lambda(\tau)} \int_{-\infty}^{\infty} d\omega (1 - n_\lambda(\omega)) J_\lambda(\omega,t,s) e^{-i\omega(t-s)}, \tag{3.3.5}$$

$$\alpha_{\lambda 2}(t,s) = e^{ie\int_s^t d\tau V_\lambda(\tau)} \int_{-\infty}^{\infty} d\omega n_\lambda(\omega) J_\lambda^*(\omega,t,s) e^{i\omega(t-s)}. \tag{3.3.6}$$

## 3.4 Summary

In this chapter, we first introduce the density operator to deal with the average of some phyical quantities of a specific ensemble. In general, we don't need the infromation of the whole system, so we introduce the reduced density operator by tracing over the degrees of freedom of the bath. Thus, the information of the bath is included in the reduced density operator as a number. We can consider the time evolution of the system we are concerned by the time evolution equation of the reduced density operator, in other words, the master equation.

Then in section 3.2, we derive the exact master equation. First we trace over the degrees of freedom of the bath and get the reduced density operator. Then by some mathematical trick, we represent the reduced density operator as the the statistical mean of the operator: $\langle zw| \Psi_t(t)\rangle \langle\Psi_t(t)| -z-w\rangle$ over the random Grassmann variables: $\rho(t) = M[\langle zw| \Psi_t(t)\rangle \langle\Psi_t(t)| -z-w\rangle]$. Then we differentiate the reduced density operator $\rho(t)$ and get the exact master equation. We then simplify the master equation by Novikov theorem.

Finally, we introduce the correlation function for later calculation. One noticing thing is that if we turn off all the time dependence and take the wide band limit, it can be easily demonstrated that the two time correlation of $t$ and $\tau$ will proportional to $\delta(t-\tau)$. It is exactly the Markovian limit. So, wide band limit can somewhat be treated as the Makovian limit.

# 4 Transient Current into a Single-Energy-Level Quantum Dot

## 4.1 Introduction

In the previous chapter, we have shown up the exact master equation for the reduced density operator by some mathematical tricks. Since we know the time evolution of the reduced density operator, we can discuss the behavior of the physical quantities we are interested. In this chapter, we focus on the transient current flowing from the left bath and the right bath. The definition of current is $I_\lambda = -e\frac{dn_\lambda}{dt} = -e\frac{d}{dt}\langle N_\lambda(t)\rangle$. In section 4.2, it takes us several pages to demonstrate the detailed derivation of the current formula. In the bottom of section4.2, we deduce that:

$$O_{L2} = O_{R2} = O_2,$$

$$O_{L1} = O_{R1} = O_1,$$

by some arguments. We propose the assumption of the Grassman average of the $O_1$ , $O_2$ operators, $Q_1$, $Q_2$:

$$Q_1(t,s) \equiv M[O_1(t,s,z^*,w^*)P_t] = A_1^*(t,s)c\rho(t) + A_2^*(t,s)\rho(t)c,$$

$$Q_2(t,s) \equiv M[O_2(t,s,z^*,w^*)P_t] = B_2(t,s)c^+\rho(t) + B_1(t,s)\rho(t)c^+.$$

with $A_1$, $A_2$, $B_1$, $B_2$ to be determined. Although we have derived the time evolution equation of $O_{\lambda 1}$ and $O_{\lambda 2}$, it is not so convenient to use due to the fact that there is $\overline{O}_{\lambda 2}$ term in the equation of $O_{\lambda 1}$ and vice versa. In other words, the time evolution equation of $O_{\lambda 1}(O_{\lambda 2})$ is mixed with the term $\overline{O}_{\lambda 2}(\overline{O}_{\lambda 1})$. In section 4.3, we refer to part 2. D in [25] to derive the pure time evolution equation for $O_1$ and $O_2$. The method used in [25] is mainly dealing with the propagator. Through this method, we can derive the time evolution equation of the undetermined coefficients $A_1$, $A_2$, $B_1$, $B_2$ and finally solve $Q_1$ and $Q_2$ operators.

## 4.2 The Transient Current

We apply the NMQSD to the research on the transient current through the single quantum dot. The current flowing from the $\lambda$-side lead is as follows:

$$I_\lambda = -e\frac{d}{dt}\left\langle N_\lambda^H(t)\right\rangle$$

$$= -e\frac{d}{dt}(Tr_{S\otimes R}[N_\lambda^H(t)\rho^H]). \tag{4.2.1}$$

Here we use the Heisenberg picture for the convenience that the density operator in the Heisenberg picture is time-independent. Eq. (4.2.1) then becomes:

$$-eTr_{S\otimes R}[\frac{dN_\lambda^H(t)}{dt}\rho^H]$$

$$= \frac{-e}{i\hbar}Tr_{S\otimes R}([N_\lambda^H(t)\,,\,H^H(t)]\rho^H). \tag{4.2.2}$$

Because we use interaction picture in the previous text, we introduce the transformation betweern the Heisenberg picture and the bath interaction picture as follows:

$$O^H = \widetilde{U}^{+} O^I \widetilde{U}, \tag{4.2.3}$$

$$\rho^H = \widetilde{U}^{+} \rho^I \widetilde{U}, \tag{4.2.4}$$

where $\widetilde{U} \equiv e^{\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau}(Te^{-\frac{i}{\hbar}\int_0^t H^{'}(\tau)d\tau})$. This is the Hermitian conjugate of the transformation operator between the Schrödinger picture and the bath interaction picture $U_B^{+}$ times the transformation operator between the Schrödinger picture and the Heisenberg picture $U$. Then we use Eq. (4.2.3) and Eq. (4.2.4) to transfrom Eq. (4.2.2) to $I_\lambda = \frac{ie}{\hbar} Tr_{S\otimes R}[[N_\lambda^I(t), H^I(t)]\rho^I(t)]$ easily. We now ignore the superscript $I$ and adopt the bath interaction picture in the followings: $H^I(t) \to H(t)$, $N_\lambda^I(t) \to N_\lambda(t)$ but still use $\rho^I(t) = \left|\Psi_t^I(t)\right\rangle \left\langle \Psi_t^I(t)\right| \to \left|\Psi_t(t)\right\rangle \left\langle \Psi_t(t)\right|$ in order to distinguish from the reduced density operator $\rho(t)$. The next step is to deal with $I_\lambda$. We now briefly calculate the operators in $I_\lambda$:

$$N_\lambda(t) = e^{\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau} \sum_k (d_{\lambda k}^{+} d_{\lambda k} + e_{\lambda k} e_{\lambda k}^{+}) e^{-\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau}$$

$$= \sum_k (d_{\lambda k}^{+} d_{\lambda k} + e_{\lambda k} e_{\lambda k}^{+}), \tag{4.2.5}$$

$$H(t) = e^{\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau} (H_S(t) + H_R^{'}(t) + H_{SR}^{'}(t)) e^{-\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau}.$$

The $e^{\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau}(H_S(t)+H_{SR}^{'}(t))e^{-\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau}$ term is exactly the $H_T(t)$ in Eq. (2.3.23) and $H_R^{'}(t) = \sum_{\lambda k}[\hbar\omega_{\lambda k}(t)(d_{\lambda k}^{+} d_{\lambda k} + e_{\lambda k} e_{\lambda k}^{+})]$. So,

$$H(t) = H_T(t) + e^{\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau} H_R^{'}(t) e^{-\frac{i}{\hbar}\int_0^t H_R^{'}(\tau)d\tau}$$

$$= H_S(t)+\sum_{\lambda' k'}(g_{\lambda' k'}(t)\sqrt{1-n_{\lambda' k'}}c^+ d_{\lambda' k'}e^{-i\varpi_{\lambda' k'}(t)}+g_{\lambda' k'}(t)\sqrt{n_{\lambda' k'}}e^{-i\varpi_{\lambda' k'}(t)}e^+_{\lambda' k'}c^+ +H.c.)+H'_R(t). \tag{4.2.6}$$

The commutator

$$[N_\lambda(t)\,,\,H(t)]$$

$$= [\sum_k (d^+_{\lambda k}d_{\lambda k}+e_{\lambda k}e^+_{\lambda k})\,,\,\sum_{\lambda' k'}(g_{\lambda' k'}(t)\sqrt{1-n_{\lambda' k'}}c^+ d_{\lambda' k'}e^{-i\varpi_{\lambda' k'}(t)}$$

$$+g_{\lambda' k'}(t)\sqrt{n_{\lambda' k'}}e^{-i\varpi_{\lambda' k'}(t)}e^+_{\lambda' k'}c^+ + H.c.)]$$

$$= \sum_{\lambda', k, k'}[d^+_{\lambda k}d_{\lambda k}+e_{\lambda k}e^+_{\lambda k}\,,\,g_{\lambda' k'}(t)\sqrt{1-n_{\lambda' k'}}c^+ d_{\lambda' k'}e^{-i\varpi_{\lambda' k'}(t)}$$

$$+g_{\lambda' k'}(t)\sqrt{n_{\lambda' k'}}e^{-i\varpi_{\lambda' k'}(t)}e^+_{\lambda' k'}c^+ + H.c.] \tag{4.2.7}$$

In Eq. (4.2.7), $[d^+_{\lambda k}d_{\lambda k}+e_{\lambda k}e^+_{\lambda k}\,,\,c^+d_{\lambda' k'}] = [d^+_{\lambda k}d_{\lambda k}\,,\,c^+d_{\lambda' k'}]$. If $\lambda \neq \lambda'$ or $k \neq k'$, then $[d^+_{\lambda k}d_{\lambda k}\,,\,c^+d_{\lambda' k'}] = 0$. If $\lambda = \lambda'$ and $k = k'$, $[d^+_{\lambda k}d_{\lambda k}\,,\,c^+d_{\lambda k}] = -c^+d_{\lambda k}$. So $[d^+_{\lambda k}d_{\lambda k}+e_{\lambda k}e^+_{\lambda k}\,,\,c^+d_{\lambda' k'}] = -c^+d_{\lambda k}\delta_{\lambda\lambda'}\delta_{kk'}$. Similarly, $[d^+_{\lambda k}d_{\lambda k}+e_{\lambda k}e^+_{\lambda k}\,,\,e^+_{\lambda' k'}c^+] = -e^+_{\lambda k}c^+\delta_{\lambda\lambda'}\delta_{kk'}$. For the Hermitian conjugate part, we introduce a small mathematical trick so that we don't really calculate them. The trick is that: if $A$ is a Hermitian operator, then $[A, B^+] = [A^+, B^+] = -([A, B])^+$. We can use this to simplify the Hermitian conjugate part of Eq. (4.2.7). For the sake of the Hermicity of $d^+_{\lambda k}d_{\lambda k} + e_{\lambda k}e^+_{\lambda k}$, $[d^+_{\lambda k}d_{\lambda k}+e_{\lambda k}e^+_{\lambda k}, d^+_{\lambda' k'}c] = -(-c^+d_{\lambda k}\delta_{\lambda\lambda'}\delta_{kk'})^+ = d^+_{\lambda k}c\delta_{\lambda\lambda'}\delta_{kk'}$ and $[d^+_{\lambda k}d_{\lambda k} + e_{\lambda k}e^+_{\lambda k}\,,\,ce_{\lambda' k'}] = -(-e^+_{\lambda k}c^+\delta_{\lambda\lambda'}\delta_{kk'})^+ = ce_{\lambda k}\delta_{\lambda\lambda'}\delta_{kk'}$.

Through the above argument, Eq. (4.2.7) is reduced to:

$$[N_\lambda(t)\,,\,H(t)]$$

$$=\sum_k(-g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+d_{\lambda k}e^{-i\overline{\omega}_{\lambda k}(t)}-g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(t)}e^+_{\lambda k}c^+$$

$$+g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}}d^+_{\lambda k}ce^{i\overline{\omega}_{\lambda k}(t)}+g^*_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(t)}ce_{\lambda k}). \qquad (4.2.8)$$

Using Eq. (4.2.8), the current of the $\lambda$-side lead is:

$$I_\lambda=\frac{ie}{\hbar}Tr_{S\otimes R}[-\sum_k g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+d_{\lambda k}e^{-i\overline{\omega}_{\lambda k}(t)}\rho^I(t)]$$

$$+\frac{ie}{\hbar}Tr_{S\otimes R}[-\sum_k g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(t)}e^+_{\lambda k}c^+\rho^I(t)]$$

$$+\frac{ie}{\hbar}Tr_{S\otimes R}[\sum_k g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}}d^+_{\lambda k}ce^{i\overline{\omega}_{\lambda k}(t)}\rho^I(t)]$$

$$+\frac{ie}{\hbar}Tr_{S\otimes R}[\sum g^*_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(t)}ce_{\lambda k}\rho^I(t)] \qquad (4.2.9)$$

After some calculation and simplification (see Appendix 6 for details), the current then becomes:

$$I_\lambda=\frac{ie}{\hbar}Tr_S[-\sum_k g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(t)}c^+Tr_R(d_{\lambda k}\rho^I(t))]$$

$$+\frac{ie}{\hbar}Tr_S[-\sum_k g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(t)}c^+Tr_R(\rho^I(t)e^+_{\lambda k})]$$

$$+\frac{ie}{\hbar}Tr_S[\sum_k g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}}ce^{i\overline{\omega}_{\lambda k}(t)}Tr_R(\rho^I(t)d^+_{\lambda k})]$$

$$+\frac{ie}{\hbar}Tr_S[\sum g^*_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(t)}cTr_R(e_{\lambda k}\rho^I(t))]$$

So next we need to deal with the terms $Tr_R(d_{\lambda k}\rho^I(t))$, $Tr_R(\rho^I(t)e^+_{\lambda k})$, $Tr_R(\rho^I(t)d^+_{\lambda k})$, $Tr_R(e_{\lambda k}\rho^I(t))$. We leave it in Appendix 7 and only list the results of them:

$$Tr_R(d_{\lambda k}\rho^I(t)) = M[z_{\lambda k}P_t], \tag{4.2.10}$$

$$Tr_R(\rho^I(t)d^+_{\lambda k}) = -M[P_t z^*_{\lambda k}], \tag{4.2.11}$$

$$Tr_R(e_{\lambda k}\rho^I(t)) = M[w_{\lambda k}P_t], \tag{4.2.12}$$

$$Tr_R(\rho^I(t)e^+_{\lambda k}) = -M[P_t w^*_{\lambda k}]. \tag{4.2.13}$$

So the current formula becomes:

$$I_\lambda = \frac{ie}{\hbar}Tr_S[-\sum_k g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(t)}c^+M[z_{\lambda k}P_t]]$$

$$-\frac{ie}{\hbar}Tr_S[-\sum_k g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(t)}c^+M[P_t w^*_{\lambda k}]]$$

$$-\frac{ie}{\hbar}Tr_S[\sum_k g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}}ce^{i\overline{\omega}_{\lambda k}(t)}M[P_t z^*_{\lambda k}]]$$

$$+\frac{ie}{\hbar}Tr_S[\sum g^*_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(t)}cM[w_{\lambda k}P_t]] \qquad (4.2.14)$$

Through Eq. (2.3.31) and Eq. (2.3.32), Eq. (4.2.14) becomes:

$$I_\lambda = -\frac{e}{\hbar}Tr_S[c^+M[z_\lambda(t)P_t]] - \frac{e}{\hbar}Tr_S[c^+M[P_t w^*_\lambda(t)]] + \frac{e}{\hbar}Tr_S[cM[P_t z^*_\lambda(t)]] + \frac{e}{\hbar}Tr_S[cM[w_\lambda(t)P_t]].$$

Here, we are not willing to deal with the annoying noise term $M[z_\lambda(t)P_t]$, $M[P_t w^*_\lambda(t)]$, $M[P_t z^*_\lambda(t)]$, $M[w_\lambda(t)P_t]$. Instead, we use Novikov theorem to transform these terms into other terms with $O$ operator, that is, we transform the current formula into:

$$I_\lambda = -\frac{e}{\hbar}Tr_S[c^+M[\overline{O}_{\lambda 1}P_t]] + \frac{e}{\hbar}Tr_S[c^+M[P_t\overline{O}^+_{\lambda 2}]] - \frac{e}{\hbar}Tr_S[cM[P_t\overline{O}^+_{\lambda 1}]] + \frac{e}{\hbar}Tr_S[cM[\overline{O}_{\lambda 2}P_t]]. \qquad (4.2.15)$$

In Eq. (4.2.15), we know that $\overline{O}_{\lambda n}(t, z^*, w^*) \equiv \int_0^t \alpha_{\lambda n}(t,s)O_{\lambda n}(t,s,z^*,w^*)ds$, $\overline{O}^+_{\lambda n} = \overline{O}^+_{\lambda n}(t,-z,-w) \equiv \int_0^t \alpha^*_{\lambda n}(t,s)O^+_{\lambda n}(t,s,-z,-w)ds$, $O^+_{\lambda n} = O^+_{\lambda n}(t,s,-z,-w)$ $n = 1$ , 2. As a result,

$$M[\overline{O}_{\lambda n}P_t]$$

$$= \int dz^2 dw^2 e^{-z^2-w^2}\int_0^t \alpha_{\lambda n}(t,s)O_{\lambda n}(t,s,z^*,w^*)dsP_t$$

$$= \int_0^t \alpha_{\lambda n}(t,s)M[O_{\lambda n}P_t]ds. \qquad (4.2.16)$$

$$M[P_t\overline{O}^{+}_{\lambda n}]$$

$$= \int dz^2 dw^2 e^{-z^2-w^2} P_t \int_0^t \alpha^*_{\lambda n}(t,s) O^{+}_{\lambda n}(t,s,-z,-w) ds$$

$$= \int_0^t \alpha^*_{\lambda n}(t,s) M[P_t O^{+}_{\lambda n}] ds. \tag{4.2.17}$$

Now we define $M[O_{\lambda n}(t,s,z^*,w^*)P_t]$ as $Q_{\lambda n}(t,s)$ and $Q^{+}_{\lambda n}(t,s) = M[P_t O^{+}_{\lambda n}(t,s,-z,-w)]$. After we define $Q$ operator, we jump to Eq. (2.4.7) and Eq. (2.4.8) and discover that $O_{R1}$ and $O_{L1}$ have the same time evolution equation. Besides, $O_{R1}$ and $O_{L1}$ have the same initial condition: $O_{R1}(t,t,z^*,w^*) = O_{L1}(t,t,z^*,w^*) = \frac{c}{\hbar}$ [15]. As a consequence, we can conclude that $O_{R1} = O_{L1} = O_1$ by the uniqueness of the solution of the differential equation. Likewise, for the sake of the initial condition $O_{R2}(t,t,z^*,w^*) = O_{L2}(t,t,z^*,w^*) = \frac{c^+}{\hbar}$ [15] and the same time evolution equations of $O_{R2}$ and $O_{L2}$. we can derive the same conclusion that $O_{R2} = O_{L2} = O_2$. By the above argument, we can simplify: $Q_1(t,s) = M[O_1(t,s,z^*,w^*)P_t]$ , $Q_2(t,s) = M[O_2(t,s,z^*,w^*)P_t]$ and $Q^{+}_1(t,s) = M[P_t O^{+}_1(t,s,-z,-w)]$ , $Q^{+}_2(t,s) = M[P_t O^{+}_2(t,s,-z,-w)]$. In the final step in this section, we get the current formula after numerous calculation:

$$I_\lambda = -\frac{e}{\hbar} Tr_S[c^+ \int_0^t \alpha_{\lambda 1}(t,s) Q_1(t,s) ds] + \frac{e}{\hbar} Tr_S[c^+ \int_0^t \alpha^*_{\lambda 2}(t,s) Q^{+}_2(t,s) ds]$$

$$-\frac{e}{\hbar} Tr_S[c \int_0^t \alpha^*_{\lambda 1}(t,s) Q^{+}_1(t,s) ds] + \frac{e}{\hbar} Tr_S[c \int_0^t \alpha_{\lambda 2}(t,s) Q_2(t,s) ds]. \tag{4.2.18}$$

The unknown part of Eq. (4.2.18) is the $Q$ operator. Fortunately, in [15], we find that the $Q$ operator is as follows:

$$\hbar Q_1(t,s) = A^*_1(t,s) c \rho(t) + A^*_2(t,s) \rho(t) c, \tag{4.2.19}$$

$$\hbar Q_2(t,s) = B_1(t,s)\rho(t)c^+ + B_2(t,s)c^+\rho(t). \tag{4.2.20}$$

The $A_1$, $A_2$, $B_1$, $B_2$ are the undetermined coefficients. We then substitute Eq. (4.2.19) and Eq. (4.2.20) into Eq. (4.2.18):

$$I_\lambda(t) = -\frac{e}{\hbar^2}\Gamma^*_{\lambda 1}(t)Tr_S[c^+c\rho(t)] - \frac{e}{\hbar^2}\Gamma^*_{\lambda 2}(t)Tr_S[c^+\rho(t)c] - \frac{e}{\hbar^2}\Gamma_{\lambda 1}(t)Tr_S[c\rho(t)c^+] - \frac{e}{\hbar^2}\Gamma_{\lambda 2}(t)Tr_S[cc^+\rho(t)]. \tag{4.2.21}$$

where the time-dependent coefficients are:

$$\Gamma_{\lambda 1}(t) = \int_0^t (\alpha^*_{\lambda 1}(t,s)A_1(t,s) - \alpha_{\lambda 2}(t,s)B_1(t,s))ds, \tag{4.2.22}$$

$$\Gamma_{\lambda 2}(t) = \int_0^t (\alpha^*_{\lambda 1}(t,s)A_2(t,s) - \alpha_{\lambda 2}(t,s)B_2(t,s))ds. \tag{4.2.23}$$

The trace over system degrees of freedom can be easily evaluated:

$$Tr_S[c^+c\rho(t)] = \sum_n \langle n| c^+c\rho(t) |n\rangle = \langle 0| c^+c\rho(t) |0\rangle + \langle 1| c^+c\rho(t) |1\rangle$$

$$= 0 + \langle 1| \rho(t) |1\rangle$$

$$= \rho_{11}(t), \tag{4.2.24}$$

$$Tr_S[c^+\rho(t)c] = Tr_S[cc^+\rho(t)] = \sum_n \langle n| cc^+\rho(t) |n\rangle = \langle 0| cc^+\rho(t) |0\rangle + \langle 1| cc^+\rho(t) |1\rangle$$

$$= \langle 0| \rho(t) |0\rangle + 0$$

$$= \rho_{00}(t), \tag{4.2.25}$$

$$Tr_S[c\rho(t)c^+] = Tr_S[c^+c\rho(t)] = \rho_{11}(t), \tag{4.2.26}$$

$$Tr_S[cc^+\rho(t)] = \rho_{00}(t). \tag{4.2.27}$$

Thus we can get the simplified current formula as:

$$I_\lambda(t) = -\frac{e}{\hbar^2}(\Gamma_{\lambda 1}(t) + \Gamma^*_{\lambda 1}(t))\rho_{11}(t) - \frac{e}{\hbar^2}(\Gamma_{\lambda 2}(t) + \Gamma^*_{\lambda 2}(t))\rho_{00}(t). \tag{4.2.28}$$

Besides Eq. (4.2.28), we can also bring Eq. (4.2.19) and Eq. (4.2.20) into the master equation of Eq. (3.2.6) and get the simpler form of Eq. (3.2.6):

$$\frac{\partial\rho(t)}{\partial t} = \frac{-i}{\hbar}[H_S(t), \rho(t)] + \frac{1}{\hbar^2}\sum_\lambda \Gamma_{\lambda 1}(t)[c, \rho(t)c^+] - \frac{1}{\hbar^2}\sum_\lambda \Gamma^*_{\lambda 1}(t)[c^+, c\rho(t)]$$

$$+\frac{1}{\hbar^2}\sum_\lambda \Gamma_{\lambda 2}(t)[c, c^+\rho(t)] - \frac{1}{\hbar^2}\sum_\lambda \Gamma^*_{\lambda 2}(t)[c^+, \rho(t)c]. \tag{4.2.29}$$

The first term in Eq. (4.2.29) is the free evolution of the system and other terms are caused by the interaction with the baths. The memory effects of the baths are embedded in the time-dependent coefficients $\Gamma_{\lambda 1}(t)$ , $\Gamma_{\lambda 2}(t)$. This is the case because $\Gamma_{\lambda 1}(t)$ , $\Gamma_{\lambda 2}(t)$ are integrals including all the history of the baths.

## 4.3 Heisenberg Approach to the $O_n$ Operator

In section 2.3.2, we learn that the total state of the system plus the bath is factorized: $|\Psi_t(0)\rangle = |\psi_0\rangle \otimes |0\rangle$ and $\langle zw\, |\Psi_t(t)\rangle = \langle zw| \, U_t \, |\Psi_t(0)\rangle = (\langle zw| \, U_t \, |0\rangle) \, |\psi_0\rangle$. $U_t$ is the time evolution operator at time $t$ of the total system. Here we define $G_t(z^*, w^*) = \langle zw| \, U_t \, |0\rangle$ as the stochastic propagator for the state $|\phi(t, z^*, w^*)\rangle$. Our mathod is that we first want to prove that:

$$\langle zw| \, U_t c^+(s) \, |0\rangle = \hbar O_2(t, s, z^*, w^*) G_t(z^*, w^*), \tag{4.3.1}$$

$$\langle zw| \, U_t c(s) \, |0\rangle = \hbar O_1(t, s, z^*, w^*) G_t(z^*, w^*). \tag{4.3.2}$$

Here, $c(s) \equiv U_s^+ c U_s$, $c^+(s) = U_s^+ c^+ U_s$. Next, we take the differentiation of Eq. (4.3.1) and Eq. (4.3.2) with respect to time $s$ and get the new time evolution equation of $O_1$ and $O_2$. To achieve this goal, we first find the time evolution equation of $G_t(z^*, w^*)$.

### 4.3.1 The Time Evolution of $G_t(z^*, w^*)$

The time evolution of $G_t$ is:

$$i\hbar \frac{\partial G_t}{\partial t} = i\hbar \, \langle zw| \, \frac{\partial U_t}{\partial t} \, |0\rangle \, .$$

By the Schrödinger-like equation in the bath interaction picture: $i\hbar \frac{\partial U_t |\Psi_t(0)\rangle}{\partial t} = i\hbar \frac{\partial U_t}{\partial t} \, |\Psi_t(0)\rangle = H_T(t) U_t \, |\Psi_t(0)\rangle \rightarrow i\hbar \frac{\partial U_t}{\partial t} = H_T(t) U_t$,

$$i\hbar \frac{\partial G_t}{\partial t} = \langle zw| \, H_T(t) U_t \, |0\rangle$$

$$= H_S G_t + \sum_{\lambda k} (g_{\lambda k}(t)\sqrt{1-n_{\lambda k}} c^+ e^{-i\varpi_{\lambda k}(t)} \langle zw| d_{\lambda k} U_t |0\rangle + \sum_{\lambda k} g_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{-i\varpi_{\lambda k}(t)} w^*_{\lambda k} c^+ G_t$$

$$+ \sum_{\lambda k} g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}} e^{i\varpi_{\lambda k}(t)} z^*_{\lambda k} c G_t + \sum_{\lambda k} g^*_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{i\varpi_{\lambda k}(t)} c \langle zw| e_{\lambda k} U_t |0\rangle . \quad (4.3.3)$$

In order to get the time evolution equation of $G_t$ with only $G_t$ term rather than $\langle zw| d_{\lambda k} U_t |0\rangle$ and $\langle zw| e_{\lambda k} U_t |0\rangle$, we need to transform them. The transformation techinique is as follows.

First, we define $d_{\lambda k}(t) \equiv U_t^+ d_{\lambda k} U_t$ and $e_{\lambda k}(t) \equiv U_t^+ e_{\lambda k} U_t$ and differentiate them:

$$i\hbar \frac{\partial d_{\lambda k}(t)}{\partial t} = i\hbar (\frac{\partial U_t^+}{\partial t}) d_{\lambda k} U_t + i\hbar U_t^+ d_{\lambda k} (\frac{\partial U_t}{\partial t})$$

$$= U_t^+ [d_{\lambda k} \, , \, H_T] U_t$$

$$= g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}} e^{i\varpi_{\lambda k}(t)} c(t), \quad (4.3.4)$$

$$i\hbar \frac{\partial e_{\lambda k}(t)}{\partial t} = U_t^+ [e_{\lambda k} \, , \, H_T] U_t$$

$$= g_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{-i\varpi_{\lambda k}(t)} c^+(t). \quad (4.3.5)$$

Eq. (4.3.3) is thus converted to:

$$i\hbar\frac{\partial G_t}{\partial t} = H_S G_t + \sum_{\lambda k}(g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+ e^{-i\overline{\omega}_{\lambda k}(t)}\langle zw| U_t d_{\lambda k}(t)|0\rangle - \sum_{\lambda k} g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(t)}c^+ w^*_{\lambda k}G_t$$

$$-\sum_{\lambda k} g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(t)}cz^*_{\lambda k}G_t + \sum_{\lambda k} g^*_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(t)}c\langle zw| U_t e_{\lambda k}(t)|0\rangle . \quad (4.3.6)$$

Second, we integrate Eq. (4.3.4) and Eq. (4.3.5):

$$d_{\lambda k}(t) = d_{\lambda k} - \frac{i}{\hbar}\int_0^t g^*_{\lambda k}(s)\sqrt{1-n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(s)}c(s)ds, \quad (4.3.7)$$

$$e_{\lambda k}(t) = e_{\lambda k} - \frac{i}{\hbar}\int_0^t g_{\lambda k}(s)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(s)}c^+(s)ds. \quad (4.3.8)$$

Equations (4.3.7) and (4.3.8) are what we exactly want for the reason that $d_{\lambda k}(e_{\lambda k})|0\rangle = 0$. We then put Eq. 4.3.7 and Eq. 4.3.8 into Eq. 4.3.6 and get:

$$i\hbar\frac{\partial G_t}{\partial t} = H_S G_t - \frac{i}{\hbar}c^+\sum_{\lambda}\int_0^t(\alpha_{\lambda 1}(t,s)\langle zw| U_t c(s)|0\rangle)ds$$

$$-i\sum_{\lambda}c^+ w^*_{\lambda}(t)G_t - i\sum_{\lambda}cz^*_{\lambda}(t)G_t$$

$$-\frac{i}{\hbar}c\sum_{\lambda}\int_0^t(\alpha_{\lambda 2}\langle zw| U_t c^+(s)|0\rangle)ds. \quad (4.3.9)$$

Here, $\overline{\omega}_{\lambda k}(t-s) \equiv \overline{\omega}_{\lambda k}(t) - \overline{\omega}_{\lambda k}(s)$. We know that $G_t \equiv \langle zw| U_t|0\rangle$, $|\phi\rangle = \langle zw| U_t|0\rangle|\psi_0\rangle$. Hence, $i\hbar\frac{\partial|\phi\rangle}{\partial t} = i\hbar\frac{\partial G_t}{\partial t}|\psi_0\rangle$. By comparing Eq. (2.4.9) and Eq. (4.3.9), we can immediately obtain Eq. (4.3.1) and Eq. (4.3.2):

$$\langle zw| U_t c(s) |0\rangle = \hbar O_1(t,s,z^*,w^*) G_t(z^*,w^*),$$

$$\langle zw| U_t c^+(s) |0\rangle = \hbar O_2(t,s,z^*,w^*) G_t(z^*,w^*).$$

A noted point in Eq. (4.3.1) and Eq. (4.3.2) is that if $s = t$, we find that:

$$c \langle zw| U_t |0\rangle = \hbar O_1(t,t,z^*,w^*) G_t(z^*,w^*),$$

$$c^+ \langle zw| U_t |0\rangle = \hbar O_2(t,t,z^*,w^*) G_t(z^*,w^*).$$

Because $\langle zw| U_t |0\rangle = G_t$, we can immediately get: $\hbar O_1(t,t,z^*,w^*) = c$ and $\hbar O_2(t,t,z^*,w^*) = c^+$. These are exactly the initial conditions in section 4.2.

### 4.3.2 The Time Evolution Equation of $O_1(t,s,z^*,w^*)$

We first differentiate Eq. (4.3.2) with respect to time $s$ and will get the time evolution equation of operator $O_1$ later.

$$\langle zw| U_t \frac{\partial c(s)}{\partial s} |0\rangle = \hbar \frac{\partial O_1(t,s,z^*,w^*)}{\partial s} G_t(z^*,w^*)$$

$$\frac{\partial c(s)}{\partial s} = \frac{\partial}{\partial s}(U_s^+ c U_s) = \frac{\partial U_s^+}{\partial s} c U_s + U_s^+ c \frac{\partial U_s}{\partial s} = \frac{i}{\hbar} U_s^+ [H_T(s), c] U_s.$$

Here $H_T(s) = \hbar\omega_S(s)c^+c + \sum_{\lambda k}(g_{\lambda k}(s)\sqrt{1-n_{\lambda k}}e^{-i\varpi_{\lambda k}(s)}c^+ d_{\lambda k} + g_{\lambda k}(s)\sqrt{n_{\lambda k}}e^{-i\varpi_{\lambda k}(s)}e_{\lambda k}^+ c^+ + g_{\lambda k}^*(s)\sqrt{1-n_{\lambda k}}e^{i\varpi_{\lambda k}(s)}d_{\lambda k}^+ c + g_{\lambda k}^*(s)\sqrt{n_{\lambda k}}e^{i\varpi_{\lambda k}(s)} c e_{\lambda k})$ and

$$[c^+c, c] = -c,$$

$$[c^+ d_{\lambda k}, c] = -d_{\lambda k},$$

$$[e^+_{\lambda k} c^+, c] = e^+_{\lambda k},$$

$$[d^+_{\lambda k} c, c] = [c e_{\lambda k}, c] = 0.$$

So,

$$\frac{\partial c(s)}{\partial s} = \frac{i}{\hbar} U_s^+ (-\hbar\omega_S(s) c + \sum_{\lambda k} (-g_{\lambda k}(s)\sqrt{1-n_{\lambda k}} e^{-i\varpi_{\lambda k}(s)} d_{\lambda k} + g_{\lambda k}(s)\sqrt{n_{\lambda k}} e^{-i\varpi_{\lambda k}(s)} e^+_{\lambda k})) U_s$$

$$= -i\omega_S(s) c(s) + \frac{i}{\hbar}\sum_{\lambda k}(-g_{\lambda k}(s)\sqrt{1-n_{\lambda k}} e^{-i\varpi_{\lambda k}(s)} d_{\lambda k}(s) + g_{\lambda k}(s)\sqrt{n_{\lambda k}} e^{-i\varpi_{\lambda k}(s)} e^+_{\lambda k}(s)). \tag{4.3.10}$$

$$\langle zw| U_t \frac{\partial c(s)}{\partial s} |0\rangle = \hbar \frac{\partial O_1}{\partial s} G_t = -i\omega_S(s) \langle zw| U_t c(s) |0\rangle$$

$$-\frac{i}{\hbar}\sum_{\lambda k} g_{\lambda k}(s)\sqrt{1-n_{\lambda k}} e^{-i\varpi_{\lambda k}(s)} \langle zw| U_t d_{\lambda k}(s) |0\rangle + \frac{i}{\hbar}\sum_{\lambda k} g_{\lambda k}(s)\sqrt{n_{\lambda k}} e^{-i\varpi_{\lambda k}(s)} \langle zw| U_t e^+_{\lambda k}(s) |0\rangle \tag{4.3.11}$$

By the same technique in obtaining Eq. (4.3.7) and Eq. (4.3.8), we have

$$d_{\lambda k}(s) = d_{\lambda k} - \frac{i}{\hbar}\int_0^s g^*_{\lambda k}(s^{'})\sqrt{1-n_{\lambda k}} e^{i\varpi_{\lambda k}(s^{"})} c(s^{'}) ds^{'}, \tag{4.3.12}$$

$$e^{+}_{\lambda k}(t) = e^{+}_{\lambda k}(s) + \frac{i}{\hbar}\int_s^t g^*_{\lambda k}(s^{'})\sqrt{n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(s^{'})}c(s^{'})ds^{'}. \quad (4.3.13)$$

Then we put Eq. (4.3.12) and Eq. (4.3.13) into Eq. (4.3.11), replace $\langle zw|\, U_t c(s^{'})\,|0\rangle$ by $\hbar O_1(t, s^{'}, z^*, w^*)G_t$ and get:

$$\hbar\frac{\partial O_1}{\partial s}G_t = -i\hbar\omega_S(s)O_1G_t - \frac{1}{\hbar}\sum_{\lambda k}(1-n_{\lambda k})\int_0^s g_{\lambda k}(s)g^*_{\lambda k}(s^{'})e^{-i\overline{\omega}_{\lambda k}(s-s^{'})}O_1(t, s^{'}, z^*, w^*)ds^{'}G_t$$

$$+\frac{i}{\hbar}\sum_{\lambda k} g_{\lambda k}(s)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(s)}\langle zw|\, U_t(e^{+}_{\lambda k}(t) - \frac{i}{\hbar}\int_s^t g^*_{\lambda k}(s^{'})\sqrt{n_{\lambda k}}e^{i\overline{\omega}_{\lambda k}(s^{'})}c(s^{'})ds^{'})\,|0\rangle$$

$$= -i\hbar\omega_S(s)O_1G_t - \frac{1}{\hbar}\sum_{\lambda k}(1-n_{\lambda k})\int_0^s g_{\lambda k}(s)g^*_{\lambda k}(s^{'})e^{-i\overline{\omega}_{\lambda k}(s-s^{'})}O_1(t, s^{'}, z^*, w^*)ds^{'}G_t$$

$$+\frac{i}{\hbar}\sum_{\lambda k} g_{\lambda k}(s)\sqrt{n_{\lambda k}}e^{-i\overline{\omega}_{\lambda k}(s)}w^*_{\lambda k}G_t + \frac{1}{\hbar}\sum_{\lambda k}\int_s^t g_{\lambda k}(s)g^*_{\lambda k}(s^{'})n_{\lambda k}e^{-i\overline{\omega}_{\lambda k}(s-s^{'})}O_1(t, s^{'}, z^*, w^*)ds^{'}G_t$$

Finally, we arrive at the time evolution equation of $O_1$:

$$\frac{\partial O_1}{\partial s} = -i\omega_S(s)O_1 - \frac{1}{\hbar^2}\sum_{\lambda} w^*_{\lambda}(s) - \frac{1}{\hbar^2}\sum_{\lambda}\int_0^s \alpha_{\lambda 1}(s, s^{'})O_1(t, s^{'}, z^*, w^*)ds^{'}$$

$$+\frac{1}{\hbar^2}\sum_{\lambda}\int_s^t \alpha_{\lambda 2}(s^{'}, s)O_1(t, s^{'}, z^*, w^*)ds^{'}. \quad (4.3.14)$$

### 4.3.3 The Time Evolution Equation of $O_2(t, s, z^*, w^*)$

We first differentiate Eq. (4.3.1) with respect to time $s$ and will get the time evolution equation of operator $O_2$.

$$\langle zw| U_t \frac{\partial c^+(s)}{\partial s} |0\rangle = \hbar \frac{\partial O_2(t, s, z^*, w^*)}{\partial s} G_t(z^*, w^*)$$

$$\frac{\partial c^+(s)}{\partial s} = (\frac{\partial c(s)}{\partial s})^+$$

$$= i\omega_S(s)c^+(s) + \frac{i}{\hbar}\sum_{\lambda k}(g^*_{\lambda k}(s)\sqrt{1-n_{\lambda k}}e^{i\varpi_{\lambda k}(s)}d^+_{\lambda k}(s) - g^*_{\lambda k}(s)\sqrt{n_{\lambda k}}e^{i\varpi_{\lambda k}(s)}e_{\lambda k}(s)). \tag{4.3.15}$$

$$\langle zw| U_t \frac{\partial c^+(s)}{\partial s} |0\rangle = \hbar \frac{\partial O_2}{\partial s} G_t = i\omega_S(s) \langle zw| U_t c^+(s) |0\rangle$$

$$+\frac{i}{\hbar}\sum_{\lambda k} g^*_{\lambda k}(s)\sqrt{1-n_{\lambda k}}e^{i\varpi_{\lambda k}(s)} \langle zw| U_t d^+_{\lambda k}(s) |0\rangle - \frac{i}{\hbar}\sum_{\lambda k} g^*_{\lambda k}(s)\sqrt{n_{\lambda k}}e^{i\varpi_{\lambda k}(s)} \langle zw| U_t e_{\lambda k}(s) |0\rangle \tag{4.3.16}$$

By the same technique in obtaining Eq. (4.3.7) and Eq. (4.3.8), we get

$$e_{\lambda k}(s) = e_{\lambda k} - \frac{i}{\hbar}\int_0^s g_{\lambda k}(s')\sqrt{n_{\lambda k}}e^{-i\varpi_{\lambda k}(s")}c^+(s')ds', \tag{4.3.17}$$

$$d^+_{\lambda k}(t) = d^+_{\lambda k}(s) + \frac{i}{\hbar}\int_s^t g_{\lambda k}(s')\sqrt{1-n_{\lambda k}}e^{-i\varpi_{\lambda k}(s')}c^+(s')ds'. \tag{4.3.18}$$

Then, we put Eq. (4.3.17) and Eq. (4.3.18) into Eq. (4.3.16), replace $\langle zw| U_t c^+(s') |0\rangle$ by $\hbar O_2(t, s', z^*, w^*)G_t$ and get:

$$\hbar\frac{\partial O_2}{\partial s}G_t = i\hbar\omega_S(s)O_2G_t - \frac{1}{\hbar}\sum_{\lambda k} n_{\lambda k}\int_0^s g^*_{\lambda k}(s)g_{\lambda k}(s^{'})e^{i\varpi_{\lambda k}(s-s^{'})}O_2(t,s^{'},z^*,w^*)ds^{'}G_t$$

$$+\frac{i}{\hbar}\sum_{\lambda k} g^*_{\lambda k}(s)\sqrt{1-n_{\lambda k}}e^{i\varpi_{\lambda k}(s)}\left\langle zw\right| U_t(d^+_{\lambda k}(t) - \frac{i}{\hbar}\int_s^t g_{\lambda k}(s^{'})\sqrt{1-n_{\lambda k}}e^{-i\varpi_{\lambda k}(s^{'})}c^+(s^{'})ds^{'})\left|0\right\rangle$$

$$= i\hbar\omega_S(s)O_2G_t - \frac{1}{\hbar}\sum_{\lambda k} n_{\lambda k}\int_0^s g^*_{\lambda k}(s)g_{\lambda k}(s^{'})e^{i\varpi_{\lambda k}(s-s^{'})}O_2(t,s^{'},z^*,w^*)ds^{'}G_t$$

$$+\frac{i}{\hbar}\sum_{\lambda k} g^*_{\lambda k}(s)\sqrt{1-n_{\lambda k}}e^{i\varpi_{\lambda k}(s)}z^*_{\lambda k}G_t + \frac{1}{\hbar}\sum_{\lambda k}\int_s^t g^*_{\lambda k}(s)g_{\lambda k}(s^{'})(1-n_{\lambda k})e^{i\varpi_{\lambda k}(s-s^{'})}O_2(t,s^{'},z^*,w^*)ds^{'}G_t$$

Finally, we arrive at the time evolution equation of $O_2$ by the same technique as $O_1$:

$$\frac{\partial O_2}{\partial s} = i\omega_S(s)O_2 - \frac{1}{\hbar^2}\sum_{\lambda} z^*_{\lambda}(s) - \frac{1}{\hbar^2}\sum_{\lambda}\int_0^s \alpha_{\lambda 2}(s,s^{'})O_2(t,s^{'},z^*,w^*)ds^{'}$$

$$+\frac{1}{\hbar^2}\sum_{\lambda}\int_s^t \alpha_{\lambda 1}(s^{'},s)O_2(t,s^{'},z^*,w^*)ds^{'}. \qquad (4.3.19)$$

## 4.4 Time Evolution of Undetermined Coefficients $A_1, A_2, B_1, B_2$

We made the assumption of Eq. (4.2.19) and Eq. (4.2.20),

$$\hbar Q_1(t,s) = A^*_1(t,s)c\rho(t) + A^*_2(t,s)\rho(t)c,$$

$$\hbar Q_2(t,s) = B_1(t,s)\rho(t)c^+ + B_2(t,s)c^+\rho(t).$$

If we want to know the time evolution equation of $A_1$, $A_2$, $B_1$, $B_2$, we need to find the time evolution of $Q_1$ and $Q_2$ first. It is not a difficult task for the reason that we have now the time evolution of $O_1$, $O_2$, and $Q_1(t,s) = M[O_1(t,s,z^*,w^*)P_t]$, $Q_2(t,s) = M[O_2(t,s,z^*,w^*)P_t]$ actually.

The time evolution equations of $Q_1$ and $Q_2$ are:

$$\frac{\partial Q_1}{\partial s} = M[\frac{\partial O_1}{\partial s}P_t]$$

$$= -i\omega_S(s)Q_1 + \frac{1}{\hbar^2}\sum_\lambda \int_s^t \alpha_{\lambda 2}(s',s)Q_1(t,s')ds' - \frac{1}{\hbar^2}\sum_\lambda \int_0^s \alpha_{\lambda 1}(s,s')Q_1(t,s')ds' - \frac{1}{\hbar^2}\sum_\lambda M[w_\lambda^*(s)P_t], \tag{4.4.1}$$

$$\frac{\partial Q_2}{\partial s} = M[\frac{\partial O_2}{\partial s}P_t]$$

$$= i\omega_S(s)Q_2 + \frac{1}{\hbar^2}\sum_\lambda \int_s^t \alpha_{\lambda 1}(s',s)Q_2(t,s')ds' - \frac{1}{\hbar^2}\sum_\lambda \int_0^s \alpha_{\lambda 2}(s,s')Q_2(t,s')ds' - \frac{1}{\hbar^2}\sum_\lambda M[z_\lambda^*(s)P_t]. \tag{4.4.2}$$

We use Novikov theorem to deal with $M[w_\lambda^*(s)P_t]$, $M[z_\lambda^*(s)P_t]$:

$$M[z_\lambda^*(s)P_t] = -M[P_t\widetilde{\overline{O}}{}_{\lambda 1}^{+}(t,s,-z,-w)], \tag{4.4.3}$$

$$M[w_\lambda^*(s)P_t] = -M[P_t\widetilde{\overline{O}}{}_{\lambda 2}^{+}(t,s,-z,-w)]. \tag{4.4.4}$$

Here $\widetilde{\overline{O}}{}_{\lambda 1}^{+}(t,s,-z,-w) = \int_0^t \alpha_{\lambda 1}^*(s,s')O_1^+(t,s',-z,-w)ds'$ and $\widetilde{\overline{O}}{}_{\lambda 2}^{+}(t,s,-z,-w) =$

$\int_0^t \alpha^*_{\lambda 2}(s,s^{'})O_2^{+}(t,s^{'},-z,-w)ds^{'}$. The proof of Eq. (4.4.3) and Eq. (4.4.4) is similar to the proof in section 5.5. We note that the time in $z^*_\lambda(s)$ , $w^*_\lambda(s)$ is $s$. Thus the correlation functions inside the integrals are $\alpha^*_{\lambda 1}(s,s^{'})$ and $\alpha^*_{\lambda 2}(s,s^{'})$, respectively. By Eq. (4.4.3) and Eq. (4.4.4), we can simplify Eq. (4.4.1) and Eq. (4.4.2) as :

$$\frac{\partial Q_1}{\partial s} = -i\omega_S(s)Q_1 + \frac{1}{\hbar^2}\sum_\lambda \int_s^t \alpha_{\lambda 2}(s^{'},s)Q_1(t,s^{'})ds^{'}$$

$$-\frac{1}{\hbar^2}\sum_\lambda \int_0^s \alpha_{\lambda 1}(s,s^{'})Q_1(t,s^{'})ds^{'} + \frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha^*_{\lambda 2}(s,s^{'})Q_2^{+}(t,s^{'}), \tag{4.4.5}$$

$$\frac{\partial Q_2}{\partial s} = i\omega_S(s)Q_2 + \frac{1}{\hbar^2}\sum_\lambda \int_s^t \alpha_{\lambda 1}(s^{'},s)Q_2(t,s^{'})ds^{'}$$

$$-\frac{1}{\hbar^2}\sum_\lambda \int_0^s \alpha_{\lambda 2}(s,s^{'})Q_2(t,s^{'})ds^{'} + \frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha^*_{\lambda 1}(s,s^{'})Q_1^{+}(t,s^{'})ds^{'}. \tag{4.4.6}$$

Next we take Eq. (4.2.19) and Eq. (4.2.20) into Eq. (4.4.5) and (4.4.6) respectively and obtain

$$\frac{\partial A_1^*(t,s)}{\partial s}c\rho(t) + \frac{\partial A_2^*(t,s)}{\partial s}\rho(t)c = -i\omega_S(s)(A_1^*(t,s)c\rho(t) + A_2^*(t,s)\rho(t)c)$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_s^t \alpha_{\lambda 2}(s^{'},s)(A_1^*(t,s^{'})c\rho(t) + A_2^*(t,s^{'})\rho(t)c)ds^{'}$$

$$-\frac{1}{\hbar^2}\sum_\lambda \int_0^s \alpha_{\lambda 1}(s,s^{'})(A_1^*(t,s^{'})c\rho(t) + A_2^*(t,s^{'})\rho(t)c)ds^{'}$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha^*_{\lambda 2}(s,s^{'})(B_1^*(t,s^{'})c\rho(t) + B_2^*(t,s^{'})\rho(t)c)ds^{'}, \tag{4.4.7}$$

$$\frac{\partial B_1(t,s)}{\partial s}\rho(t)c^+ + \frac{\partial B_2(t,s)}{\partial s}c^+\rho(t) = i\omega_S(s)(B_1(t,s)\rho(t)c^+ + B_2(t,s)c^+\rho(t))$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_s^t \alpha_{\lambda 1}(s^{'},s)(B_1(t,s^{'})\rho(t)c^+ + B_2(t,s^{'})c^+\rho(t))ds^{'}$$

$$-\frac{1}{\hbar^2}\sum_\lambda \int_0^s \alpha_{\lambda 2}(s,s^{'})(B_1(t,s^{'})\rho(t)c^+ + B_2(t,s^{'})c^+\rho(t))ds^{'}$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha^*_{\lambda 1}(s,s^{'})(A_1(t,s^{'})\rho(t)c^+ + A_2(t,s^{'})c^+\rho(t))ds^{'}. \qquad (4.4.8)$$

Since $c\rho(t)$ , $\rho(t)c$ , $\rho(t)c^+$ , $c^+\rho(t)$ are linealy independent. We can get the time evolution of $A_1$ , $A_2$ , $B_1$ , $B_2$ through the coefficients of $c\rho(t)$ , $\rho(t)c$ , $\rho(t)c^+$ , $c^+\rho(t)$.

For $Q_1$:

$c\rho(t)$:

$$\frac{\partial A_1(t,s)}{\partial s} = i\omega_S(s)A_1(t,s) - \frac{1}{\hbar^2}\sum_\lambda \int_0^s (\alpha_{\lambda 1}(s^{'},s) + \alpha_{\lambda 2}(s,s^{'}))A_1(t,s^{'})ds^{'}$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha_{\lambda 2}(s,s^{'})(B_1(t,s^{'}) + A_1(t,s^{'}))ds^{'}. \qquad (4.4.9)$$

$\rho(t)c$:

$$\frac{\partial A_2(t,s)}{\partial s} = i\omega_S(s)A_2(t,s) - \frac{1}{\hbar^2}\sum_\lambda \int_0^s (\alpha_{\lambda 1}(s^{'},s) + \alpha_{\lambda 2}(s,s^{'}))A_2(t,s^{'})ds^{'}$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha_{\lambda 2}(s,s^{'})(A_2(t,s^{'}) + B_2(t,s^{'}))ds^{'}. \qquad (4.4.10)$$

For $Q_2$:

$c^+\rho(t)$:

$$\frac{\partial B_1(t,s)}{\partial s} = i\omega_S(s)B_1(t,s) - \frac{1}{\hbar^2}\sum_\lambda \int_0^s (\alpha_{\lambda 1}(s',s) + \alpha_{\lambda 2}(s,s'))B_1(t,s')ds'$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha_{\lambda 1}(s',s)(A_1(t,s') + B_1(t,s'))ds'. \tag{4.4.11}$$

$\rho(t)c^+$:

$$\frac{\partial B_2(t,s)}{\partial s} = i\omega_S(s)B_2(t,s) - \frac{1}{\hbar^2}\sum_\lambda \int_0^s (\alpha_{\lambda 1}(s',s) + \alpha_{\lambda 2}(s,s'))B_2(t,s')ds'$$

$$+\frac{1}{\hbar^2}\sum_\lambda \int_0^t \alpha_{\lambda 1}(s',s)(A_2(t,s') + B_2(t,s'))ds'. \tag{4.4.12}$$

Finally, we get the time evolution of $A_1$, $A_2$, $B_1$, $B_2$. We have used the fact that $\alpha^*_{\lambda n}(s',s) = \alpha_{\lambda n}(s,s')$. This can be easily proved. Because the initial condition of $Q_1(t,s)$ and $Q_2(t,s)$ are:

$$Q_1(t,t) = M[O_1(t,t,z^*,w^*)P_t] = c\rho(t),$$

$$Q_2(t,t) = M[O_2(t,t,z^*,w^*)P_t] = c^+\rho(t).$$

We can get the initial condition as follows:

$$A_1(t,t) = B_2(t,t) = 1, \tag{4.4.13}$$

$$A_2(t,t) = B_1(t,t) = 0. \tag{4.4.14}$$

## 4.5 Summary

In the begining of this chapter, we start from the definition of the transient current flowing into the quantum dot. We calculate it in the Heisenberg picture for the convenience that the density operator in the Heisenberg picture is time-independent. After we calculate it in the Heisenberg picture, we transform the result back into the bath interaction picture. By the average of $d_{\lambda k}$ , $d^{+}_{\lambda k}$ , $e_{\lambda k}$ , $e^{+}_{\lambda k}$

$$Tr_R(d_{\lambda k}\rho^I(t)) = M[z_{\lambda k}P_t],$$

$$Tr_R(\rho^I(t)d^{+}_{\lambda k}) = -M[P_t z^{*}_{\lambda k}],$$

$$Tr_R(e_{\lambda k}\rho^I(t)) = M[w_{\lambda k}P_t],$$

$$Tr_R(\rho^I(t)e^{+}_{\lambda k}) = -M[P_t w^{*}_{\lambda k}],$$

and the Novikov theorem, we can get the final current form as

$$I_\lambda(t) = -\frac{e}{\hbar^2}(\Gamma_{\lambda 1}(t) + \Gamma^{*}_{\lambda 1}(t))\rho_{11}(t) - \frac{e}{\hbar^2}(\Gamma_{\lambda 2}(t) + \Gamma^{*}_{\lambda 2}(t))\rho_{00}(t). \tag{4.5.1}$$

In Eq. (4.5.1),

$$\Gamma_{\lambda 1}(t) = \int_0^t (\alpha^{*}_{\lambda 1}(t,s)A_1(t,s) - \alpha_{\lambda 2}(t,s)B_1(t,s))ds,$$

$$\Gamma_{\lambda 2}(t) = \int_0^t (\alpha^{*}_{\lambda 1}(t,s)A_2(t,s) - \alpha_{\lambda 2}(t,s)B_2(t,s))ds.$$

In section 4.3, we use Heisenberg approach to obtain another time evolution equation for $O_1$ and $O_2$. Through the time evolution equation for $O_1$ and $O_2$, we can then derive the time evolution equation of the undetermined coefficients $A_1$ , $A_2$ , $B_1$ , $B_2$. Thus both of the exact master equation and the current formula with time-dependent bias voltage, external time-dependent gate voltage and time-dependent transmission coefficient can be exactly determined.

# 5 Modeling of Time-dependent Coupling strength

## 5.1 Introduction

In section 3.3, we have introduced the effective transmission coefficent $\overline{V}_\lambda(t)$. This term will also determine the behavior of $\alpha_{\lambda 1}(t,s)$ and $\alpha_{\lambda 2}(t,s)$. Thus, we have to determine the form of $\overline{V}_\lambda(t)$. We use the barrier controlled by the gate voltage to vary $\overline{V}_\lambda(t)$. In our setup, the bias voltage, the system energy, the gate voltage are all time-dependent. For this reason, we need to calculate the tunneling problem which is not stationary. Our system contains the left lead, left barrier, central system, right barrier and right lead. The the method to calculate the effective transmission through the left barrier is the same as that for the right side. Hence we demonstrate the left part in this section. Figures 5.1.1 is a schematic illustration of our physical model. We refer to Ref. [16] as our prototype. In that paper, only the barrier is controlled by time-dependent gate voltage and the scattering wave function solved in that paper is approximated under the assumption that $\frac{\Delta}{\hbar\omega} \ll 1$, where $\Delta$ is the amplitude of the time-dependent voltage and $\omega$ is the oscillating frequency of the time-dependent voltage. In Ref. [26], the wave function and transmission coefficient is calculated by scattering matrix and Floquet theorem and the wavefunction solved in Ref. [26] is more accurate. In our model, we use the same approximation of wavefunction as in Ref. [16] with three regions controlled by time-dependent voltage.

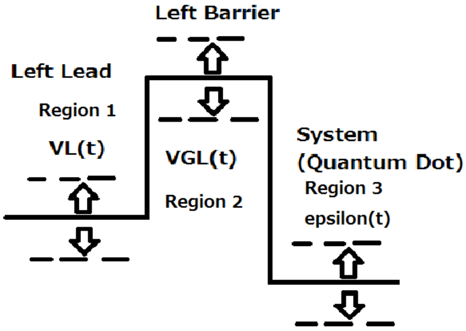


Figure 5.1.1: This is the figure of our model. The left lead region is controlled by the bias voltage. The left barrier region is controlled by the left gate voltage. The central system is controlled by the gate voltage. We only consider the left hand side of our physical model. The setup is the same as the right hand side. All the voltages are time-dependent. In the following sections, we call the left lead region1, the left barrier region2 and the system(quantum dot) region3.

## 5.2 Simple Model constructed by M. Büttiker and R. Landauer

In Ref. [16], the Hamiltonian of the barrier region is simply: $H(t) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2} + V_0 + V_1 cos(\omega t)$. By solving the Schrödinger equation: $H(t)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$, we can easily get the wavefunction $\psi(x,t,E)$

$$\psi(x,t,E) = (Be^{\kappa x} + Ce^{-\kappa x})e^{-i\frac{Et}{\hbar}}e^{-i\frac{V_1}{\hbar\omega}sin(\omega t)}. \tag{5.2.1}$$

$E$ is the incident energy. $e^{-i\frac{V_1}{\hbar\omega}sin(\omega t)}$ can be expanded as $\sum_{n=-\infty}^{\infty} J_n(\frac{V_1}{\hbar\omega})e^{-in\omega t}$ [27], where $J_n(x)$ is the Bessel function. $\psi(x,t,E)$ is thus $(Be^{\kappa x}+Ce^{-\kappa x})\sum_{n=-\infty}^{\infty} J_n(\frac{V_1}{\hbar\omega})e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}$. We can see that if the wavefunction is incident from the left lead with energy $E$, it will be transferred to another sideband $E + n\hbar\omega$. Because there are now other sidebands in the barrier $(Be^{\kappa x} + Ce^{-\kappa x})J_n(\frac{V_1}{\hbar\omega})e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}$, we need to add the term $(B_n e^{\kappa_n x} + C_n e^{-\kappa_n x})e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}$, where $\kappa_n \equiv \sqrt{\frac{2m(V_0-(E+n\hbar\omega))}{\hbar^2}}$. This is an analogy to the stationary quantum tunneling. The generation of sidebands in the barrier will produce reflected waves and transmitted waves at the energies $E+n\hbar\omega$. The general wavefunction solutions in regions 1, 2, 3: $\psi_1$ , $\psi_2$ , $\psi_3$ are, respectively,

$$\psi_1(x,t) = (e^{ikx} + Ae^{-ikx})e^{-i\frac{Et}{\hbar}} + \sum_{n=-\infty,n\neq 0}^{\infty} (A_n e^{-ik_n x} e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}), \tag{5.2.2}$$

$$\psi_2(x,t) = (Be^{\kappa x}+Ce^{-\kappa x}) \sum_{n=-\infty}^{\infty} J_n(\frac{V_1}{\hbar\omega})e^{\frac{-i(n\hbar\omega+E)t}{\hbar}} + \sum_{n=-\infty,n\neq 0}^{\infty} (B_n e^{\kappa_n x}+C_n e^{-\kappa_n x})e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}, \tag{5.2.3}$$

$$\psi_3(x,t) = De^{ikx}e^{-i\frac{Et}{\hbar}} + \sum_{n=-\infty,n\neq 0}^{\infty} (D_n e^{ik_n x} e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}), \tag{5.2.4}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$, $k_n \equiv \sqrt{\frac{2m(E+n\hbar\omega)}{\hbar^2}}$. In the model of the paper of Ref. [16], the potentials in region 1 and 3 are 0 as in Fig. 5.2.1. By the boundary condition: $\psi_1(0,t) = \psi_2(0,t)$, $\psi_2(L,t) = \psi_3(L,t)$, $\frac{\partial\psi_1(x,t)}{\partial x}|_{x=0} = \frac{\partial\psi_2(x,t)}{\partial x}|_{x=0}$, $\frac{\partial\psi_2(x,t)}{\partial x}|_{x=L} = \frac{\partial\psi_3(x,t)}{\partial x}|_{x=L}$ and the linear independence of $e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}$, we can solve the coefficients $A$ , $B$ , $C$ , $D$ , $A_n, B_n$ , $C_n$ , $D_n$. We now take a look on a simple property of Bessel function. We know from Ref. [28] that

$$J_n(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{s!(n+s)!}(\frac{x}{2})^{n+2s}, \tag{5.2.5}$$

$$J_{-n}(x) = (-1)^n J_n(x), \tag{5.2.6}$$

where $n$ is an integer. Therefore, if $\frac{V_1}{\hbar\omega} \ll 1$, $J_n(\frac{V_1}{\hbar\omega}) \approx \frac{1}{n!}(\frac{V_1}{2\hbar\omega})^n$ and $J_{-n}(\frac{V_1}{\hbar\omega}) \approx (-1)^n\frac{1}{n!}(\frac{V_1}{2\hbar\omega})^n$ for $n \geq 0$. Thus,

$$\psi_2(x,t) \approx (Be^{\kappa x} + Ce^{-\kappa x})(\sum_{n=0}^{\infty} \frac{1}{n!}(\frac{V_1}{2\hbar\omega})^n e^{\frac{-i(n\hbar\omega+E)t}{\hbar}} + \sum_{n=1}^{\infty} (-1)^n \frac{1}{n!}(\frac{V_1}{2\hbar\omega})^n e^{\frac{-i(-n\hbar\omega+E)t}{\hbar}})$$

$$+ \sum_{n=-\infty, n\neq 0}^{\infty} (B_n e^{\kappa_n x} + C_n e^{-\kappa_n x}) e^{\frac{-i(n\hbar\omega+E)t}{\hbar}}$$

$$\approx (Be^{\kappa x}+Ce^{-\kappa x})e^{-i\frac{Et}{\hbar}}(1+\frac{V_1}{2\hbar\omega}e^{\frac{-i(\hbar\omega+E)t}{\hbar}}-\frac{V_1}{2\hbar\omega}e^{\frac{-i(-\hbar\omega+E)t}{\hbar}})+(B_1e^{\kappa_1 x}+C_1e^{-\kappa_1 x})e^{\frac{-i(\hbar\omega+E)t}{\hbar}}$$

$$+(B_{-1}e^{\kappa_{-1}x} + C_{-1}e^{-\kappa_{-1}x})e^{\frac{-i(-\hbar\omega+E)t}{\hbar}}. \tag{5.2.7}$$

In other words, we can for $V_1 \ll \hbar\omega$ consider only the contribution from $n = -1$ to $n = 1$, and the wavefunctions$\psi_1$ and $\psi_3$ are then

$$\psi_1(x,t) \approx (e^{ikx} + Ae^{-ikx})e^{-i\frac{Et}{\hbar}} + A_1 e^{-i\frac{(\hbar\omega+E)t}{\hbar}} e^{-ik_1 x} + A_{-1} e^{-i\frac{(-\hbar\omega+E)t}{\hbar}} e^{-ik_{-1}x}, \tag{5.2.8}$$

$$\psi_3(x,t) \approx De^{ikx}e^{-i\frac{Et}{\hbar}} + D_1 e^{-i\frac{(\hbar\omega+E)t}{\hbar}} e^{ik_1 x} + D_{-1} e^{-i\frac{(-\hbar\omega+E)t}{\hbar}} e^{ik_{-1}x} \tag{5.2.9}$$

This approximation can greatly simplify the problem. We will find its benefit when this method is applied in our model in section 5.3.

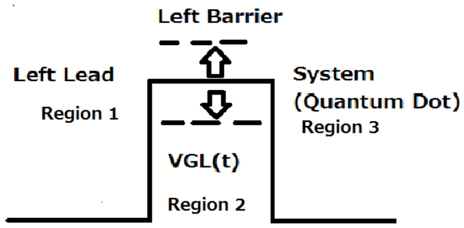


Figure 5.2.1: This is the figure of the model of M. Büttiker and R. Landauer. The left lead region and the central system is at zero potential. The left barrier region is controlled by the time-dependent left gate voltage.

## 5.3 Model of Calculating Effective Transmission Coefficient $\overline{V}_\lambda(t)$

In this section, we generalize the method described in section 5.2. That is, the potentials at regions 1, 2, 3 are all time-dependent as in Fig. 5.1.1. In our model we add time-dependent potentials $V_L = \Delta_1 cos(\omega_1 t)$, $V_{GL} = \Delta_2 cos(\omega_2 t)$ and $\epsilon(t) = \Delta_3 cos(\omega_3 t)$ on regions 1, 2, 3, respectively. Similar to section 5.2, we can write

the wavefunction $\psi_1(x,t)$ as

$$\psi_1(x,t) = (e^{ik_1x} + Ae^{-ik_1x})e^{-i\frac{\mu_L t}{\hbar}}(1+\frac{\Delta_1}{2\hbar\omega_1}e^{-i\omega_1 t} - \frac{\Delta_1}{2\hbar\omega_1}e^{i\omega_1 t}) + A_{11,1}e^{-ik_{11,1}x}e^{-i\frac{(\mu_L+\hbar\omega_1)t}{\hbar}}$$

$$+A_{11,-1}e^{-ik_{11,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_1)t}{\hbar}} + A_{21,1}e^{-ik_{21,1}x}e^{-i\frac{(\mu_L+\hbar\omega_2)t}{\hbar}} + A_{21,-1}e^{-ik_{21,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_2)t}{\hbar}}$$

$$+A_{31,1}e^{-ik_{31,1}x}e^{-i\frac{(\mu_L+\hbar\omega_3)t}{\hbar}}+A_{31,-1}e^{-ik_{31,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_3)t}{\hbar}}, \quad (5.3.1)$$

the wavefunction $\psi_2(x,t)$ as

$$\psi_2(x,t)=(Be^{\kappa_2 x}+Ce^{-\kappa_2 x})e^{-i\frac{\mu_L t}{\hbar}}(1+\frac{\Delta_2}{2\hbar\omega_2}e^{-i\omega_2 t}-\frac{\Delta_2}{2\hbar\omega_2}e^{i\omega_2 t})$$

$$+(B_{22,-1}e^{\kappa_{22,-1}x}+C_{22,-1}e^{-\kappa_{22,-1}x})e^{-i\frac{(\mu_L-\hbar\omega_2)t}{\hbar}}+(B_{32,1}e^{\kappa_{32,1}x}+C_{32,1}e^{-\kappa_{32,1}x})e^{-i\frac{(\mu_L+\hbar\omega_3)t}{\hbar}}$$

$$+(B_{32,-1}e^{\kappa_{32,-1}x}+C_{32,-1}e^{-\kappa_{32,-1}x})e^{-i\frac{(\mu_L-\hbar\omega_3)t}{\hbar}}+(B_{12,1}e^{\kappa_{12,1}x}+C_{12,1}e^{-\kappa_{12,1}x})e^{-i\frac{(\mu_L+\hbar\omega_1)t}{\hbar}}$$

$$+(B_{12,-1}e^{\kappa_{12,-1}x}+C_{12,-1}e^{-\kappa_{12,-1}x})e^{-i\frac{(\mu_L-\hbar\omega_1)t}{\hbar}}+(B_{22,1}e^{\kappa_{22,1}x}+C_{22,1}e^{-\kappa_{22,1}x})e^{-i\frac{(\mu_L+\hbar\omega_2)t}{\hbar}} \quad (5.3.2)$$

and the wavefunction $\psi_3(x,t)$ as

$$\psi_3(x,t)=De^{ik_3 x}e^{-i\frac{\mu_L t}{\hbar}}(1+\frac{\Delta_3}{2\hbar\omega_3}e^{-i\omega_3 t}-\frac{\Delta_3}{2\hbar\omega_3}e^{i\omega_3 t})+D_{33,1}e^{ik_{33,1}x}e^{-i\frac{(\mu_L+\hbar\omega_3)t}{\hbar}}$$

$$+D_{33,-1}e^{ik_{33,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_3)t}{\hbar}}+D_{23,1}e^{ik_{23,1}x}e^{-i\frac{(\mu_L+\hbar\omega_2)t}{\hbar}}+D_{23,-1}e^{ik_{23,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_2)t}{\hbar}}$$

$$+D_{13,1}e^{ik_{13,1}x}e^{-i\frac{(\mu_L+\hbar\omega_1)t}{\hbar}}+D_{13,-1}e^{ik_{13,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_1)t}{\hbar}} \quad (5.3.3)$$

in regions 1, 2, 3 respectively. Here, $k_1 = \sqrt{\frac{2m\mu_L}{\hbar^2}}$ , $\kappa_2 = \sqrt{\frac{2m(V_0-\mu_L)}{\hbar^2}}$ , $k_3 = \sqrt{\frac{2m(\mu_L-\epsilon_0)}{\hbar^2}} k_{n1,\pm 1} = \sqrt{\frac{2m(\mu_L \pm \hbar\omega_n)}{\hbar^2}}$, $\kappa_{n2,\pm 1} = \sqrt{\frac{2m(V_0-(\mu_L \pm \hbar\omega_n))}{\hbar^2}}$, and $k_{n3,\pm 1} = \sqrt{\frac{2m(\mu_L \pm \hbar\omega_n - \epsilon_0)}{\hbar^2}}$. In section 5.2, we know that the oscillating potential will produce reflected waves and transmitted waves at the energies $E + \hbar\omega$, $E - \hbar\omega$. In this section, we apply time-dependent potentials in regions 1, 2, 3. Thus, the oscillating potential in region 1 will produce sideband contributions on region 2: $(B_{12,1}e^{\kappa_{12,1}x} + C_{12,1}e^{-\kappa_{12,1}x})e^{-i\frac{(\mu_L+\hbar\omega_1)t}{\hbar}} + (B_{12,-1}e^{\kappa_{12,-1}x} + C_{12,-1}e^{-\kappa_{12,-1}x})e^{-i\frac{(\mu_L-\hbar\omega_1)t}{\hbar}}$ and on region 3: $D_{13,1}e^{ik_{13,1}x}e^{-i\frac{(\mu_L+\hbar\omega_1)t}{\hbar}} + D_{13,-1}e^{ik_{13,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_1)t}{\hbar}}$, the oscillating potential in region 3 will produce sideband contributions on region 1: $A_{31,1}e^{-ik_{31,1}x}e^{-i\frac{(\mu_L+\hbar\omega_3)t}{\hbar}} + A_{31,-1}e^{-ik_{31,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_3)t}{\hbar}}$ and on region 2: $(B_{32,1}e^{\kappa_{32,1}x} + C_{32,1}e^{-\kappa_{32,1}x})e^{-i\frac{(\mu_L+\hbar\omega_3)t}{\hbar}} + (B_{32,-1}e^{\kappa_{32,-1}x} + C_{32,-1}e^{-\kappa_{32,-1}x})e^{-i\frac{(\mu_L-\hbar\omega_3)t}{\hbar}}$ and the oscillating potential in region 2 will produce sideband contrivutions on region 1: $A_{21,1}e^{-ik_{21,1}x}e^{-i\frac{(\mu_L+\hbar\omega_2)t}{\hbar}} + A_{21,-1}e^{-ik_{21,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_2)t}{\hbar}}$ and on region 3: $D_{23,1}e^{ik_{23,1}x}e^{-i\frac{(\mu_L+\hbar\omega_2)t}{\hbar}} + D_{23,-1}e^{ik_{23,-1}x}e^{-i\frac{(\mu_L-\hbar\omega_2)t}{\hbar}}$. The coefficients in Eq. (5.3.1), Eq. (5.3.2) and Eq. (5.3.3) can be solved similar to section 5.2 by the boundary condition: $\psi_1(0,t) = \psi_2(0,t)$, $\psi_2(L,t) = \psi_3(L,t)$, $\frac{\partial\psi_1(x,t)}{\partial x}|_{x=0} = \frac{\partial\psi_2(x,t)}{\partial x}|_{x=0}$, $\frac{\partial\psi_2(x,t)}{\partial x}|_{x=L} = \frac{\partial\psi_3(x,t)}{\partial x}|_{x=L}$ and the linear independence of $e^{\frac{-i(\pm\hbar\omega_m+\mu_L)t}{\hbar}}$. Recall now that in quantum mechanics [29], the transmission coefficient is defined as $T \equiv \sqrt{\frac{J_3}{J_1}}$. $J_1$ is the incident probability current density and $J_3$ is the probability current density after tunneling. Here we find the effective transmission coefficient by the same definition as before.

$$\overline{V}_\lambda(t) = \sqrt{\frac{J_3}{J_1}}|_{x=L} \tag{5.3.4}$$

$$J_3 = \frac{\hbar}{2m}(i\psi_3\frac{\partial\psi_3^*}{\partial x} + c.c), \tag{5.3.5}$$

$$J_1 = \frac{\hbar}{2m}(i\psi_{1i}\frac{\partial\psi_{1i}^*}{\partial x} + c.c), \tag{5.3.6}$$

where $\psi_{1i} = e^{ikx} e^{-i\frac{\mu_L t}{\hbar}} (1 + \frac{\Delta_1}{2\hbar\omega_1} e^{-i\omega_1 t} - \frac{\Delta_1}{2\hbar\omega_1} e^{i\omega_1 t})$ is the incident wavefunction.

## 5.4 Summary

In this chapter, we have found the effective transmission coefficients. We first introduce how M. Büttiker and R. Landauer dealt with the tunneling problem with an oscillating barrier. We imitate their method, that is, we only consider the contributions from the sidebands $n = -1$ , $n = 1$ under the approximation $\frac{\Delta_1}{\hbar\omega_1}$ , $\frac{\Delta_2}{\hbar\omega_2}$ , $\frac{\Delta_3}{\hbar\omega_3} \ll 1$, and apply it to our model in section 5.3. In the general case, we should consider all the sidebands and the coefficients of $e^{-in\omega t}$ in the expansion $e^{-i\frac{V}{\hbar\omega} sin(\omega t)} = \sum_{n=-\infty}^{\infty} J_n(\frac{V}{\hbar\omega}) e^{-in\omega t}$. However, we can still use this method to discuss the current under this approximation. There is another approximation in Ref. [30]. In that paper, if the oscillation of the potential is not so rapid: $\omega\tau \ll 1$, $\tau$ is the traversal time through the potential barrier [16], the tunneling problem can be treated as quasi-stationary. In the quasi-stationary approximation, one can just use the result in stationary tunneling problem and change the time-independent potential to time-dependent case, i.e., $V \rightarrow V(t)$. In Eq. 5.3.4, $\sqrt{\frac{J_3}{J_1}}$ is in general a function of $x$ and $t$. We take its value at $x = L$, which is just the position the wavefunction tunnel through the barrier as our transmission coefficient. Our method is an approximated method to discuss the time-dependent effective transmission and we can get more accurate result by taking into account more terms in the sideband contributions.

# 6 Numerical Result and Discussion

## 6.1 Numerical method

In this chapter, we use nature unit $\hbar = e = k_B = 1$ for simplicity. From Eq. (4.2.28) and Eq. (4.2.29), we know the current is:

$$I_\lambda(t) = -(\Gamma_{\lambda 1}(t) + \Gamma^*_{\lambda 1}(t) - \Gamma_{\lambda 2}(t) - \Gamma^*_{\lambda 2}(t))\rho_{11}(t) - (\Gamma_{\lambda 2}(t) + \Gamma^*_{\lambda 2}(t)). \tag{6.1.1}$$

$$\frac{\partial \rho_{11}(t)}{\partial t} = -\sum_\lambda (\Gamma_{\lambda 1}(t) + \Gamma^*_{\lambda 1}(t) - \Gamma_{\lambda 2}(t) - \Gamma^*_{\lambda 2}(t))\rho_{11}(t) - (\Gamma_{\lambda 2}(t) + \Gamma^*_{\lambda 2}(t)) \tag{6.1.2}$$

Here we have used the fact that $Tr_S(\rho(t)) = \rho_{00}(t) + \rho_{11}(t) = 1$. Therefore, if we know $\rho_{11}(t)$ , $\Gamma_{\lambda 1}(t) + \Gamma^*_{\lambda 1}(t) - \Gamma_{\lambda 2}(t) - \Gamma^*_{\lambda 2}(t)$ , $\Gamma_{\lambda 2}(t) + \Gamma^*_{\lambda 2}(t)$, we can exactly determine the current. Fortunately, we find in [9] that the current is as follows:

$$I_\lambda(t) = -(\lambda_\lambda(t) + \lambda^*_\lambda(t) + (\kappa_\lambda(t) + \kappa^*_\lambda(t))\rho_{11}(t)). \tag{6.1.3}$$

We can get that $\kappa_\lambda(t) + \kappa^*_\lambda(t) = \Gamma_{\lambda 1}(t) + \Gamma^*_{\lambda 1}(t) - \Gamma_{\lambda 2}(t) - \Gamma^*_{\lambda 2}(t)$ and $\lambda_\lambda(t) + \lambda^*_\lambda(t) = \Gamma_{\lambda 2}(t) + \Gamma^*_{\lambda 2}(t)$. Hence if we solve $\kappa_\lambda(t)$ and $\lambda_\lambda(t)$, we can get the current. The numerical details can be found in [9], [31] and [30]. We ignore the lengthy calculation here.

## 6.2 Numerical Result

Here, $m$ is the effective mass in GaAs $0.067m_e$, $m_e$ is the rest mass of electron and the energy unit $\Gamma = 1meV$. In this section, we use all the controlling voltage as sine function form. In this section, we do numerical analysis with high frequency bias voltage and high frequency system voltage respectively and the effective transmission coefficient.

### 6.2.1 Investigation of Wide Band Limit

In this subsection, we use asymmetric setup to see the relation between wideband limit and Markovian limit. We use the asymmetric setup as Fig. 6.2.1.

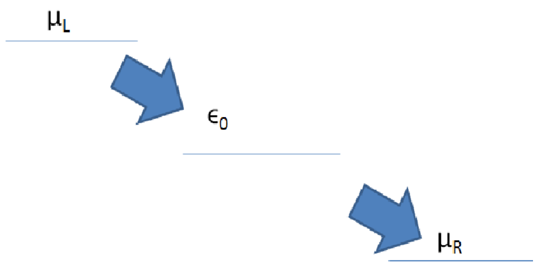


Figure 6.2.1: The symbolic figure of the asymmetric setup. $\mu_L = 3\Gamma$, $\mu_R = 1\Gamma$, $\epsilon_0 = 2\Gamma$

Here, we fix the chemical potential of the left lead: $\mu_L = 3\Gamma$, the right lead: $\mu_R = 1\Gamma$ and the system energy $\epsilon_0 = 2\Gamma$. In Fig. 6.2.2, we take the wideband limit, that is, bandwidth $W_L = W_R = 80\Gamma$and we compare it with Fig. 6.2.3, whcih has bandwidth $W_L = W_R = \Gamma$. The blue curve is for $I_L(t)$, and the green one is for $I_R(t)$. In these two figures, you can find immediately that the currents $I_L(t)$ , $I_R(t)$ both decay more rapidly in Fig. 6.2.2 than in Fig. 6.2.3. This manifests clearly the Markovian limit, that is, without the memory effect of the bath, the current flowing into the system will reach steady state more rapidly.

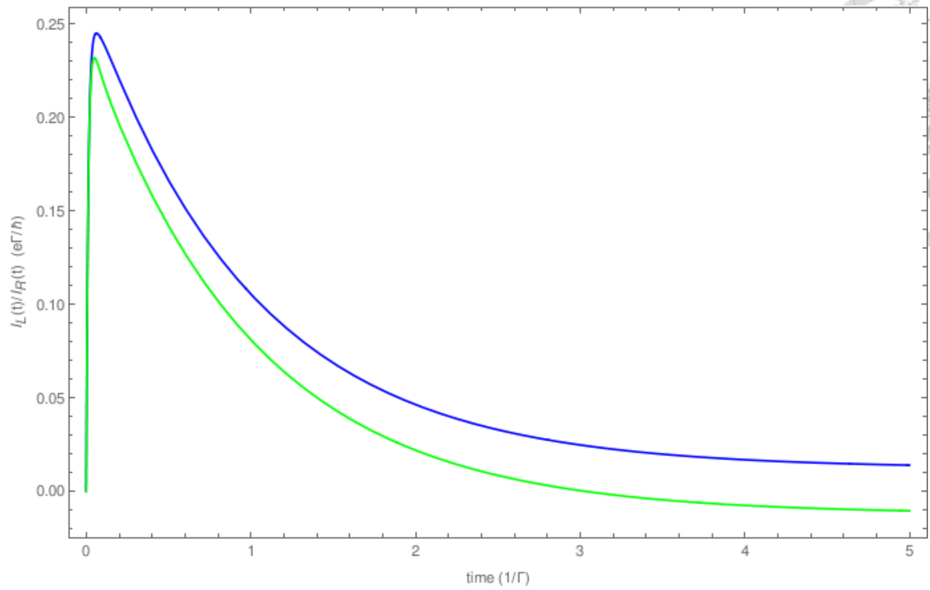


Figure 6.2.2: $I_R$ (the green one) and $I_L$ (the blue one) with bandwith $W_L = W_R = 80\Gamma$, chemical potential $\mu_L = 3\Gamma$ , $\mu_R = \Gamma$ and system energy $\epsilon_0 = 2\Gamma$

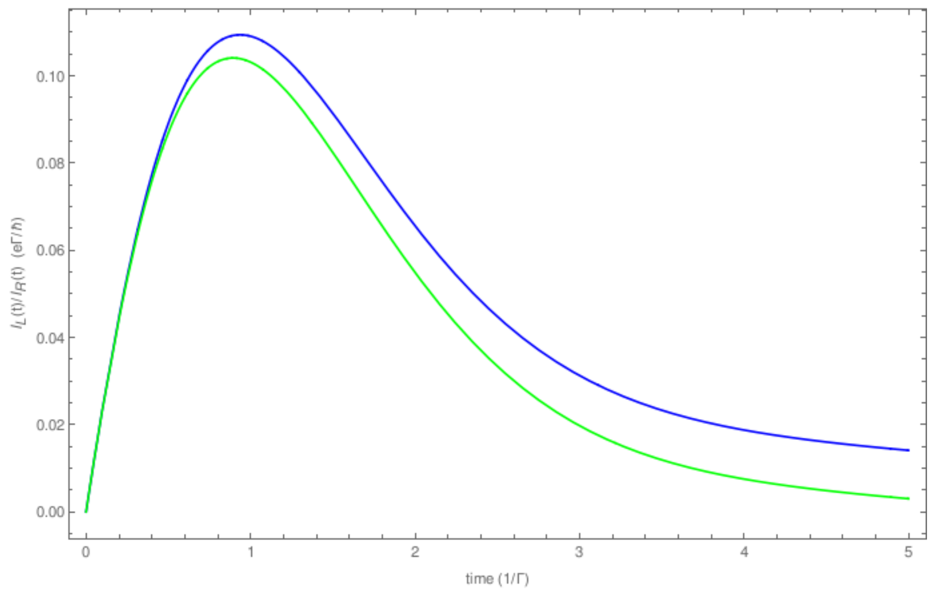


Figure 6.2.3: $I_R$(the green one) and $I_L$ (the blue one) with bandwith $W_L = W_R = \Gamma$, other parameters are the same as Fig. 6.2.2

## 6.3 Investigation on Time-Dependent gate voltage on the system

In this section, we discuss the behavior when we apply time-dependent gate voltage on the system without applying time-dependent bias voltage. Here, we set the chemical potential of the left lead $\mu_L = 3\Gamma$, the chemical potential of the right lead $\mu_R = \Gamma$ and apply gate voltage $\epsilon_s(t) = \epsilon_0 + \epsilon_c cos(\omega_s t)$ on the system, $\epsilon_c$ is $\Gamma$ such that the maximum of $\epsilon_s(t)$ is equal to $\mu_L$ and the minimum of $\epsilon_s(t)$ is equal to $\mu_R$. When $\epsilon_s(t)$ reach its maximum, the current flowing from the left lead can be ignored when it is compared with the current flowing from the system to the right lead. Thus the net current $I_{net}(t) \equiv I_L(t) - I_R(t)$ is dominated by $I_R(t)$. And due to the large value of energy difference between $\epsilon_s(t)$ and $\mu_R$, we can get the conclusion that the magnitude of the net current has the maximum value. The case in Fig. 6.3.1 occurs at time $t = \frac{2n\pi}{\omega_s}$, with n a nonnegatice integer. These times correspond to the first peak of the net current $I_{net}(t)$.

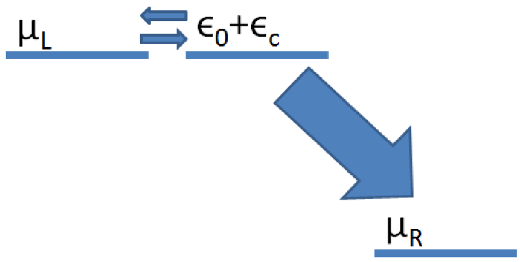


Figure 6.3.1: The picture representing the flow of the current when $\epsilon_s(t)$ reaches its maximum. The current between the left lead and the system is negligible compared with the current flowing from the system into the right lead.

Similar to Fig. 6.3.1, in Fig. 6.3.2, when $\epsilon_s(t)$ reaches its minimum, the current flowing from the right lead can be ignored when it is compared with the current flowing from the left lead to the system. Thus the net current $I_{net}(t) \equiv I_L(t) - I_R(t)$ is dominated by

$I_L(t)$. And the net current has the maximum value in Fig. 6.3.2 for the same reason as Fig. 6.3.1. The case in Fig. 6.3.2 occurs at time $t = \frac{(2n-1)\pi}{\omega_s}$ with n a positive integer These times correspond to the second peak of the net current $I_{net}(t)$.

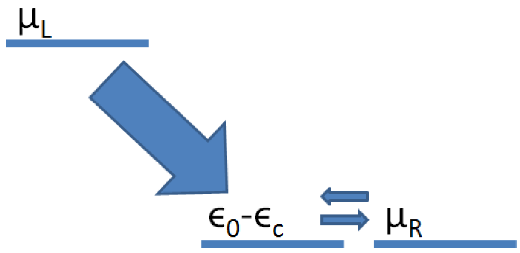


Figure 6.3.2: The picture representing the flow of the current when $\epsilon_s(t)$ reaches its minimum. The current between the right lead and the system is negligible compared with the current flowing from the left lead to the system.

In the following, we do some numerical simulation to examine our argument. It can be seen obviously in Fig. that when the magnitude of $I_R$ is minimum, the $I_L$ has maximum and vice versa. In Fig. 6.3.4 and Fig. 6.3.5, we plot the net current and set the bandwidth $W_L = W_R = 5\Gamma$. The chemical potential of the left, the right lead is $\mu_L = 3\Gamma$ and $\mu_R = 1\Gamma$ respectively.

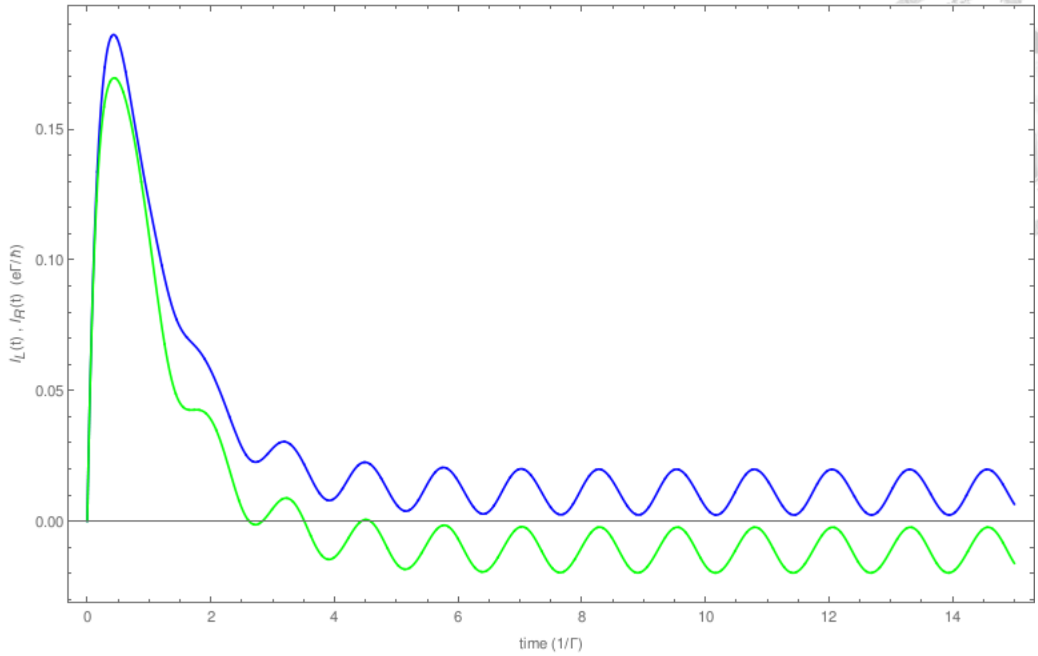


Figure 6.3.3: The $I_R$(the green one) and $I_L$(the blue one) when we apply time-dependent gate voltage on the system $\epsilon_s(t) = \epsilon_0 + \epsilon_c cos(\omega_s t)$, $\epsilon_0 = 2\Gamma$, $\epsilon_c = \Gamma$, $\mu_L = 3\Gamma$, $\mu_R = 1\Gamma$. The other parameters are as follows: $W_L = W_R = 5\Gamma$, $\Gamma_L = \Gamma_R = 0.5\Gamma$, $\omega_s = 5\Gamma$, $\beta = \frac{0.1}{\Gamma}$

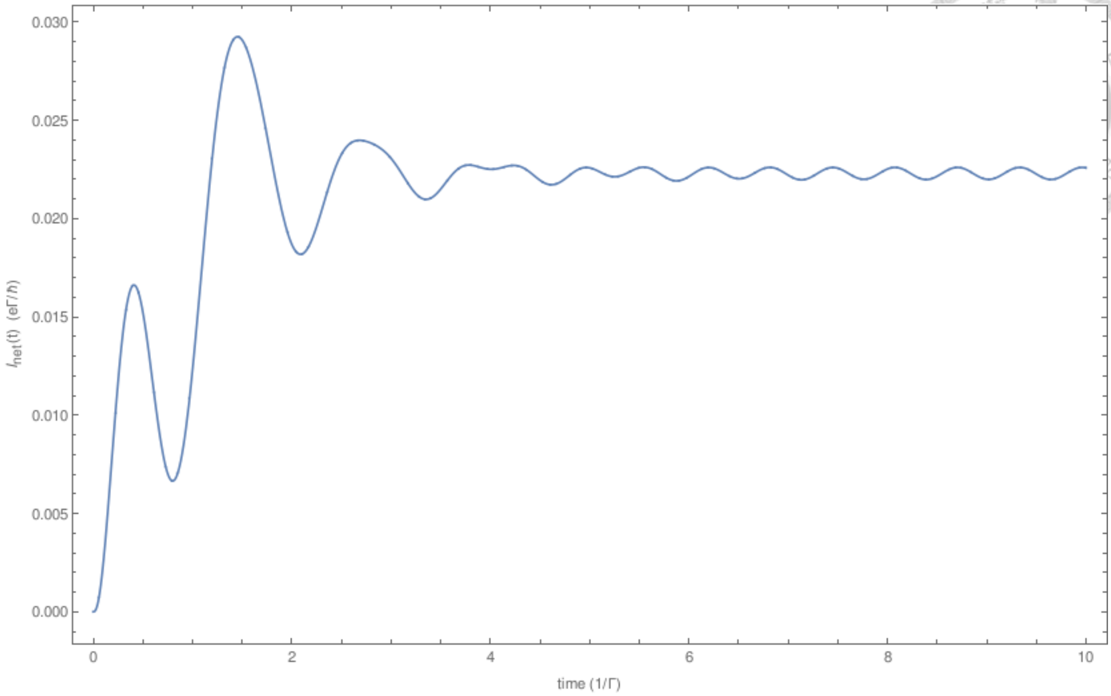


Figure 6.3.4: The net current when we apply a time-dependent gate voltage on the system $\epsilon_s(t) = \epsilon_0 + \epsilon_c cos(\omega_s t)$, $\epsilon_0 = 2\Gamma$, $\epsilon_c = \Gamma$, $\mu_L = 3\Gamma$, $\mu_R = 1\Gamma$. The other parameters are as follows: $W_L = W_R = 5\Gamma$, $\Gamma_L = \Gamma_R = 0.5\Gamma$, $\omega_s = 5\Gamma$, $\beta = \frac{0.1}{\Gamma}$

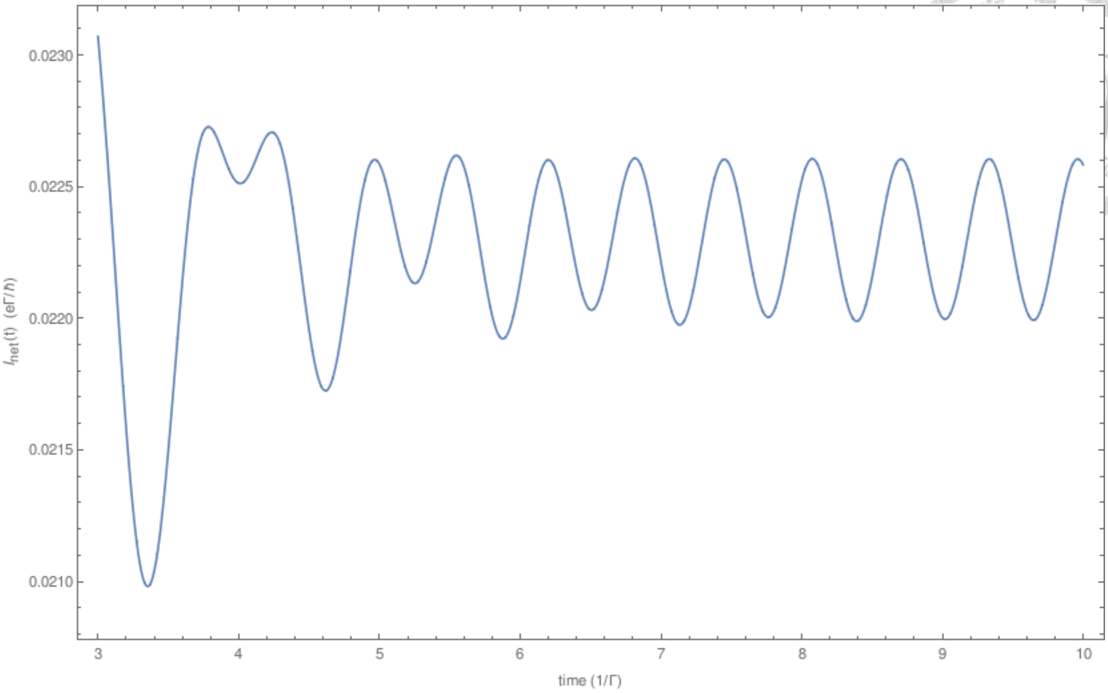


Figure 6.3.5: The picture showing the details of Fig. 6.3.4 from time $t = \frac{3}{\Gamma}$ to $t = \frac{10}{\Gamma}$

In Fig. 6.3.4, the first local maximum is at $t = \frac{3.7845}{\Gamma}$ and the next local maximum are as follows: $t = \frac{4.2349}{\Gamma}$ , $\frac{4.9662}{\Gamma}$ , $\frac{5.5463}{\Gamma}$ , $\frac{6.2005}{\Gamma}$. These values are very close to $\frac{6\pi}{5\Gamma}$ , $\frac{7\pi}{5\Gamma}$ , .... And the minimum is at $t = \frac{3.3533}{\Gamma}(\frac{(2*6-1)\pi}{2*\omega_s} = \frac{11\pi}{10\Gamma} \approx \frac{3.4558}{\Gamma})$ , $\frac{4.0108}{\Gamma}(\frac{13\pi}{10\Gamma} \approx \frac{4.0841}{\Gamma})$ , $\frac{4.6168}{\Gamma}(\frac{15\pi}{10\Gamma} \approx \frac{4.7124}{\Gamma})$... The result match our previous argument perfectly. In Fig. 6.3.6 and Fig. 6.3.7, we plot $I_L$ , $I_R$ and $I_{net}$ and find the net current reaches maximum at times very close to $\frac{6\pi}{5\Gamma}$ , $\frac{7\pi}{5\Gamma}$ , ... , which is the same as Fig. 6.3.4.

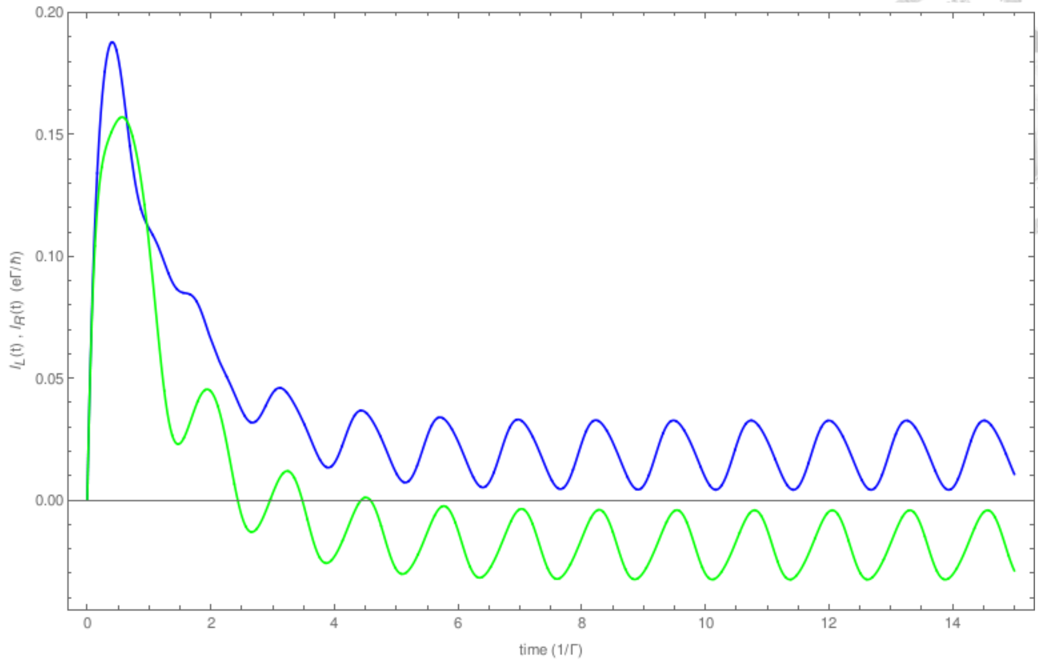


Figure 6.3.6: The $I_R$(the green one) and $I_L$(the blue one) when we apply time-dependent gate voltage on the system $\epsilon_s(t) = \epsilon_0 + \epsilon_c cos(\omega_s t)$, $\epsilon_0 = 4\Gamma$, $\epsilon_c = 2\Gamma$, $\mu_L = 6\Gamma$, $\mu_R = 2\Gamma$. The other parameters are as follows: $W_L = W_R = 5\Gamma$, $\Gamma_L = \Gamma_R = 0.5\Gamma$, $\omega_s = 5\Gamma$, $\beta = \frac{0.1}{\Gamma}$

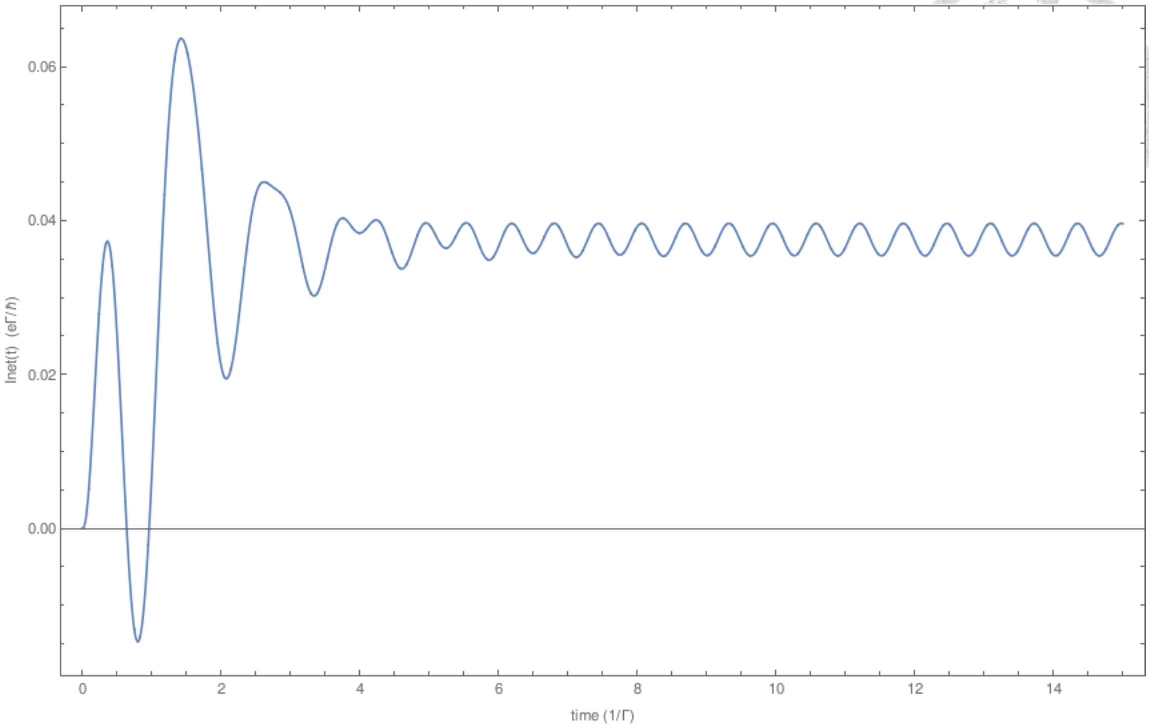


Figure 6.3.7: The net current when we apply a time-dependent gate voltage on the system $\epsilon_s(t) = \epsilon_0 + \epsilon_c cos(\omega_s t)$, $\epsilon_0 = 4\Gamma$, $\epsilon_c = 2\Gamma$, $\mu_L = 6\Gamma$, $\mu_R = 2\Gamma$. The other parameters are as follows: $W_L = W_R = 5\Gamma$, $\Gamma_L = \Gamma_R = 0.5\Gamma$, $\omega_s = 5\Gamma$, $\beta = \frac{0.1}{\Gamma}$

## 6.4 Investigation on Time-Dependent Efficient Transmission Coefficient

In this section, we take a look at the behavior of the time-dependent transmission coefficient $\overline{V}_\lambda(t)$ as the Fig. 6.4.1.

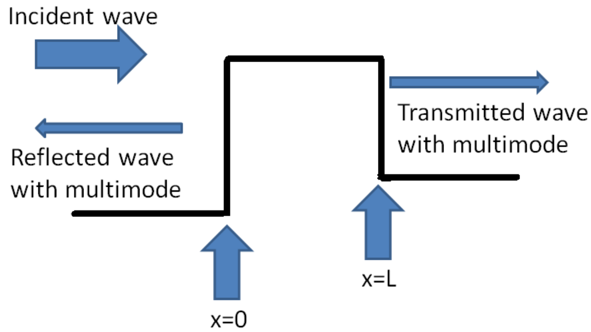


Figure 6.4.1: The left barrier and the parameters are as follows $L = 10^{-9}m$ [26]

In the following, we only show the transmission coefficient of the left barrier. The transmission coefficient of the right barrier can be obtained by the same method as the left barrier. In Fig. 6.4.2, we choose $\Delta_1 = \Gamma$, $\Delta_2 = 2\Gamma$, $\Delta_3 = \Gamma$ and $\omega_1 = 4.22\Gamma$, $\omega_2 = 5.275\Gamma$, $\omega_3 = 1.055\Gamma$ and we take the potential in region 1 as reference so that the potential is 0 in region 1 and the potential in region 2 without bias voltage is $V_0$, the potential in region 3 without gate voltage is $\epsilon_0$.

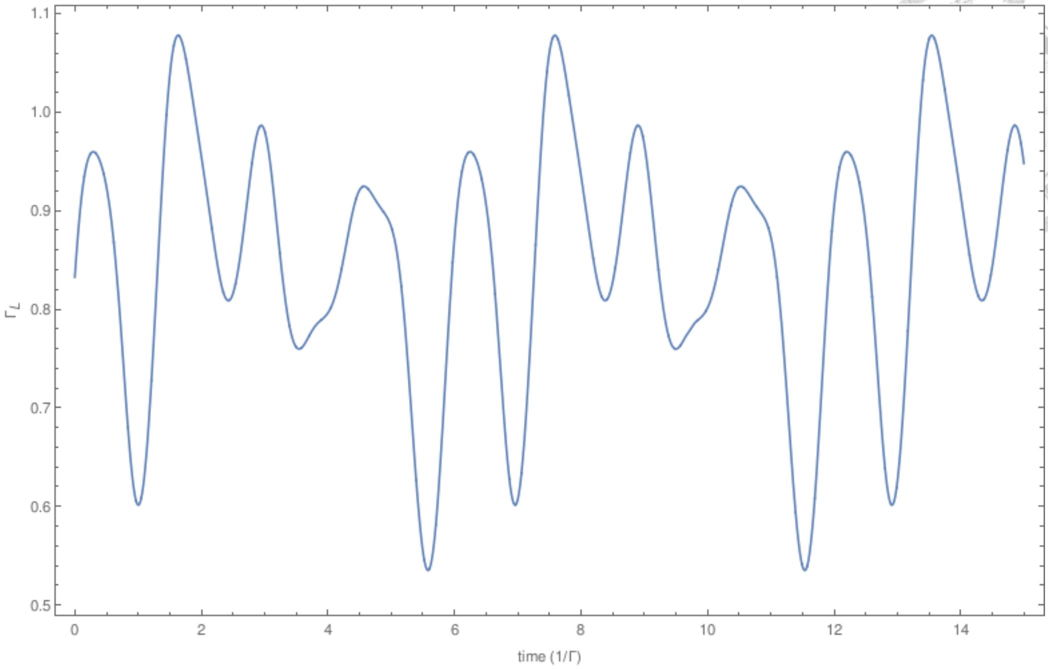


Figure 6.4.2: The effective transmission coefficient with $\Delta_1 = \Gamma$, $\Delta_2 = 2\Gamma$, $\Delta_3 = \Gamma$ and $\omega_1 = 4.22\Gamma$, $\omega_2 = 5.275\Gamma$, $\omega_3 = 1.055\Gamma$ and $V_0 = 5\Gamma$, $\epsilon_0 = \Gamma$.

However, it contradicts our intuition that the transmission coefficient $> 1$. It is because that in this case $\frac{\Delta_n}{\omega_n} \sim 1$, this does not obey our assumption that $\frac{\Delta_n}{\omega_n} \ll 1$. If $\frac{\Delta_n}{\omega_n} \sim 1$, we need to consider more terms in section 5.3 so that we would not lose information of the incident wave and the transmitted wave. In Fig. 6.4.3, we choose $\Delta_1 = \Gamma$, $\Delta_2 = 2\Gamma$, $\Delta_3 = \Gamma$ and $\omega_1 = 4220\Gamma$, $\omega_2 = 5275\Gamma$, $\omega_3 = 1055\Gamma$ and $V_0 = 5\Gamma$ so that these parameters satisfy the condition $\frac{\Delta_n}{\omega_n} \ll 1$.

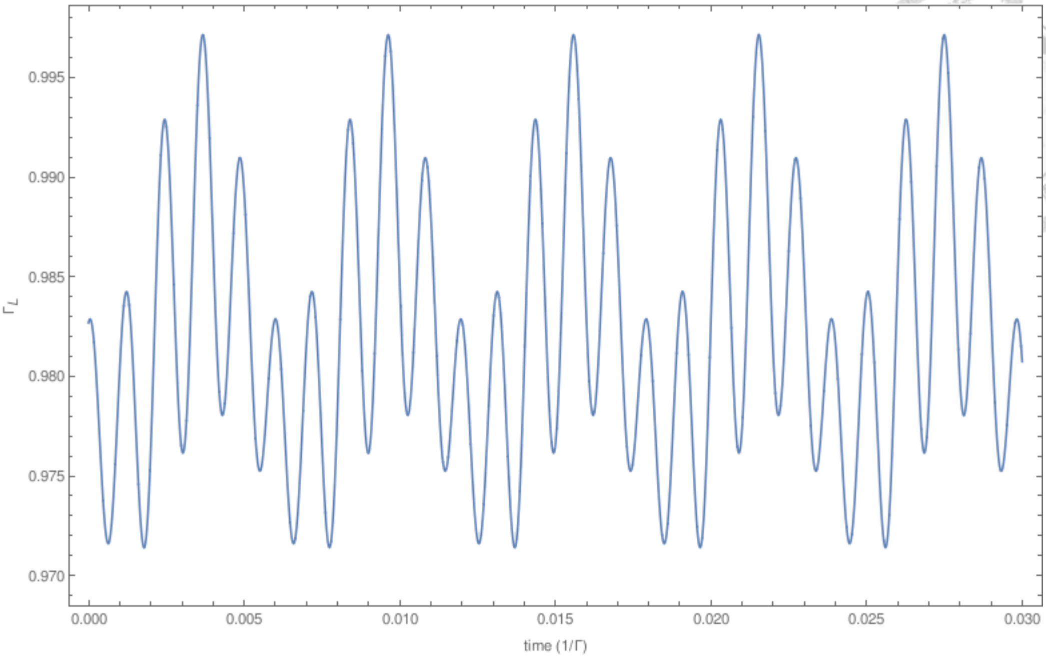


Figure 6.4.3: The effective transmission coefficient with $\Delta_1 = \Gamma$, $\Delta_2 = 2\Gamma$, $\Delta_3 = \Gamma$ and $\omega_1 = 4220\Gamma$, $\omega_2 = 5275\Gamma$, $\omega_3 = 1055\Gamma$ and $V_0 = 5\Gamma$, $\epsilon_0 = \Gamma$.

## 6.5 Electron Switch

In this section, we control the left and the right barrier oscillating in a $\pi$ phase shift, that is, applying the left gate voltage and the right gate voltage $V_{GL} = \Delta cos(\omega t + \pi)$ and $V_{GR} = \Delta cos(\omega t)$ on the left and the right barrier respectively. We fix the chemical potential of the left lead $\mu_L = 2\Gamma$, the chemical potential potential of the right lead $\mu_R = 2\Gamma$and the quantum dot energy $\epsilon_0 = 1\Gamma$. $\Delta = 2\Gamma$ and $\omega = 40\Gamma$. Here, we plot the $I_L$, $I_R$ and $I_{net}$ in Fig. 6.5.2 and Fig. 6.5.3. The pictures of $I_L$, $I_R$ and $I_{net}$ from the time $t = \frac{8}{\Gamma}$ to the time $t = \frac{10}{\Gamma}$ are showed in Fig. and Fig.

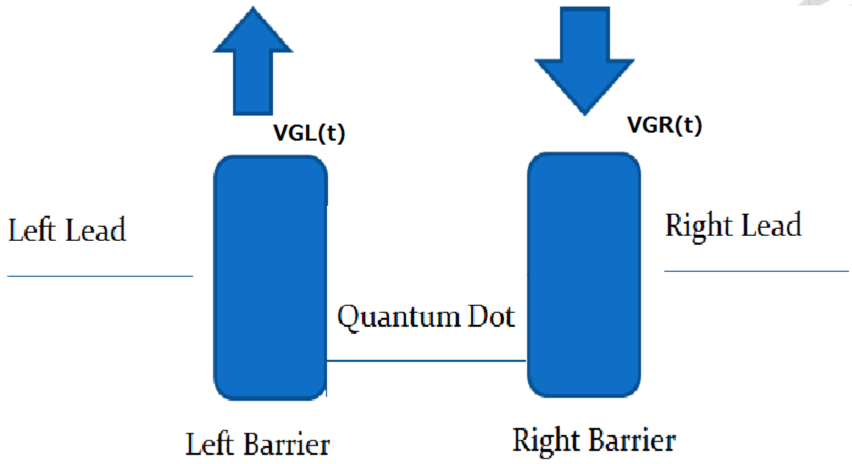


Figure 6.5.1: We apply the left gate voltage $V_{GL} = \Delta cos(\omega t + \pi)$ and the right gate voltage $V_{GR} = \Delta cos(\omega t)$ on the left and the right barrier respectively. The other parameters are $\mu_L = 2\Gamma$, $\mu_R = 2\Gamma$, $\epsilon_0 = 1\Gamma$. $\Delta = 2\Gamma$, $\omega = 40\Gamma$, $W_L = W_R = 5\Gamma$ and $\Gamma_L = \Gamma_R = 0.5\Gamma$ and the width of the left and the right barrier are both $L = 5nm$

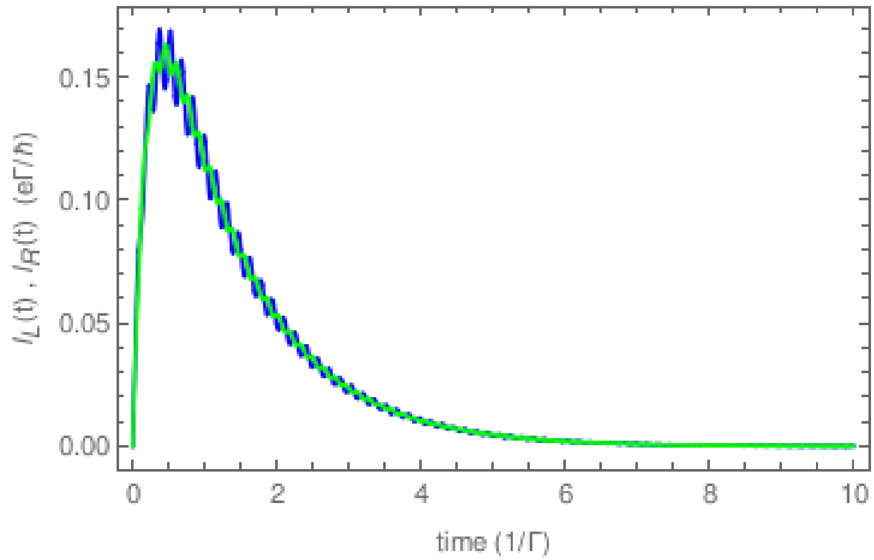


Figure 6.5.2: $I_R$ (green one) and $I_L$ (blue one) when we apply the left gate voltage $V_{GL} = \Delta cos(\omega t + \pi)$ and the right gate voltage $V_{GR} = \Delta cos(\omega t)$ on the left and the right barrier respectively. The other parameters are $\mu_L = 2\Gamma$, $\mu_R = 2\Gamma$, $\epsilon_0 = 1\Gamma$. $\Delta = 2\Gamma$, $\omega = 40\Gamma$, $W_L = W_R = 5\Gamma$ and $\Gamma_L = \Gamma_R = 0.5\Gamma$ and the width of the left and the right barrier are both $L = 5nm$

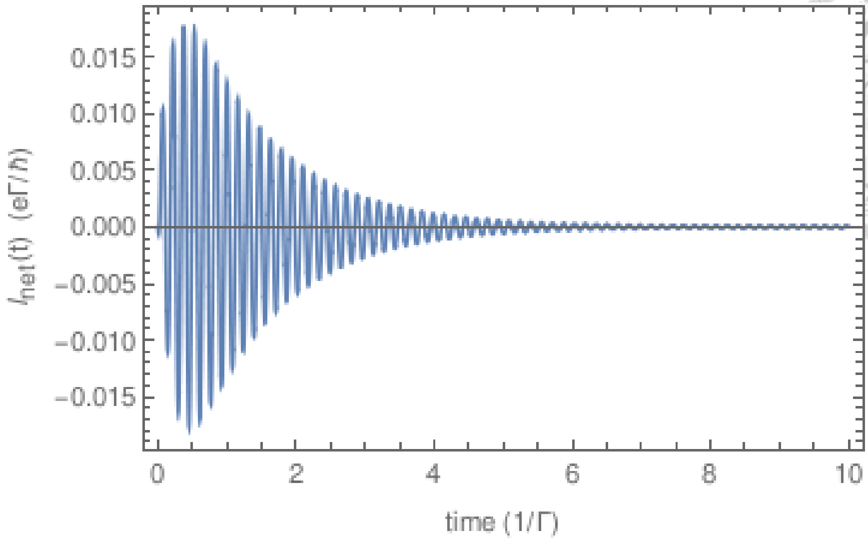


Figure 6.5.3: $I_{net}$ when we apply the left gate voltage $V_{GL} = \Delta cos(\omega t + \pi)$ and the right gate voltage $V_{GR} = \Delta cos(\omega t)$ on the left and the right barrier respectively. The other parameters are $\mu_L = 2\Gamma$, $\mu_R = 2\Gamma$, $\epsilon_0 = 1\Gamma$. $\Delta = 2\Gamma$, $\omega = 40\Gamma$, $W_L = W_R = 5\Gamma$ and $\Gamma_L = \Gamma_R = 0.5\Gamma$ and the width of the left and the right barrier are both $L = 5nm$

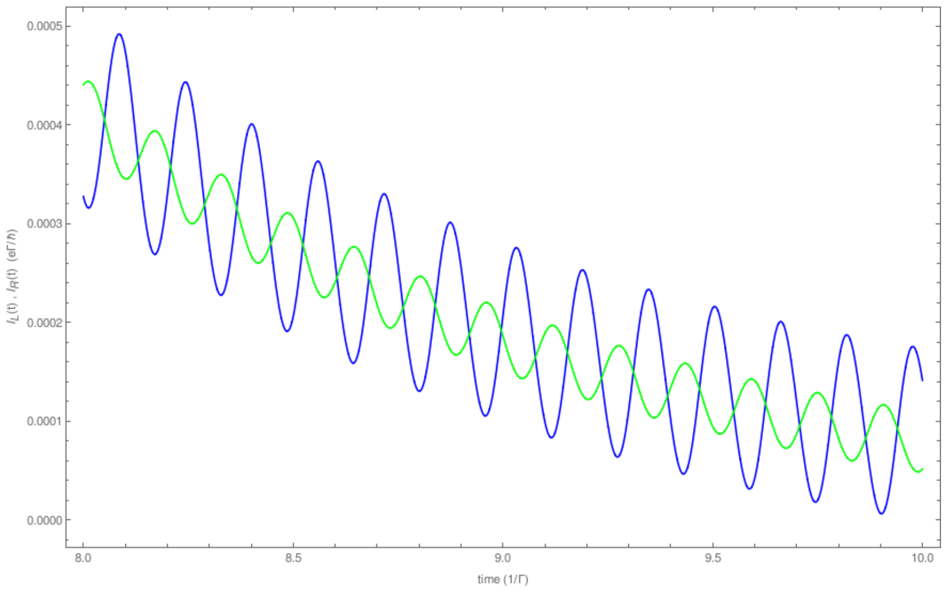


Figure 6.5.4: $I_R$ (green one) and $I_L$ (blue one) from the time $t = \frac{8}{\Gamma}$ to the time $t = \frac{10}{\Gamma}$. The other parameters are the same as Fig. 6.5.2.

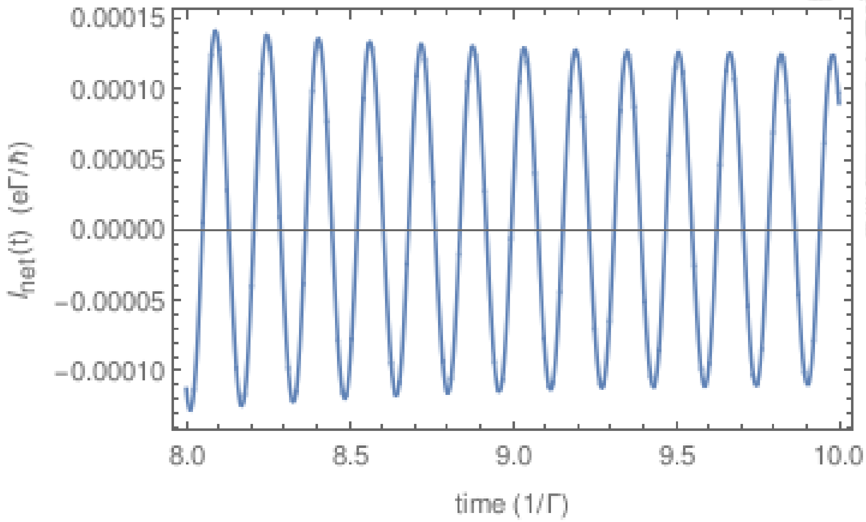


Figure 6.5.5: $I_{net}$ from the time $t = \frac{8}{\Gamma}$ to the time $t = \frac{10}{\Gamma}$. The other parameters are the same as Fig. 6.5.3.

From Fig. 6.5.4, we can obtain that when $I_R$ reaches its maximum, $I_L$ reaches its minimum and vice versa. Thus, we achieve our goal that we can control the current like a switch. One noting point is that the shpae of $I_L$ is a different from $I_R$. There may be two reasons for this. First, in our simulation, we need to expand our correlation function $\alpha_{\lambda 1}(t, s)$ and it would take a long time to do this simulation. Thus, we only expand it to 50 terms that is not enough. Second, although the left and the right gate voltage are cosine functions with only a $\pi$ phase shift, the wavefunctions in the left and the right barrier would contain contributions from the sidebands. Thus, the behavior of $I_R$ and $I_L$ would be different.

# 7 Conclusion and Future Work

In this thesis, we apply the fermionic NMQSD to describe the transport dynamics of an open quantum dot under the time-dependent bias voltage on the left lead (drain) and the right lead (source) and the time-dependent gate voltage on the single-energy-level quantum dot (system). We not only derive the fermionic NMQSD but also use it to obtain the exact master equation for transport dynamics. We then use the master equation to derive the transient current formula.

In the numerical aspect, we have proved that the transient current formula is equivalent to the Feynman-Vernon influence functional theorem. We also derive the time-dependent effective transmission coefficient so that we can deal with the transport problem with time-dependent coupling strength. However, in this case, we assume the barrier potential, system energy and bias energy have the same phase (we assume it to be 0). In the future work, for more general cases, we need to obtain the efficient transmission coefficient under the time-dependent voltages with different phases.

With the derived master equation, one can then describe and then control the dynamics of the quantum dot for various time-dependent voltage applied to the source and the drain, to the energy level of the quantum dot system as well as to the tunnel barriers.

# 8 Appendix

## 8.1 Markovian Limit

In the open quantum dynamics, the Markovian dynamics is easier under the Markovian limit [32],

$$\alpha(t,t^{'}) \equiv \left\langle \hat{R}_i(t)\,\hat{R}_j(t^{'}) \right\rangle_R \propto \delta(t-t^{'}) \tag{8.1.1}$$

In this formula, $\alpha(t,t^{'})$ is defined as the two-time correlation of $\hat{R}_i(t)$ and $\hat{R}_j(t^{'})$, $\langle * \rangle_R$ means average over bath degrees, i.e. take trace of $*$over a set of basis states of the bath. This means that $\hat{R}_i(t)$ and $\hat{R}_j(t^{'})$ have correlation only when $t = t^{'}$.When $t \neq t^{'}$, $\left\langle \hat{R}_i(t)\,\hat{R}_j(t^{'}) \right\rangle_R = 0$ which means that the environmental bath at $t$ won't be affected by the previous bath at $t^{'}$. As a result, the interaction of the system and the environmental will not be affected by the previous bath, too. There will not be memory terms in the time-evolution equation. We will see its simplicity in the non Markovian dynamics wich has a memory kernel.

## 8.2 Transforming the Hamiltonian into the Interaction Picture

We now shoe the detailed proof of $H_T$ in the interaction picture:

$$H_T = e^{\frac{i}{\hbar}\int_0^t dt' H_R'(t')}(H_S(t) + H_{SR}'(t))e^{-\frac{i}{\hbar}\int_0^t dt' H_R'(t')}. \tag{8.2.1}$$

$$H_R'(t) = \sum_{\lambda' k'} \hbar\omega_{\lambda' k'}(t)(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'}) \tag{8.2.2}$$

By definition $\overline{\omega}_{\lambda' k'}(t) \equiv \int_0^t dt' \omega_{\lambda' k'}(t')$

$$H_T = e^{i\sum_{\lambda' k'} \overline{\omega}_{\lambda' k'}(t)(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'})}(\hbar\omega_S(t)c^+c + \sum_{\lambda k}(\sqrt{n_{\lambda k}}g^*_{\lambda k} c e_{\lambda k} +$$

$$\sqrt{1-n_{\lambda k}}g_{\lambda k} c^+_{\lambda} d_{\lambda k} + H.c))e^{-i\sum_{\lambda' k'} \overline{\omega}_{\lambda' k'}(t)(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'})} \tag{8.2.3}$$

Because $[d^+_{\lambda' k'} d_{\lambda' k'}\ (e_{\lambda' k'} e^+_{\lambda' k'}),\, c^+c] = 0$ and $[d^+_{\lambda' k'} d_{\lambda' k'}\ (e_{\lambda' k'} e^+_{\lambda' k'}),\, c^+\ (c)] = 0$,

$$H_T = \hbar\omega_S(t)c^+c + e^{i\sum_{\lambda' k'} \overline{\omega}_{\lambda' k'}(t)(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'})}(\sum_{\lambda k}(\sqrt{n_{\lambda k}}g^*_{\lambda k} c e_{\lambda k} +$$

$$\sqrt{1-n_{\lambda k}}g_{\lambda k} c^+_{\lambda} d_{\lambda k} + H.c)e^{-i\sum_{\lambda' k'} \overline{\omega}_{\lambda' k'}(t)(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'})} \tag{8.2.4}$$

Now, we need to proof that:

$$[e^{i\sum_{\lambda' k'} \overline{\omega}_{\lambda' k'}(t)(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'})}][e_{\lambda k}][e^{-i\sum_{\lambda' k'} \overline{\omega}_{\lambda' k'}(t)(d^+_{\lambda' k'} d_{\lambda' k'} + e_{\lambda' k'} e^+_{\lambda' k'})}] = e^{i\overline{\omega}_{\lambda k}(t)} e_{\lambda k} \tag{8.2.5}$$

*Proof* :

Because $[d^{+}_{\lambda'k'}d_{\lambda'k'}\,,\,e_{\lambda k}]=0$ and $[e_{\lambda'k'}e^{+}_{\lambda'k'}\,,\,e_{\lambda k}]=0$ for $\lambda \neq \lambda'$or $k \neq k'$. Hence, the above equation can be written as:

$$[e^{i(\sum_{\lambda'\neq\lambda\, or\, k'\neq k}\overline{\omega}_{\lambda'k'}(t)(d^{+}_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^{+}_{\lambda'k'}))+d^{+}_{\lambda k}d_{\lambda k}}][e^{i\overline{\omega}_{\lambda k}(t)e_{\lambda k}e^{+}_{\lambda k}}][e_{\lambda k}][e^{-i\overline{\omega}_{\lambda k}(t)e_{\lambda k}e^{+}_{\lambda k}}]$$

$$*[e^{-i(\sum_{\lambda'\neq\lambda\, or\, k'\neq k}\overline{\omega}_{\lambda'k'}(t)(d^{+}_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^{+}_{\lambda'k'}))-d^{+}_{\lambda k}d_{\lambda k}}]$$

We first deal with the $\lambda k$ part:

$$(e^{i\overline{\omega}_{\lambda k}(t)e_{\lambda k}e^{+}_{\lambda k}})e_{\lambda k}(e^{-i\overline{\omega}_{\lambda k}(t)e_{\lambda k}e^{+}_{\lambda k}})$$

$$=(\sum_{n}\frac{1}{n!}(i\overline{\omega}_{\lambda k}(t))^{n}(e_{\lambda k}e^{+}_{\lambda k})^{n})e_{\lambda k}(e^{-i\overline{\omega}_{\lambda k}(t)e_{\lambda k}e^{+}_{\lambda k}})$$

And

$$(e_{\lambda k}e^{+}_{\lambda k})^{n}e_{\lambda k}=(e_{\lambda k}e^{+}_{\lambda k})^{n-1}(e_{\lambda k}e^{+}_{\lambda k})e_{\lambda k}$$

$$=(e_{\lambda k}e^{+}_{\lambda k})^{n-1}(1-e^{+}_{\lambda k}e_{\lambda k})e_{\lambda k}$$

$$= (e_{\lambda k} e^{+}_{\lambda k})^{n-1} e_{\lambda k}.$$

$$\ldots\ldots$$

By the same step, we can get the same result of $n-2$, $n-3$, ..., 0. And finally arrive at:

$$= e_{\lambda k} \; for \; every \; n$$

So, the $\lambda k$ part is

$$(e^{i\overline{\omega}_{\lambda k}(t) e_{\lambda k} e^{+}_{\lambda k}}) e_{\lambda k} (e^{-i\overline{\omega}_{\lambda k}(t) e_{\lambda k} e^{+}_{\lambda k}})$$

$$= (\sum_n \frac{1}{n!} (i\overline{\omega}_{\lambda k}(t))^n (e_{\lambda k} e^{+}_{\lambda k})^n) e_{\lambda k} (e^{-i\overline{\omega}_{\lambda k}(t) e_{\lambda k} e^{+}_{\lambda k}})$$

$$= \sum_n \frac{1}{n!} (i\overline{\omega}_{\lambda k}(t))^n e_{\lambda k} (e^{-i\overline{\omega}_{\lambda k}(t) e_{\lambda k} e^{+}_{\lambda k}})$$

$$= e^{i\overline{\omega}_{\lambda k}(t)} e_{\lambda k} \sum_m \frac{1}{m!} (-i\overline{\omega}_{\lambda k}(t))^m (e_{\lambda k} e^{+}_{\lambda k})^m$$

$$= e^{i\overline{\omega}_{\lambda k}(t)} e_{\lambda k}$$

Finally,

$$[e^{i\sum_{\lambda'k'}\overline{\omega}_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}][e_{\lambda k}][e^{-i\sum_{\lambda'k'}\overline{\omega}_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}]$$

$$= [e^{i(\sum_{\lambda'\neq\lambda\, or\, k'\neq k}\overline{\omega}_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'}))+d^+_{\lambda k}d_{\lambda k}}]e^{i\overline{\omega}_{\lambda k}(t)}e_{\lambda k}$$

$$*[e^{-i(\sum_{\lambda'\neq\lambda\, or\, k'\neq k}\overline{\omega}_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'}))-d^+_{\lambda k}d_{\lambda k}}]$$

$$= e^{i\overline{\omega}_{\lambda k}(t)}e_{\lambda k}\ qed$$

We prove that:

$$[e^{i\sum_{\lambda'k'}\overline{\omega}_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}][e_{\lambda k}][e^{-i\sum_{\lambda'k'}\overline{\omega}_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}] = e^{i\overline{\omega}_{\lambda k}(t)}e_{\lambda k} \quad (8.2.5)$$

For $d_{\lambda k}$ part is similar, we only simply manifest the part $(e^{i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})d_{\lambda k}(e^{-i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})$:

$$(e^{i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})d_{\lambda k}(e^{-i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})$$

$$= (e^{i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})d_{\lambda k}(\sum_n \frac{1}{n!}(-i\overline{\omega}_{\lambda k}(t))^n(d^+_{\lambda k}d_{\lambda k})^n)$$

And



$$d_{\lambda k}(d^+_{\lambda k}d_{\lambda k})^n = d_{\lambda k}(d^+_{\lambda k}d_{\lambda k})(d^+_{\lambda k}d_{\lambda k})^{n-1}$$

$$= d_{\lambda k}(1 - d_{\lambda k}d^+_{\lambda k})(d^+_{\lambda k}d_{\lambda k})^{n-1}$$

$$= d_{\lambda k}(d^+_{\lambda k}d_{\lambda k})^{n-1}$$

$$\cdots\cdots$$

By the same step, we can get the same result of $n-2$ , $n-3$ , ..., 0. And finally arrive at:

$$= d_{\lambda k} \ for \ every \ n$$

So, the $\lambda k$ part is

$$(e^{i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})d_{\lambda k}(e^{-i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})$$

$$= (e^{i\overline{\omega}_{\lambda k}(t)d^+_{\lambda k}d_{\lambda k}})d_{\lambda k}\sum_n \frac{1}{n!}(-i\overline{\omega}_{\lambda k}(t))^n$$

$$= d_{\lambda k}e^{-i\overline{\omega}_{\lambda k}(t)}.$$

So,

$$[e^{i\sum_{\lambda'k'}\varpi_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}][d_{\lambda k}][e^{-i\sum_{\lambda'k'}\varpi_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}] = d_{\lambda k}e^{-i\varpi_{\lambda k}(t)} \tag{8.2.6}$$

The Hermitian conjugate (H.c.) of Eq. (8.2.5) and Eq. (8.2.6) are

$$[e^{i\sum_{\lambda'k'}\varpi_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}][e^+_{\lambda k}][e^{-i\sum_{\lambda'k'}\varpi_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}] = e^+_{\lambda k}e^{-i\varpi_{\lambda k}(t)}, \tag{8.2.7}$$

$$[e^{i\sum_{\lambda'k'}\varpi_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}][d^+_{\lambda k}][e^{-i\sum_{\lambda'k'}\varpi_{\lambda'k'}(t)(d^+_{\lambda'k'}d_{\lambda'k'}+e_{\lambda'k'}e^+_{\lambda'k'})}] = e^{i\varpi_{\lambda k}(t)}d^+_{\lambda k}, \tag{8.2.8}$$

respectively. Through Eq. (8.2.5) and Eq. (8.2.6) and their Hermitian conjugate parts, we can get the simplified Hamiltonian $H_T$ in the interaction picture:

$$H_T(t) = H_S(t)+\sum_{\lambda k}(g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+d_{\lambda k}e^{-i\varpi_{\lambda k}(t)}+g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\varpi_{\lambda k}(t)}e^+_{\lambda k}c^+ + H.c.)\ qed$$

## 8.3 Derivation of the Fermionic Non-Markovian Quantum State Diffusion

We are now to simplify the following equation:

$$\langle zw| \frac{\partial}{\partial t} |\Psi_t(t)\rangle = -i\frac{1}{\hbar} \langle zw| H_T(t) |\Psi_t(t)\rangle$$

$$= -i\frac{1}{\hbar}(\langle zw| H_S(t)+\sum_{\lambda k}(g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+ d_{\lambda k}e^{-i\varpi_{\lambda k}(t)}+g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\varpi_{\lambda k}(t)}e^+_{\lambda k}c^+ +H.c.) |\Psi_t(t)\rangle) \tag{8.3.1}$$

Because $\langle zw|$is independent of time $t$, $\langle zw| \frac{\partial}{\partial t} |\Psi_t(t)\rangle = \frac{\partial}{\partial t}(\langle zw| \Psi_t(t)\rangle)$. And $|zw\rangle$ is the bath state vector, the $H_S(t)$ system Hamiltonian is only acting on the system state vector, so $|zw\rangle$ and $H_S(t)$ are commute:

$$\frac{\partial}{\partial t} |\phi(t, z^*, w^*)\rangle = -\frac{i}{\hbar} H_S(t) |\phi(t, z^*, w^*)\rangle$$

$$-i\frac{1}{\hbar}(\langle zw| \sum_{\lambda k}(g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+ d_{\lambda k}e^{-i\varpi_{\lambda k}(t)} + g_{\lambda k}(t)\sqrt{n_{\lambda k}}e^{-i\varpi_{\lambda k}(t)}e^+_{\lambda k}c^+ + H.c.) |\Psi_t(t)\rangle) \tag{8.3.2}$$

To simplify Eq. (8.3.2), we need to introduce some properties when fermionic operators act on the fermionic coherent states:

$$\langle zw| d^+_{\lambda k} = \langle zw| z^*_{\lambda k} \tag{8.3.3}$$

$$\langle zw| d_{\lambda k} = \frac{\partial}{\partial z^*_{\lambda k}} \langle zw| \tag{8.3.4}$$

$$\langle zw| e^+_{\lambda k} = \langle zw| w^*_{\lambda k} \tag{8.3.5}$$

$$\langle zw| e_{\lambda k} = \frac{\partial}{\partial w^*_{\lambda k}} \langle zw| \tag{8.3.6}$$

the above equations can be easily proved by the definition of fermionic coherent state. We don't put too much emphasis on it. Before we use Eq. (8.3.3) to (8.3.6) to simplfy Eq. (8.3.2), we demonstrate how the memory effect rises by the functional derivative:

$$\frac{\partial}{\partial z^*_{\lambda k}} = \int_0^t ds \frac{\partial z^*_\lambda(s)}{\partial z^*_{\lambda k}} \frac{\delta}{\delta z^*_\lambda(s)} = \int_0^t ds(-i\sqrt{1-n_{\lambda k}} g^*_{\lambda k}(s) e^{i\varpi_{\lambda k}(s)}) \frac{\delta}{\delta z^*_\lambda(s)} \tag{8.3.7}$$

$$\frac{\partial}{\partial w^*_{\lambda k}} = \int_0^t ds \frac{\partial w^*_\lambda(s)}{\partial w^*_{\lambda k}} \frac{\delta}{\delta w^*_\lambda(s)} = \int_0^t ds(-i\sqrt{n_{\lambda k}} g_{\lambda k}(s) e^{-i\varpi_{\lambda k}(s)}) \frac{\delta}{\delta w^*_\lambda(s)} \tag{8.3.8}$$

By Eq. (8.3.3) to (8.3.6), Eq. (8.3.7) and Eq. (8.3.8), we can finally get the fermionic NMQSD:

$$\frac{\partial}{\partial t} |\phi(t,z^*,w^*)\rangle = -\frac{i}{\hbar} H_S(t) |\phi(t,z^*,w^*)\rangle - \frac{1}{\hbar} \sum_\lambda c^+ \int_0^t \alpha_{\lambda 1}(t,s) \frac{\delta |\phi(t,z^*,w^*)\rangle}{\delta z^*_\lambda(s)} ds$$

$$-\frac{1}{\hbar}\sum_\lambda c \int_0^t \alpha_{\lambda 2}(t,s) \frac{\delta |\phi(t,z^*,w^*)\rangle}{\delta w^*_\lambda(s)} ds - \frac{1}{\hbar}\sum_\lambda c^+ w^*_\lambda(t) |\phi(t,z^*,w^*)\rangle - \frac{1}{\hbar}\sum_\lambda c z^*_\lambda(t) |\phi(t,z^*,w^*)\rangle . \tag{8.3.9}$$

## 8.4 The Transformation of the Reduced Density Operator

We now derive how the density operator $\rho(t) = Tr_R(|\Psi_t(t)\rangle \langle \Psi_t(t)|)$ be transformed to $M[\langle zw|\ \Psi_t(t)\rangle \langle \Psi_t(t)|\ -z-w\rangle]$.

$$\rho(t) = Tr_R(|\Psi_t(t)\rangle \langle \Psi_t(t)|)$$

$$= \sum_n \langle n | \Psi_t(t) \rangle \langle \Psi_t(t) | n \rangle \tag{8.4.1}$$

To prove Eq. (3.2.1), we calculate $M[\langle zw | \Psi_t(t)\rangle \langle \Psi_t(t)| -z-w\rangle]$ and show that it is the $Tr_R(|\Psi_t(t)\rangle \langle \Psi_t(t)|)$.

*Proof* :

$$M[\langle zw | \Psi_t(t)\rangle \langle \Psi_t(t)| -z-w\rangle]$$

$$= \int dz^2 dw^2 e^{-z^2-w^2} \langle zw | \Psi_t(t)\rangle \langle \Psi_t(t)| -z-w\rangle \tag{8.4.2}$$

Here, $dz^2 \equiv \prod_{\lambda k} dz^*_{\lambda k} dz_{\lambda k}$, $dw^2 \equiv \prod_{\lambda k} dw^*_{\lambda k} dw_{\lambda k}$, $e^{-z^2-w^2} \equiv e^{-z^*_{\lambda k} z_{\lambda k}} e^{-w^*_{\lambda k} w_{\lambda k}}$

$$\langle zw | = \langle 0 | \prod_{\lambda k} (1 - e_{\lambda k} w^*_{\lambda k})(1 - d_{\lambda k} z^*_{\lambda k})$$

$$= (\otimes_{\lambda k} \langle 0|_{\lambda k e} (1 - e_{\lambda k} w^*_{\lambda k})) \otimes (\otimes_{\lambda k} \langle 0|_{\lambda k d} (1 - d_{\lambda k} z^*_{\lambda k}))$$

$$|-z-w\rangle = \prod_k (1 + z_{\lambda k} d^+_{\lambda k}) \prod_l (1 + w_{\lambda k} e^+_{\lambda k}) |0\rangle$$

$$= (\otimes_{\lambda k} (1 + z_{\lambda k} d^+_{\lambda k}) |0\rangle_{\lambda k d}) \otimes (\otimes_{\lambda k} (1 + w_{\lambda k} e^+_{\lambda k})) |0\rangle_{\lambda k e})$$

Here, we argue that the vaccum state is separable in different modes: $|0\rangle = (\otimes_{\lambda k} |0\rangle_{\lambda k d}) \otimes (\otimes_{\lambda k} |0\rangle_{\lambda k e})$. It is resonable in the reason that there is no entanglement between different modes when the bath is in the vaccum state. So we can write the vaccum state $|0\rangle$ in a separable way of different modes. The above argument makes Eq. (8.4.2) become:

$$M[\langle zw | \Psi_t(t)\rangle \langle \Psi_t(t)| -z-w\rangle]$$

$$= \int dz^2 dw^2 e^{-z^2-w^2} (\otimes_{\lambda k} \langle 0|_{\lambda ke} (1 - e_{\lambda k} w^*_{\lambda k})) \otimes (\otimes_{\lambda k} \langle 0|_{\lambda kd} (1 - d_{\lambda k} z^*_{\lambda k})) |\Psi_t(t)\rangle$$

$$\langle \Psi_t(t)| (\otimes_{\lambda k} (1 + z_{\lambda k} d^+_{\lambda k}) |0\rangle_{\lambda kd}) \otimes (\otimes_{\lambda k} (1 + w_{\lambda k} e^+_{\lambda k})) |0\rangle_{\lambda ke}). \tag{8.4.3}$$

So that we can deal with the integral in the Hilbert space of different modes respectively. We demonstrate the calculation of one specific mode and the other modes can be derived in the same way.

$$\int dz^*_{\lambda k} dz_{\lambda k} (1 - z^*_{\lambda k} z_{\lambda k}) \langle 0|_{\lambda kd} (1 - d_{\lambda k} z^*_{\lambda k}) |\Psi_t(t)\rangle \langle \Psi_t(t)| (1 + z_{\lambda k} d^+_{\lambda k}) |0\rangle_{\lambda kd}$$

$$= \int dz^*_{\lambda k} dz_{\lambda k} (1 - z^*_{\lambda k} z_{\lambda k}) (\langle 0|_{\lambda kd} |\Psi_t(t)\rangle - \langle 0|_{\lambda kd} d_{\lambda k} z^*_{\lambda k} |\Psi_t(t)\rangle) (\langle \Psi_t(t) |0\rangle_{\lambda kd} + \langle \Psi_t(t)| z_{\lambda k} d^+_{\lambda k} |0\rangle_{\lambda kd})$$

$$= \int dz^*_{\lambda k} dz_{\lambda k} (1 - z^*_{\lambda k} z_{\lambda k}) (\langle 0|_{\lambda kd} |\Psi_t(t)\rangle \langle \Psi_t(t) |0\rangle_{\lambda kd} + \langle 0|_{\lambda kd} |\Psi_t(t)\rangle \langle \Psi_t(t)| z_{\lambda k} d^+_{\lambda k}) |0\rangle$$

$$- \langle 0|_{\lambda kd} d_{\lambda k} z^*_{\lambda k} |\Psi_t(t)\rangle \langle \Psi_t(t) |0\rangle_{\lambda kd} - \langle 0|_{\lambda kd} d_{\lambda k} z^*_{\lambda k} |\Psi_t(t)\rangle \langle \Psi_t(t)| z_{\lambda k} d^+_{\lambda k} |0\rangle_{\lambda kd})$$

$$= \langle 0|_{\lambda kd} |\Psi_t(t)\rangle \langle \Psi_t(t) |0\rangle_{\lambda kd} + \langle 0|_{\lambda kd} d_{\lambda k} |\Psi_t(t)\rangle \langle \Psi_t(t)| d^+_{\lambda k} |0\rangle_{\lambda kd}. \tag{8.4.4}$$

Here, the state $d^+_{\lambda k} |0\rangle_{\lambda kd}$ is $|1\rangle_{\lambda kd}$. $|1\rangle_{\lambda kd}$ represent the one particle state in the $\lambda k$

mode.

The next mode $\lambda^{'}k^{'}$becomes:

$$\langle 0|_{\lambda kd}\int dz^{*}_{\lambda^{'}k^{'}}dz_{\lambda^{'}k^{'}}(1-z^{*}_{\lambda^{'}k^{'}}z_{\lambda^{'}k^{'}})\,\langle 0|_{\lambda^{'}k^{'}d}\,(1-d_{\lambda^{'}k^{'}}z^{*}_{\lambda^{'}k^{'}})\,|\Psi_t(t)\rangle\,\langle\Psi_t(t)|\,(1+z_{\lambda^{'}k^{'}}d^{+}_{\lambda^{'}k^{'}})\,|0\rangle_{\lambda^{'}k^{'}d}\,|0\rangle_{\lambda kd}$$

$$+\,\langle 1|_{\lambda kd}\int dz^{*}_{\lambda^{'}k^{'}}dz_{\lambda^{'}k^{'}}(1-z^{*}_{\lambda^{'}k^{'}}z_{\lambda^{'}k^{'}})\,\langle 0|_{\lambda^{'}k^{'}d}\,(1-d_{\lambda^{'}k^{'}}z^{*}_{\lambda^{'}k^{'}})\,|\Psi_t(t)\rangle\,\langle\Psi_t(t)|\,(1+z_{\lambda^{'}k^{'}}d^{+}_{\lambda^{'}k^{'}})\,|0\rangle_{\lambda^{'}k^{'}d}\,|1\rangle_{\lambda kd}$$

$$=\langle 0|_{\lambda kd}\,\langle 0|_{\lambda^{'}k^{'}d}\,|\Psi_t(t)\rangle\,\langle\Psi_t(t)\;|0\rangle_{\lambda^{'}k^{'}d}\,|0\rangle_{\lambda kd}+\langle 0|_{\lambda kd}\,\langle 1|_{\lambda^{'}k^{'}d}\,|\Psi_t(t)\rangle\,\langle\Psi_t(t)\;|1\rangle_{\lambda^{'}k^{'}d}\,|0\rangle_{\lambda kd}$$

$$+\,\langle 1|_{\lambda kd}\,\langle 0|_{\lambda^{'}k^{'}d}\,|\Psi_t(t)\rangle\,\langle\Psi_t(t)\;|0\rangle_{\lambda^{'}k^{'}d}\,|1\rangle_{\lambda kd}+\langle 1|_{\lambda kd}\,\langle 1|_{\lambda^{'}k^{'}d}\,|\Psi_t(t)\rangle\,\langle\Psi_t(t)\;|1\rangle_{\lambda^{'}k^{'}d}\,|1\rangle_{\lambda kd}$$

$$\cdots\cdots$$

By integrating all the modes in the $z_{\lambda k}$ part, we can easily get: $\sum_{n_z}\langle n_z\;|\Psi_t(t)\rangle\,\langle\Psi_t(t)|\;n_z\rangle$. It's the same for the $w_{\lambda k}$ part and we finally get:

$$M[\langle zw|\;\Psi_t(t)\rangle\,\langle\Psi_t(t)|\;-z-w\rangle]=\sum_{n_z,n_w}\langle n_z|\,\langle n_w\;|\Psi_t(t)\rangle\,\langle\Psi_t(t)|\;n_w\rangle\,|n_z\rangle \tag{8.4.5}$$

So Eq. (8.4.3) becomes:

$$\sum_{n}\langle n\;|\Psi_t(t)\rangle\,\langle\Psi_t(t)\;n\rangle| \tag{8.4.6}$$

And eq, (8.4.6) is exactly $\sum_n \langle n|\ \Psi_t(t)\rangle \langle \Psi_t(t)\ |n\rangle = Tr_R(|\Psi_t(t)\rangle \langle \Psi_t(t)|) = \rho(t)$. Thus, $\rho(t) = M[\langle zw|\ \Psi_t(t)\rangle \langle \Psi_t(t)|\ -z-w\rangle]$. Here, we define $P_t \equiv \langle zw|\ \Psi_t(t)\rangle \langle \Psi_t(t)|\ -z-w\rangle$ so that $\rho(t) = M[P_t]$ for simplicity.

## 8.5 Derivation of Eq. (3.2.6) and Novikov Theorem

$$\frac{\partial \rho(t)}{\partial t} = \frac{\partial M[\langle zw|\ \Psi_t(t)\rangle \langle \Psi_t(t)|\ -z-w\rangle]}{\partial t} = \frac{\partial M[|\phi\rangle \langle \phi|]}{\partial t} = M[|\phi\rangle \frac{\partial \langle \phi|}{\partial t} + \frac{\partial |\phi\rangle}{\partial t} \langle \phi|]$$

By Eq. (2.4.9):

$$\frac{\partial |\phi\rangle}{\partial t} = -\frac{i}{\hbar} H_S |\phi\rangle - \frac{1}{\hbar}\sum_\lambda c^+ \overline{O}_{\lambda 1}(t, z^*, w^*)|\phi\rangle - \frac{1}{\hbar}\sum_\lambda c\overline{O}_{\lambda 2}(t, z^*, w^*)|\phi\rangle$$

$$-\frac{1}{\hbar}\sum_\lambda c^+ w_\lambda^*(t)|\phi\rangle - \frac{1}{\hbar}\sum_\lambda c z_\lambda^*(t)|\phi\rangle,$$

and Eq. (3.2.5)

$$\frac{\partial \langle \phi|}{\partial t} = \frac{i}{\hbar}\langle \phi| H_S - \frac{1}{\hbar}\sum_\lambda \langle \phi| \overline{O}^+_{\lambda 1}(t, -z, -w)c - \frac{1}{\hbar}\sum_\lambda \langle \phi| \overline{O}^+_{\lambda 2}(t, -z, -w)c^+$$

$$+\frac{1}{\hbar}\sum_\lambda \langle \phi| w_\lambda(t) c + \frac{1}{\hbar}\sum_\lambda \langle \phi| z_\lambda(t) c^+.$$

The master equation becomes:

$$\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H_S, \rho(t)] - \frac{1}{\hbar}\sum_\lambda M[P_t\overline{O}^+_{\lambda 1}]c - \frac{1}{\hbar}\sum_\lambda M[P_t\overline{O}^+_{\lambda 2}]c^+ + \frac{1}{\hbar}\sum M[P_{t\lambda} w_\lambda(t)]c + \frac{1}{\hbar}\sum_\lambda M[P_t z_\lambda(t)]c^+$$

$$-\frac{1}{\hbar}\sum_{\lambda} c^{+}M[\overline{O}_{\lambda 1}P_t] - \frac{1}{\hbar}\sum_{\lambda} cM[\overline{O}_{\lambda 2}P_t] - \frac{1}{\hbar}\sum_{\lambda} c^{+}M[w^*_{\lambda}(t)P_t] - \frac{1}{\hbar}\sum_{\lambda} cM[z^*_{\lambda}(t)P_t]. \tag{8.5.1}$$

Because we don't need the troublesome noise term $w_\lambda(t)$, $z_\lambda(t)$, $w^*_\lambda(t)$, $z^*_\lambda(t)$, we now introduce Novikov theorem that represent the relation between the noise and the $O$ operator:

Novikov theorem:

$$M[P_t z_\lambda(t)] = M[\overline{O}_{\lambda 1}P_t] \tag{8.5.2}$$

$$M[P_t w_\lambda(t)] = M[\overline{O}_{\lambda 2}P_t] \tag{8.5.3}$$

$$M[w^*_\lambda(t)P_t] = -M[P_t\overline{O}^{+}_{\lambda 2}] \tag{8.5.4}$$

$$M[z^*_\lambda(t)P_t] = -M[P_t\overline{O}^{+}_{\lambda 1}] \tag{8.5.5}$$

We only prove $M[P_t z_\lambda(t)] = M[\overline{O}_{\lambda 1}P_t]$. To prove $M[P_t z_\lambda(t)] = M[\overline{O}_{\lambda 1}P_t]$, we first prvoe that:

$$\int dz^2 dw^2 e^{-z^2-w^2} P_t w_{\lambda k} = \int dz^2 dw^2 e^{-z^2-w^2} \frac{\partial P_t}{\partial w^*_{\lambda k}}$$

It is obvious that for modes different from $\lambda k$, the left hand side is equal to the right hand side. Thus, we only deal with the mode $w_{\lambda k}$:

The left hand side:

$$\int dw^*_{\lambda k} dw_{\lambda k} (1 - w^*_{\lambda k} w_{\lambda k}) \langle 0| (1 - e_{\lambda k} w^*_{\lambda k}) |\Psi_t(t)\rangle \langle \Psi_t(t)| (1 + w_{\lambda k} e^+_{\lambda k}) |0\rangle w_{\lambda k}$$

$$= \langle 0| e_{\lambda k} |\Psi_t(t)\rangle \langle \Psi_t(t)| 0\rangle$$

The right hand side:

$$\int dw^*_{\lambda k} dw_{\lambda k} (1 - w^*_{\lambda k} w_{\lambda k}) \langle 0| e_{\lambda k} |\Psi_t(t)\rangle \langle \Psi_t(t)| (1 + w_{\lambda k} e^+_{\lambda k}) |0\rangle$$

$$= \langle 0| e_{\lambda k} |\Psi_t(t)\rangle \langle \Psi_t(t)| 0\rangle .$$

So the right hand side is equal to the left hand side and we prove that $\int dz^2 dw^2 e^{-z^2 - w^2} P_t w_{\lambda k} = \int dz^2 dw^2 e^{-z^2 - w^2} \frac{\partial P_t}{\partial w^*_{\lambda k}}$

Then,

$$M[P_t w_\lambda(t)] = i \sum_k \sqrt{n_{\lambda k}} g^*_{\lambda k}(t) e^{i\varpi_{\lambda k}(t)} \int dz^2 dw^2 e^{-z^2 - w^2} P_t w_{\lambda k}$$

$$= i \sum_k \sqrt{n_{\lambda k}} g^*_{\lambda k}(t) e^{i\varpi_{\lambda k}(t)} \int dz^2 dw^2 e^{-z^2 - w^2} \frac{\partial P_t}{\partial w^*_{\lambda k}}$$

$$= i \sum_k \sqrt{n_{\lambda k}} g^*_{\lambda k}(t) e^{i\varpi_{\lambda k}(t)} \int dz^2 dw^2 e^{-z^2 - w^2} (\int_0^t ds \frac{\partial w^*_\lambda(s)}{\partial w^*_{\lambda k}} \frac{\delta P_t}{\delta w^*_\lambda(s)})$$

$$= i \sum_k \sqrt{n_{\lambda k}} g^*_{\lambda k}(t) e^{i\varpi_{\lambda k}(t)} \int dz^2 dw^2 e^{-z^2 - w^2} (\int_0^t ds (-i \sqrt{n_{\lambda k}} g_{\lambda k}(s) e^{-i\varpi_{\lambda k}(s)}) \frac{\delta P_t}{\delta w^*_\lambda(s)})$$

$$= \int dz^2 dw^2 e^{-z^2-w^2} (\int_0^t ds (\sum_k n_{\lambda k} g^*_{\lambda k}(t) g_{\lambda k}(s) e^{i\overline{\omega}_{\lambda k}(t-s)}) O_{\lambda 2} P_t)$$

Here, $(\int_0^t ds(\sum_k n_{\lambda k} g^*_{\lambda k}(t) g_{\lambda k}(s) e^{i\overline{\omega}_{\lambda k}(t-s)}) O_{\lambda 2} = \int_0^t ds \alpha_{\lambda 2}(t,s) O_{\lambda 2} = \overline{O}_{\lambda 2}$. Thus, $M[P_t w_\lambda(t)] = \int dz^2 dw^2 e^{-z^2-w^2} \overline{O}_{\lambda 2} P_t) = M[\overline{O}_{\lambda 2} P_t]$.Similarly, $M[P_t z_\lambda(t)] = M[\overline{O}_{\lambda 1} P_t]$. Then we deal with $M[w^*_\lambda(t) P_t] = -M[P_t \overline{O}^+_{\lambda 2}]$. First we calculate:

$$(M[P_t w_\lambda(t)])^+ = (M[\langle zw | \Psi_t(t)\rangle \langle \Psi_t(t)| -z-w\rangle w_\lambda(t)])^+$$

$$= M[w^*_\lambda(t) \langle -z-w | \Psi_t(t)\rangle \langle \Psi_t(t)| zw\rangle]$$

$$= (M[\overline{O}_{\lambda 2} P_t])^+ = M[\langle -z-w | \Psi_t(t)\rangle \langle \Psi_t(t)| zw\rangle \overline{O}^+_{\lambda 2}].$$

Then we change variables: $z_{\lambda k} \to -z_{\lambda k}$ , $w_{\lambda k} \to -w_{\lambda k}$,

$$-M[w^*_\lambda(t) \langle zw | \Psi_t(t)\rangle \langle \Psi_t(t)| -z-w\rangle] = M[\langle zw | \Psi_t(t)\rangle \langle \Psi_t(t)| -z-w\rangle \overline{O}^+_{\lambda 2}]$$

$$\to M[w^*_\lambda(t) P_t] = -M[P_t \overline{O}^+_{\lambda 2}(t, -z, -w)].$$

Finally, by substituting from Eq. (8.5.2) to Eq. (8.5.5) in Eq. (8.5.1), we can easily get:

$$\frac{\partial \rho(t)}{\partial t} = \frac{-i}{\hbar}[H_S(t), \rho(t)] + \frac{1}{\hbar}\sum_\lambda ([c, M[P_t \overline{O}^+_{\lambda 1}(t, -z, -w)]] - [c^+, M[\overline{O}_{\lambda 1}(t, z^*, w^*) P_t]]$$

$$-[c, M[\overline{O}_{\lambda 2}(t, z^*, w^*)P_t]] + [c^+, M[P_t\overline{O}^+_{\lambda 2}(t, -z, -w)]]).$$

## 8.6 Simplification of Eq. (4.2.9)

First, we use $Tr(AB) = Tr(BA)$. Eq. (4.2.9) becomes:

$$I_\lambda = \frac{ie}{\hbar} Tr_{S\otimes R}[-\sum_k g_{\lambda k}(t)\sqrt{1-n_{\lambda k}}c^+ d_{\lambda k} e^{-i\overline{\omega}_{\lambda k}(t)}\rho^I(t)]$$

$$+\frac{ie}{\hbar} Tr_{S\otimes R}[-\sum_k g_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{-i\overline{\omega}_{\lambda k}(t)}\rho^I(t) e^+_{\lambda k} c^+]$$

$$+\frac{ie}{\hbar} Tr_{S\otimes R}[\sum_k g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}} e^{i\overline{\omega}_{\lambda k}(t)}\rho^I(t) d^+_{\lambda k} c]$$

$$+\frac{ie}{\hbar} Tr_{S\otimes R}[\sum g^*_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{i\overline{\omega}_{\lambda k}(t)} c e_{\lambda k}\rho^I(t)]$$

Then, by Eq. (3.1.2), the current finally becomes:

$$I_\lambda = \frac{ie}{\hbar} Tr_S[-\sum_k g_{\lambda k}(t)\sqrt{1-n_{\lambda k}} e^{-i\overline{\omega}_{\lambda k}(t)} c^+ Tr_R(d_{\lambda k}\rho^I(t))]$$

$$+\frac{ie}{\hbar} Tr_S[-\sum_k g_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{-i\overline{\omega}_{\lambda k}(t)} Tr_R(\rho^I(t) e^+_{\lambda k}) c^+]$$

$$+\frac{ie}{\hbar} Tr_S[\sum_k g^*_{\lambda k}(t)\sqrt{1-n_{\lambda k}} e^{i\overline{\omega}_{\lambda k}(t)} Tr_R(\rho^I(t) d^+_{\lambda k}) c]$$

$$+\frac{ie}{\hbar} Tr_S[\sum g^*_{\lambda k}(t)\sqrt{n_{\lambda k}} e^{i\overline{\omega}_{\lambda k}(t)} c Tr_R(e_{\lambda k}\rho^I(t))]$$

## 8.7 Bath Ensemble Average of $d_{\lambda k}$ , $e_{\lambda k}$ , $d^+_{\lambda k}$ , $e^+_{\lambda k}$

$$Tr_R(d_{\lambda k}\rho^I(t)) = Tr_R(d_{\lambda k}\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|)$$

$$= \sum_n \langle n| \int dz^2 dw^2 e^{-z^2-w^2} d_{\lambda k}\left|zw\right\rangle\left\langle zw\right|\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|n\rangle . \qquad (8.7.1)$$

As in appendix 5.4, we consider different modes respectively. Eq. (8.7.1) in mode $w_{\lambda k}$ is :

$$\sum_{n_{\lambda kd}} \langle n|_{\lambda kd} \int dz^*_{\lambda k} dz_{\lambda k} z_{\lambda k}(1 - z_{\lambda k} d^+_{\lambda k})\left|0\right\rangle_{\lambda kd}\left\langle 0\right|_{\lambda kd}(1 - d_{\lambda k} z^*_{\lambda k})\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|n\rangle_{\lambda kd}$$

$$= \langle 0|_{\lambda kd} \int dz^*_{\lambda k} dz_{\lambda k} z_{\lambda k}(1 - z_{\lambda k} d^+_{\lambda k})\left|0\right\rangle_{\lambda kd}\left\langle 0\right|_{\lambda kd}(1 - d_{\lambda k} z^*_{\lambda k})\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|0\rangle_{\lambda kd}$$

$$+ \langle 1|_{\lambda kd} \int dz^*_{\lambda k} dz_{\lambda k} z_{\lambda k}(1 - z_{\lambda k} d^+_{\lambda k})\left|0\right\rangle_{\lambda kd}\left\langle 0\right|_{\lambda kd}(1 - d_{\lambda k} z^*_{\lambda k})\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|1\rangle_{\lambda kd}$$

$$= \langle 0|_{\lambda kd}\left|0\right\rangle_{\lambda kd}\left\langle 0\right|_{\lambda kd} d_{\lambda k}\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|0\rangle_{\lambda kd} + \langle 1|_{\lambda kd}\left|0\right\rangle_{\lambda kd}\left\langle 0\right|_{\lambda kd} d_{\lambda k}\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|1\rangle_{\lambda kd}$$

And we note that in mode $w_{\lambda k}$:

$$\sum_{n_{\lambda kd}} \int dz^*_{\lambda k} dz_{\lambda k} z_{\lambda k}\left\langle 0\right|_{\lambda kd}(1 - d_{\lambda k} z^*_{\lambda k})\left|\Psi_t(t)\right\rangle\left\langle\Psi_t(t)\right|n\rangle_{\lambda kd}\left\langle n\right|_{\lambda kd}(1 + z_{\lambda k} d^+_{\lambda k})\left|0\right\rangle_{\lambda kd}$$

$$= \langle 0|_{\lambda kd}\, d_{\lambda k} \,|\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, 0\rangle_{\lambda kd} \,\langle 0|_{\lambda kd}\, |0\rangle_{\lambda kd} + \langle 0|_{\lambda kd}\, d_{\lambda k} \,|\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, 1\rangle_{\lambda kd} \,\langle 1|_{\lambda kd}\, |0\rangle_{\lambda kd}$$

$$= \langle 0|_{\lambda kd}\, |0\rangle_{\lambda kd} \,\langle 0|_{\lambda kd}\, d_{\lambda k} \,|\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, 0\rangle_{\lambda kd} + \langle 1|_{\lambda kd}\, |0\rangle_{\lambda kd} \,\langle 0|_{\lambda kd}\, d_{\lambda k} \,|\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, 1\rangle_{\lambda kd} .$$

Because $\langle 0|_{\lambda kd}\, |0\rangle_{\lambda kd}$ and $\langle 1|_{\lambda kd}\, |0\rangle_{\lambda kd}$ are all just numbers. For the other modes, it is just the case in the appendix 5.4. Thus we finally prove that:

$$Tr_R(d_{\lambda k}\rho^I(t)) = \int dz^2 dw^2 e^{-z^2-w^2} z_{\lambda k} \sum_n \langle zw\, |\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, n\rangle \,\langle n|\, -z-w\rangle$$

$$= \int dz^2 dw^2 e^{-z^2-w^2} z_{\lambda k} \,\langle zw\, |\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, -z-w\rangle$$

$$= M[z_{\lambda k} P_t] \tag{8.7.2}$$

by virtue of $\sum_n |n\rangle \langle n| = I$. Taking the Hermitian conjugate of Eq. (8.7.2):

$$Tr_R(\rho^I(t) d^+_{\lambda k}) = M[\langle -z-w\, |\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, zw\rangle\, z^*_{\lambda k}].$$

Then we change variables: $z_{\lambda k} \to -z_{\lambda k}$ , $w_{\lambda k} \to -w_{\lambda k}$,

$$Tr_R(\rho^I(t) d^+_{\lambda k}) = -M[\langle zw\, |\Psi_t(t)\rangle \,\langle \Psi_t(t)|\, -z-w\rangle\, z^*_{\lambda k}] = -M[P_t z^*_{\lambda k}].$$

Similarly,

$$Tr_R(e_{\lambda k}\rho^I(t)) = Tr_R(e_{\lambda k} \,|\Psi_t(t)\rangle \,\langle \Psi_t(t)|)$$

$$= M[w_{\lambda k} P_t],$$

$$Tr_R(\rho^I(t) e^{+}_{\lambda k}) = -M[\langle zw \left|\Psi_t(t)\right\rangle \left\langle \Psi_t(t)\right| -z - w\rangle \, w^{*}_{\lambda k}] = -M[P_t w^{*}_{\lambda k}].$$

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