

Classical Reduction of Quantum Master
Equations as Similarity Transformation
Department of Physics and Astronomy, Kyoto University

Norikazu Kamiya

Abstract

A general method of quantum-to-classical reduction of quantum dynamics is described. The key aspect of our method is the similarity transformation of the Liouvillian, which provides a new perspective. In conventional studies of quantum energy transport, the rotating wave approximation has been frequently regarded as an inappropriate approach because it causes the energy flow through the system to vanish. Our formulation elucidates as to why this unphysical result occurs and provides a solution for the problem. Moreover, we show that quantum dynamics can be “exactly” replaced with the classical equation for the calculation of the transport efficiency. This exact replacement is applied to the quantum transport efficiency problem, which gives an intuitive picture of the problem.

Acknowledgements

I would like to thank my supervisor Dr Shinji Takesue for his support and encouragement during this work.

Contents

1	Introduction	5
1.1	Quantum Open Systems	5
1.2	Quantum Master Equation	6
1.3	The Lindblad Form	7
1.4	Quantum System in Contact with Heat Reservoir	8
1.5	Studies of Quantum Energy Transport	9
1.6	Quantum Transport Efficiency	10
1.7	Aims of the Thesis	11
1.8	Organization of the Thesis	12
2	Reduction as Similarity Transformation	13
2.1	Projection-Operator Technique	13
2.2	Reduction of Hamiltonian	14
2.3	Reduction of Liouvillian by Similarity Transformation	15
2.4	Example	19
3	Quantum Energy Transport and the RWA	22
3.1	Energy Transport and RWA	22
3.2	Example	24
4	Quantum Transport Efficiency	26
4.1	Basic Settings	26
4.2	Exact Replacement with Population Dynamics	27
4.3	ENAQT in ordered systems	30
5	Conclusions	34

Chapter 1

Introduction

1.1 Quantum Open Systems

The study of an open quantum system is a challenging and a comparatively new problem. Quantum phenomena widely appear in both artificial and biological systems. Principles of future technologies such as quantum computers and quantum communication are based on the nature of quantum mechanics. Quantum effects are seen not only in these artificial systems but in natural systems. Recently, long-lived excitonic coherence has been observed in experimental studies of photosynthetic light-harvesting complexes [1, 2]. It indicates that we should model these systems as quantum system with its noisy environment.

A quantum system interacts with its environment in varying degrees. There are mainly two types of roles of environment. One is dissipation accompanied with irreversible exchange of conserving quantities (for e.g., energy), and the other is decoherence that implies the loss of quantum interference. Decoherence is caused by an environmental noise, and it is frequently a crucial factor in quantum phenomena. In general experiments of quantum systems are very sensitive to environmental noise, which is a barrier to the realization of quantum computers. In such cases, environmental noise is desired to be removed. However, in the following case, environment acts on the transport in a different way. The study of quantum transport efficiency in light-harvesting complexes has been attractive in the past few years, because it motivates the wide area of science including physics, chemistry, and biology. The role of environment on the quantum transport efficiency has

been discussed [3,4]. As a result, it has been found that the environment can enhance the transport of excitons. Thus, understanding of an open-quantum system has become increasingly important.

1.2 Quantum Master Equation

In principle, all the information of an open quantum system is contained in the von Neumann equation for the total Hamiltonian that includes the system, the environment, and the coupling between them. However, it is impossible to solve the equation due to the enormous degrees of freedom. Instead, the strategy of “reduction” has been commonly undertaken. That is, the reduction of the dynamics of the full Hamiltonian to the dynamics of the remarked system is performed, assuming the separation of the time-scales. The resulting equation is called quantum-master-equation. The difference between a quantum master equation and a classical master equation is the existence of the off-diagonal elements of the density matrix. Provided additional conditions (such as strong decoherence) are met, we can obtain the effective classical master equation. That is, “reduction” from a quantum master equation to the corresponding classical master equation can be carried out.

These two reductions should be technically distinguished. The former case involves the compression of direct products of wave functions, that is, we extract a system state $|\psi\rangle_S$ from the original state $|\psi\rangle_S \otimes |\psi\rangle_E$, where the suffixes S and E denote the system and the environment, respectively. On the other hand, the latter case leads to the compression of the dimension of the system wave function. Nevertheless, with a suitable definition of the projection operator, the two types of reductions are described by the same method, widely known as projection-operator technique [5]. The projection-operator method is to extract dynamics of the relevant space, and the operators that operate on the irrelevant space are eliminated. However, there is a case wherein the irrelevant-space operators contain the essences of the problem. For example, in the case of energy transport through a many-body system, an internal energy current is represented as an off-diagonal matrix in the energy basis. On the other hand, if we employ the rotating wave approximation (RWA) on the quantum master equation, time evolution of the density matrix is closed in the diagonal space. Formally, the RWA is described by the projection-operator technique, resulting in the elimination of the off-

diagonal elements. Thus, the internal energy current operator has no sense in the RWA [6]. Only the bath-to-system current can be correctly computed, for example, by the generalized quantum master equation approach [7, 8]. This fact is highly unphysical for the energy-conducting model (hereinafter we refer to this problem as the current vanishing problem). We will discuss this problem in detail in section 3.1.

1.3 The Lindblad Form

There is an important class of quantum master equations called the Lindblad form, which is described as [5, 9]

$$\frac{d}{dt}\rho = i[\rho, H] + \sum_k \gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right), \quad (1.1)$$

where γ_k is a positive constant and L_k denotes an arbitrary operator. H is a Hermitian operator, and it usually coincides with the system Hamiltonian. A master equation that is written in the Lindblad form ensures the trace preserving property and complete positivity of the density matrix, both of which are required for the probabilistic interpretation of the density matrix. Although quantum master equations are usually derived from the unitary time evolution of the total Hamiltonian including the environment, approaches that start from the quantum master equation are frequently taken. In both cases, the fact that the quantum master equation is of the Lindblad form is a crucial aspect for the validity of the model.

The Lindblad equation is also important in terms of numerical calculations. For the Lindblad equation, the stochastic Schrödinger equation method can be applied. In this method not the density matrix but the wave function is computed [5]. If the dimension of the density matrix is D , the dimension of the wave function is $D^{1/2}$. Thus, the cost of the numerical calculation decreases. This fact is important especially in the case of a quantum spin chain, because the dimension of the system increases exponentially as a function of the system size.

Thus, the Lindblad form is quite important both in terms of the validity of the master equation and in terms of the numerical calculation.

1.4 Quantum System in Contact with Heat Reservoir

Here, we briefly review how we derive the Lindblad equation for the system in contact with the heat reservoir.

Consider the system which is expressed by

$$H_{\text{tot}} = H_S + \lambda H_{\text{SB}} + H_B, \quad (1.2)$$

where H_S , H_B , and H_{SB} are the system Hamiltonian, the bath Hamiltonian, and the interaction Hamiltonian, respectively. We here assume

$$H_{\text{SB}} = X \otimes Y, \quad (1.3)$$

where X and Y are operators in the system and in the bath, respectively. The time evolution of the density matrix of the total system is given by the von Neumann equation:

$$\frac{d}{dt}\rho = i[\rho, H_{\text{tot}}]. \quad (1.4)$$

The non-reversible quantum master equation is obtained by assuming weak system-bath coupling λ and tracing out the degrees of freedom of the reservoir. The resulting equation is called the Redfield equation, which is not of the Lindblad form and is given as

$$\frac{d}{dt}\rho_S = i[\rho_S, H_S] + \pi\lambda^2 \sum_{i,j} (\Gamma_{i,j} \langle \epsilon_i | X | \epsilon_j \rangle [|\epsilon_i\rangle \langle \epsilon_j| \rho_S, X] + h.c.), \quad (1.5)$$

where ρ_S denotes the reduced density matrix and $\Gamma_{i,j}$ is a Fourier transformation of the reservoir correlation function. The state $|\epsilon_i\rangle$ is the eigenstate of the system Hamiltonian that has the eigenvalue ϵ_i . To obtain the Lindblad equation, the RWA has to be taken, and we have

$$\frac{d}{dt}\rho_S = i[\rho_S, H_S] + \pi\lambda^2 \sum_{i,j} (\Gamma_{i,j} [\langle \epsilon_i | X | \epsilon_j \rangle |\epsilon_i\rangle \langle \epsilon_j| \rho_S, \langle \epsilon_j | X | \epsilon_i \rangle |\epsilon_j\rangle \langle \epsilon_i|] + h.c.). \quad (1.6)$$

The above equation is of the Lindblad form because $\Gamma_{i,j}$ is positive. Moreover, the above RWA-equation has an interesting property. That is, the

dynamics of the diagonal and the off-diagonal elements are decoupled. Thus, the classical rate equation is derived as

$$\frac{d}{dt}P_k(t) = 2\pi\lambda^2 \sum_{i,k} \left(\Gamma_{k,i} |\langle \epsilon_k | X | \epsilon_i \rangle|^2 P_i(t) - \Gamma_{i,k} |\langle \epsilon_i | X | \epsilon_k \rangle|^2 P_k(t) \right), \quad (1.7)$$

where $P_k = \langle \epsilon_k | \rho_S | \epsilon_k \rangle$.

Thus, the RWA results in the Lindblad equation, and moreover the RWA can be regarded as a classical reduction of the quantum master equation.

1.5 Studies of Quantum Energy Transport

Understanding of energy transport is an important problem in non-equilibrium statistical physics. One of the main motivations of these studies is to unravel Fourier's law of heat conduction. Though Fourier's law has been widely used, its validity has not been understood completely. For classical systems, many efforts have been made, and it is revealed that the dimension of the system is an important factor for Fourier's law [10]. A harmonic chain is a simple and easy model to study the energy transport in low dimensional systems. The corresponding quantum chain is also solved in the same way as in the classical system. In contrast, a quantum spin chain does not have the corresponding classical model. To study energy transport through a quantum spin chain, the quantum-master-equation approach has been by many researchers [11–21]. Solving quantum master equations is difficult in general because the dimension of the density matrix increases exponentially as a function of the system size N . Moreover, the quantum master equations that have been used in the studies of energy transport through a spin chain have some defects as follows.

The RWA leads to a quantum master equation of the Lindblad form. Moreover, the quantum master equation with the RWA has the Gibbs state as an equilibrium solution. Therefore, the RWA-equation appears to be an appropriate model to study the quantum system in contact with heat reservoirs. However, the RWA does not present non-zero heat current as mentioned in section 1.2. For this reason, instead of the RWA, two approaches are proposed to investigate quantum energy transport.

One is to start with the Lindblad equation that without derivation from the total unitary evolution [11, 13–16, 19]. In this approach the Lindblad operators are chosen to be local, that is, they only act on the ends of the

	Redfield equation	assumed Lindblad equation
physical picture	clear	unclear
equilibrium solution	Gibbs state	not Gibbs state
numerical calculation	difficult	easy
positivity	not ensured	ensured

Table 1.1: Comparison table between the Redfield equation and the assumed Lindblad equation.

chain. The dissipation processes can have the Gibbs state as an equilibrium solution only if the system consists of a single spin. However, the advantage of this method is the simplicity of the dissipation processes, which enables the calculation of large systems ($N \simeq 100$). Because this Lindblad equation is not derived from the total Hamiltonian, the physical meaning of the master equation is not clear. It is reported that the statistical average of an observable can be approximated by the average with respect to the Gibbs state, if the system internal couplings are sufficiently weak [19]. Another interpretation of this Lindblad equation can be obtained by the quantum repeated interaction model (QRIM) if the system Hamiltonian conserved the total spin [22–24]. However, the QRIM does not conserve energy, therefore, it is inappropriate to use in the study of energy transport.

The other approach to study quantum energy transport is the use of the Redfield equation [12, 17, 21]. The Redfield equation is derived from the total Hamiltonian. If we employ the RWA on the Redfield equation, we obtain the Lindblad-type master equation. In contrast to the former assumed Lindblad-equation approach, the physical view of the master equation is clear in this case. However, the Redfield equation does not ensure the positivity of the density matrix. Moreover, it is very difficult to solve the Redfield equation, which restricts the study to small systems. ($N \simeq 10$).

Thus, each of the two approaches has defects as a model of quantum energy transport (Table 1.1).

1.6 Quantum Transport Efficiency

Studies of the quantum transport efficiency have been active in recent years [3, 4, 25–33]. The main motivation of these studies is to understand the mechanism of highly efficient excitonic energy transport in light-harvesting

complexes.

At the first stage of photosynthesis, light-harvesting complexes absorb light to create an exciton. The exciton is then transferred to a reaction center where the further process of photosynthesis is done. The transport efficiency is defined by the rate that the exciton arrives at the reaction center.

It has been considered that the quantum nature of the exciton on the light-harvesting complex can be neglected because of the vibrations of pigment molecules. The vibration of a pigment molecule is usually treated as a phonon reservoir, which involves decoherence processes, and the coherent nature of the exciton decreases. However, recent experimental studies have confronted us with the evidence of surprisingly long-lived excitonic coherence, which implies that we should model the system as a quantum system.

In studies of quantum transport efficiency based on the quantum master equation, it has been recognized that the environment can enhance the displacement of the exciton, which is frequently called environment-assisted quantum transport (ENAQT). The main ENAQT scenario is the suppression of the Anderson localization. The environmental noise destroys the coherent localization due to the disorder of the system, which results in the enhancement of the displacement of the exciton. Though this scenario is intuitively understandable, ENAQT phenomena are also observed even in ordered systems where the wave function is not localized [31]. Thus, the unified understandable picture is needed.

1.7 Aims of the Thesis

One of the aims of this thesis is to present a new formulation of quantum-to-classical reduction of master equations that recovers the physical meaning of the eliminated observables, which gives the solution of the current vanishing problem. The fundamental idea of the method is the similarity transformation both of the Liouvillian and the Physical quantities. The RWA or the conventional projection-operator technique and the similarity transformation produce the same classical Liouvillian. In the conventional approaches, the classical master equation is considered as merely an approximation for the density matrix and physical observables remain unchanged. On the other hand, the similarity transformation changes the basis of the Liouvillian space, which naturally leads to the idea that physical observables should also be transformed. The solution of the current vanishing problem

has much significance in the study of quantum energy transport because the RWA equation ensures the positivity of the density matrix, and at the same time, it has a clear physical picture.

For the quantum transport efficiency problem, we show that the exact replacement of a quantum master equation by the corresponding classical master equation can be carried out for the problem like quantum transport efficiency. This provides a unified understanding of the mechanism of ENAQT phenomena.

1.8 Organization of the Thesis

The rest of this thesis is organized as follows. In chapter 2, we describe our method based on the similarity transformation. In chapter 3, we apply the method to a certain quantum energy transport problem. The RWA method is briefly reviewed, and we show that our method by the similarity transformation gives a solution of the current vanishing problem in the RWA. In chapter 4, we show that the quantum master equation can be exactly replaced with the classical master equation for the calculation of the transport efficiency. Summary and conclusions are given In chapter 5.

Chapter 2

Reduction as Similarity Transformation

2.1 Projection-Operator Technique

Here, we review the Nakajima–Zwanzig method as a general formula to obtain reduced equations.

First, let us consider the quantum system described as

$$\frac{d}{dt}\rho = \mathcal{L}\rho, \quad (2.1)$$

where ρ and $\mathcal{L}$ denote the (reduced) density matrix of the system and the Liouvillian, respectively. Let us introduce the projection superoperator $\mathcal{P}$ and its complement $\mathcal{Q} = 1 - \mathcal{P}$. Utilizing these superoperators, we obtain the following equation for $\mathcal{P}\rho$ from Eq. (2.1):

$$\frac{d}{dt}\mathcal{P}\rho = \mathcal{P}\mathcal{L}\mathcal{P}\rho + \mathcal{P}\mathcal{L}\mathcal{Q} \int_0^t ds e^{\mathcal{Q}\mathcal{L}\mathcal{Q}s} \mathcal{Q}\mathcal{L}\mathcal{P}\rho(t-s). \quad (2.2)$$

The sub-space $\mathcal{P}\rho$ denotes the relevant space (e.g., population space). The above equation is formally derived and the practical usability is not assured. Usually, the separation of the time scales between the relevant space and the irrelevant one is assumed. Let us assume that the reduced density matrix $\mathcal{P}\rho$ varies in a slow time scale and that the generator $e^{\mathcal{Q}\mathcal{L}\mathcal{Q}s}$ stands for decay in a fast time scale. Consequently, Eq. (2.2) becomes as

$$\frac{d}{dt}\mathcal{P}\rho = [\mathcal{P}\mathcal{L}\mathcal{P} - \mathcal{P}\mathcal{L}\mathcal{Q} \frac{1}{\mathcal{Q}\mathcal{L}\mathcal{Q}} \mathcal{Q}\mathcal{L}\mathcal{P}] \mathcal{P}\rho. \quad (2.3)$$

This is a convenient form because the difficulty in calculation is confined to the inverse of the superoperator $Q\mathcal{L}Q$.

2.2 Reduction of Hamiltonian

The strategy of “reduction” is one of the most fundamental idea widely-seen in physics. The reduction from the Dirac equation to the Schrödinger equation is such an example. Here we review the reduction of the Hamiltonian.

Assume that the Dirac equation is presented in the form of coupled equations for 2-spinors:

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} \psi \\ \bar{\psi} \end{pmatrix} = E \begin{pmatrix} \psi \\ \bar{\psi} \end{pmatrix}, \quad (2.4)$$

where E denotes the energy and $H_{i,j}$ ($i, j = 1, 2$) denotes the sub-matrices of the Hamiltonian. $\bar{\psi}$ corresponds to the anti-matter space. If the Hamiltonian is block-diagonal ($H_{12} = H_{21} = 0$), we obtain the eigenvalue problem only for ψ , which can be regarded as the Schrödinger equation.

Naively, one might try to obtain the effective Schrödinger equation by solving the above coupled equation, resulting in the following equation:

$$\left(H_{11} + H_{12} \frac{1}{E - H_{22}} H_{21} \right) \psi = E \psi. \quad (2.5)$$

Although this is the most straightforward way, the above equation produces an unphysical complex-value of the energy.

The first step to overcome this problem is to reconsider the procedure we have done in a different way. In fact, the procedure from equation (2.4) to equation (2.5) can be described by the similarity transformation of the equation (2.4) with the matrix S :

$$S = \begin{pmatrix} I & 0 \\ -(E - H_{22})^{-1} & I \end{pmatrix}, \quad (2.6)$$

where I denotes identity. The inverse operator of S is presented as

$$S^{-1} = \begin{pmatrix} I & 0 \\ (E - H_{22})^{-1} & I \end{pmatrix}. \quad (2.7)$$

Here we should note that the matrix S is not a unitary matrix in general. This is the reason why equation (2.5) does not preserve a physical value of

the energy. To address the problem, the way to construct a suitable unitary transformation has been developed [34, 35].

In the following, we show that the perspective of the similarity transformation is also important in the reduction of master equations.

2.3 Reduction of Liouvillian by Similarity Transformation

In this section, we present a method to extract the effective classical Liouvillian for a quantum system. Our strategy is to split the eigenvalue problem of the Liouvillian into the population part and the coherent part in a certain basis. We show that the splitting procedure can be carried out by a similarity transformation.

First, we define the inner product of operators (A, B) as

$$(A, B) = \text{Tr}[A^\dagger B] \quad (2.8)$$

where A and B denote arbitrary operators. With the definition, we represent the quantum Markovian master equation in the block matrix form:

$$\frac{d}{dt}\rho = \mathcal{L}\rho = \begin{pmatrix} \mathcal{L}_{PP} & \mathcal{L}_{PC} \\ \mathcal{L}_{CP} & \mathcal{L}_{CC} \end{pmatrix} \begin{pmatrix} \rho_P \\ \rho_C \end{pmatrix}. \quad (2.9)$$

Here, ρ_P and ρ_C denote the diagonal and off-diagonal components, respectively, in a certain basis of the density matrix ρ . Since in the present paper, we treat superoperators as matrices and operators as vectors, in order to avoid confusion, we call the subspace spanned by the diagonal components of operators as “P-space” and the remnant space “C-space.” The dynamics is called classical if it is closed in P-space.

We assume that the minimum value of the diagonal components of the superoperator $\mathcal{L}_{CC}$ (say M) is much larger than the maximum of the other components of $\mathcal{L}$ (say m). That is, we assume the relative relation between the diagonal components of $\mathcal{L}_{CC}$ and all the other components of $\mathcal{L}$. This is the condition of application for the method in this study. For example, if the energy levels of the system are not degenerate and the unitary part of the Liouvillian is large compared to other parts, the diagonal components of $\mathcal{L}_{CC}$ in the energy representation have large values, which is also the condition of application for the RWA. In this case, the minimum of the energy level

spacings corresponds to M . In the following, without loss of generality, we set $M = \Gamma$ and $m = 1$ for simplicity.

The solution of the quantum master equation (2.9) is related to the eigenvalue problem

$$\begin{pmatrix} \mathcal{L}_{\text{PP}} & \mathcal{L}_{\text{PC}} \\ \mathcal{L}_{\text{CP}} & \mathcal{L}_{\text{CC}} \end{pmatrix} \begin{pmatrix} \rho_{\text{P}}^E \\ \rho_{\text{C}}^E \end{pmatrix} = E \begin{pmatrix} \rho_{\text{P}}^E \\ \rho_{\text{C}}^E \end{pmatrix}, \quad (2.10)$$

where $\rho^E = (\rho_{\text{P}}^E, \rho_{\text{C}}^E)^T$ denotes the eigenvector corresponding to the eigenvalue E . The above equation can be solved formally, and we obtain the equation for ρ_{P}^E as

$$(\mathcal{L}_{\text{PP}} + \mathcal{L}_{\text{PC}} \frac{1}{E - \mathcal{L}_{\text{CC}}} \mathcal{L}_{\text{CP}}) \rho_{\text{P}}^E = E \rho_{\text{P}}^E. \quad (2.11)$$

The eigenvalues of $\mathcal{L}$ are divided into two groups. One consists of the eigenvalues of $\mathcal{O}(\Gamma^0)$ and the other those of $\mathcal{O}(\Gamma)$. The latter is related to coherence decaying or fast rotating wave dynamics and the time scale is fast. Therefore, the dynamics can be regarded as a classical one when we focus only on phenomena occurring at sufficiently large time scales. For an eigenvalue ϵ that has an $\mathcal{O}(\Gamma^0)$ value, the following equation approximately holds:

$$\left(\mathcal{L}_{\text{PP}} - \mathcal{L}_{\text{PC}} \frac{1}{\mathcal{L}_{\text{CC}}} \mathcal{L}_{\text{CP}} \right) \rho_{\text{P}}^\epsilon = \epsilon \rho_{\text{P}}^\epsilon + \mathcal{O}(\Gamma^{-2}). \quad (2.12)$$

The above procedure can be understood in terms of a similarity transformation of $\mathcal{L}$. The eigenvalue problem expressed by Eq. (2.10) is transformed by an arbitrary non-singular matrix (superoperator) $\mathcal{S}$ without any changes in the eigenvalue:

$$\mathcal{S} \begin{pmatrix} \mathcal{L}_{\text{PP}} & \mathcal{L}_{\text{PC}} \\ \mathcal{L}_{\text{CP}} & \mathcal{L}_{\text{CC}} \end{pmatrix} \mathcal{S}^{-1} \mathcal{S} \begin{pmatrix} \rho_{\text{P}}^E \\ \rho_{\text{C}}^E \end{pmatrix} = E \mathcal{S} \begin{pmatrix} \rho_{\text{P}}^E \\ \rho_{\text{C}}^E \end{pmatrix}. \quad (2.13)$$

Let us define the transformed Liouvillian $\mathcal{L}' \equiv \mathcal{S} \mathcal{L} \mathcal{S}^{-1}$ and the new density matrix $\rho^{E'} \equiv \mathcal{S} \rho^E$. We note that the transformation may violate the property of positive mapping, and in fact, there exists a transformation from a positive mapping Liouvillian to a non-positive mapping Liouvillian. If we choose $\mathcal{S}$ as

$$\mathcal{S} = \begin{pmatrix} I & 0 \\ -(E - \mathcal{L}_{\text{CC}})^{-1} \mathcal{L}_{\text{CP}} & I \end{pmatrix}, \quad (2.14)$$

then, the density matrix is transformed as

$$\rho^{E'} = \mathcal{S}\rho^E = \begin{pmatrix} \rho_P^E \\ 0 \end{pmatrix}. \quad (2.15)$$

This is because the equality

$$\rho_C^E = \frac{1}{E - \mathcal{L}_{CC}} \mathcal{L}_{CP} \rho_P^E \quad (2.16)$$

holds from Eq. (2.10). The transformed Liouvillian $\mathcal{L}'$ is expressed as

$$\mathcal{L}' = \begin{pmatrix} \mathcal{J} & \mathcal{L}_{PC} \\ \mathcal{L}_{CP} + \mathcal{L}_{CC}\mathcal{A} - \mathcal{A}\mathcal{J} & -\mathcal{A}\mathcal{L}_{PC} + \mathcal{L}_{CC} \end{pmatrix}, \quad (2.17)$$

where $\mathcal{A} = (E - \mathcal{L}_{CC})^{-1} \mathcal{L}_{CP}$ and $\mathcal{J} = \mathcal{L}_{PP} + \mathcal{L}_{PC}\mathcal{A}$. Utilizing Eq. (2.10), the following equality holds:

$$(\mathcal{L}_{CP} + \mathcal{L}_{CC}\mathcal{A} - \mathcal{A}\mathcal{J})\rho_P^E = 0. \quad (2.18)$$

For an eigenvalue ϵ , $\mathcal{S}$ approximately becomes

$$\mathcal{S} \simeq \begin{pmatrix} I & 0 \\ \mathcal{L}_{CC}^{-1} \mathcal{L}_{CP} & I \end{pmatrix}, \quad (2.19)$$

which does not depend on eigenvalues. All the eigenvectors of $\mathcal{O}(\Gamma^0)$ are transformed as Eq. (2.15).

Next, let us consider the time evolution of the density matrix. A density matrix is expanded by the eigenvectors of the Liouvillian, and its time evolution can be expressed as

$$\rho(t) = e^{\mathcal{L}t} \rho(0) = e^{\mathcal{L}t} \left(\sum_{\alpha} C_{\alpha} \rho^{\alpha} + \sum_{\beta} C'_{\beta} \rho^{\beta} \right), \quad (2.20)$$

where the ρ^{α} values denote the eigenvectors of the Liouvillian, which correspond to the eigenvalues of $\mathcal{O}(\Gamma^0)$, and the ρ^{β} values denote the eigenvectors corresponding to the eigenvalues of $\mathcal{O}(\Gamma)$. C_{α} and C'_{β} denote the coefficients of the expansion. We can ignore the summation over β in Eq. (2.20) because the time evolution of ρ^{β} is fast-decaying in the case wherein the real parts of the eigenvalues are large or the time evolution is fast-rotating if the imaginary parts of the eigenvalues are large. Consequently, this density matrix is transformed into

$$\mathcal{S}\rho(0) \simeq \begin{pmatrix} \rho_P^{(0)} \\ 0 \end{pmatrix}. \quad (2.21)$$

The Liouvillian is transformed by $\mathcal{S}$ in Eq. (2.19) into

$$\mathcal{L}' = \mathcal{S}\mathcal{L}\mathcal{S}^{-1} \simeq \begin{pmatrix} \mathcal{L}_{\text{PP}} - \mathcal{L}_{\text{PC}}\mathcal{L}_{\text{CC}}^{-1}\mathcal{L}_{\text{CP}} & \mathcal{L}_{\text{PC}} \\ \mathcal{L}_{\text{CC}}^{-1}\mathcal{L}_{\text{CP}}(\mathcal{L}_{\text{PP}} - \mathcal{L}_{\text{PC}}\mathcal{L}_{\text{CC}}^{-1}\mathcal{L}_{\text{CP}}) & \mathcal{L}_{\text{CC}}^{-1}\mathcal{L}_{\text{CP}}\mathcal{L}_{\text{PC}} + \mathcal{L}_{\text{CC}} \end{pmatrix}. \quad (2.22)$$

We can regard the left-bottom block of $\mathcal{L}'$ in Eq. (2.22) as zero matrix because we ignore the β -summation part and the left-bottom block of $\mathcal{L}'$ does not affect the dynamics by virtue of Eqs. (2.17)–(2.19). From Eqs. (2.15), (2.19), and (2.21), we obtain the following equation:

$$\mathcal{S}\rho(t) = e^{\mathcal{L}'t}\mathcal{S}\rho(0) \simeq \begin{pmatrix} e^{\mathcal{L}_{\text{eff}}t}\rho_{\text{P}}(0) \\ 0 \end{pmatrix}, \quad (2.23)$$

where we define the superoperator $\mathcal{L}_{\text{eff}}$ as

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\text{PP}} - \mathcal{L}_{\text{PC}}\mathcal{L}_{\text{CC}}^{-1}\mathcal{L}_{\text{CP}}. \quad (2.24)$$

This expression is equivalent to Eq. (2.12). As can be inferred from the following sections, the effective classical Liouvillian $\mathcal{L}_{\text{eff}}$ thus defined is a generalization including the results of previous studies [40, 41] and the RWA.

The foregoing formulation utilizing a similarity transformation provides an important perspective on the calculation of physical quantities. The statistical average of an arbitrary physical observable A can be written as:

$$\text{Tr}[A\rho(t)] = \text{Tr}[\mathcal{A}\mathcal{S}^{-1}\mathcal{S}\rho(t)] = \text{Tr}[\mathcal{A}\mathcal{S}^{-1}e^{\mathcal{L}_{\text{eff}}t}\rho_{\text{P}}(0)]. \quad (2.25)$$

Thus, when we reduce the quantum master equation to the classical one, the observable A also should be transformed to $\tilde{A}$ as:

$$\tilde{A} = \mathcal{A}\mathcal{S}^{-1} = \{\mathcal{S}^{-1}\}^\dagger A, \quad (2.26)$$

where we introduce the adjoint superoperator for convenience, which is defined for an arbitrary superoperator $\mathcal{K}$ as [5, 24]

$$\text{Tr}[A\mathcal{K}\rho] = \text{Tr}[(\mathcal{K}^\dagger A)\rho]. \quad (2.27)$$

From Eq. (2.19), $\tilde{A}$ is written as

$$\tilde{A} = \{1 - \mathcal{P}\mathcal{L}^\dagger\{(1 - \mathcal{P})\mathcal{L}^\dagger(1 - \mathcal{P})\}^{-1}\}A, \quad (2.28)$$

where the superoperator $\mathcal{P}$ represents the projection superoperator onto the P-space. If A has no C-space components, it is not changed by $\mathcal{S}$. The transformation given by Eq. (2.28) is a novel and important outcome of our formulation, and it explains why the RWA results in problems in the study of energy transport and further explains how the physical consistency can be recovered.

2.4 Example

In this section, we apply the method described in the previous section to a simple physical system. We consider a single particle hopping on a one-dimensional lattice with a periodic boundary condition, which is given by the Hamiltonian:

$$H = \sum_{k=1}^N (|k\rangle \langle k+1| + |k+1\rangle \langle k|), \quad (2.29)$$

where the ket-vector $|k\rangle$ represents the particle being at the site k and $|N+1\rangle = |1\rangle$. We assume that the system is influenced by its environment and the dynamics is described by the following Lindblad equation:

$$\frac{d}{dt}\rho = i[\rho, H] + \Gamma \sum_{k=1}^N (n_k \rho n_k - \frac{1}{2} \{n_k, \rho\}), \quad (2.30)$$

where $n_k = |k\rangle \langle k|$ and $\{.,.\}$ denotes the anticommutator. The non-unitary part in Eq. (2.30) is called “pure dephasing,” which is one of the simplest models of the environmental noise, and it has been frequently used in studies of quantum transport efficiency [3, 30–32] and quantum transport in the stationary state [36–39].

Here, we represent the Liouvillian with the basis $\{|k\rangle \langle j|\}$ ($k, j = 1, 2, \dots, N$). Consequently, the diagonal components of the matrix $\mathcal{L}_{CC}$ are $-\Gamma$. Thus, we can apply our method if $\Gamma \gg 1$, which results in

$$\frac{d}{dt}\rho_P = \mathcal{L}_{\text{eff}}\rho_P = -\mathcal{L}_{PC}\mathcal{L}_{CC}^{-1}\mathcal{L}_{CP}\rho_P. \quad (2.31)$$

Let us next consider the operation of $\mathcal{L}_{\text{eff}}$ on n_k . The superoperator $\mathcal{L}_{CP}$ yields

$$\mathcal{L}_{CP}n_k = i(|k\rangle \langle k-1| - |k-1\rangle \langle k|) - i(|k+1\rangle \langle k| - |k\rangle \langle k+1|). \quad (2.32)$$

Although calculating the inverse operator $\mathcal{L}_{CC}^{-1}$ is difficult in general, it is approximately given by

$$\mathcal{L}_{CC}^{-1} |k\rangle \langle k+1| = -\frac{1}{\Gamma} |k\rangle \langle k+1| + \mathcal{O}(\frac{1}{\Gamma^2}). \quad (2.33)$$

Using Eqs. (2.31)–(2.33), we obtain

$$\mathcal{L}_{\text{eff}}n_k = \frac{2}{\Gamma}(n_{k-1} - 2n_k + n_{k+1}). \quad (2.34)$$

This can be rewritten in the following Lindblad form

$$\frac{d}{dt}\rho_{\text{P}} = \frac{2}{\Gamma} \sum_{k=1}^N \sum_{i=L,R} (L_{k,k+1}^{(i)} \rho_{\text{P}} L_{k,k+1}^{(i)\dagger} - \frac{1}{2} \{L_{k,k+1}^{(i)\dagger} L_{k,k+1}^{(i)}, \rho_{\text{P}}\}), \quad (2.35)$$

where

$$L_{k,k+1}^{(L)} = |k\rangle \langle k+1|, \quad L_{k,k+1}^{(R)} = |k+1\rangle \langle k|. \quad (2.36)$$

Thus, the population dynamics shows a diffusive behaviour that obeys Eq. (2.34). This result agrees with those of previous works [37, 38, 40, 41].

We next compare the original quantum dynamics with the classical reduction. We consider the case wherein the particle is initially at site N . In our study, we numerically calculated the population at site 1, $P_1(t) = \text{Tr}[n_1 \rho(t)]$ for the system size $N = 5$ and three different values of the dephasing rate Γ (Fig. 2.1). In all cases, the population P_1 converges to $1/5$. However, the intermediate behaviour of the reduced equation is different from the original quantum dynamics for $\Gamma = 0.1$ and $\Gamma = 1$. In contrast, for the case of $\Gamma = 10$, the classical and the quantum time evolutions agree with each other. This is because quantum effects decreases as the dephasing rate increases.

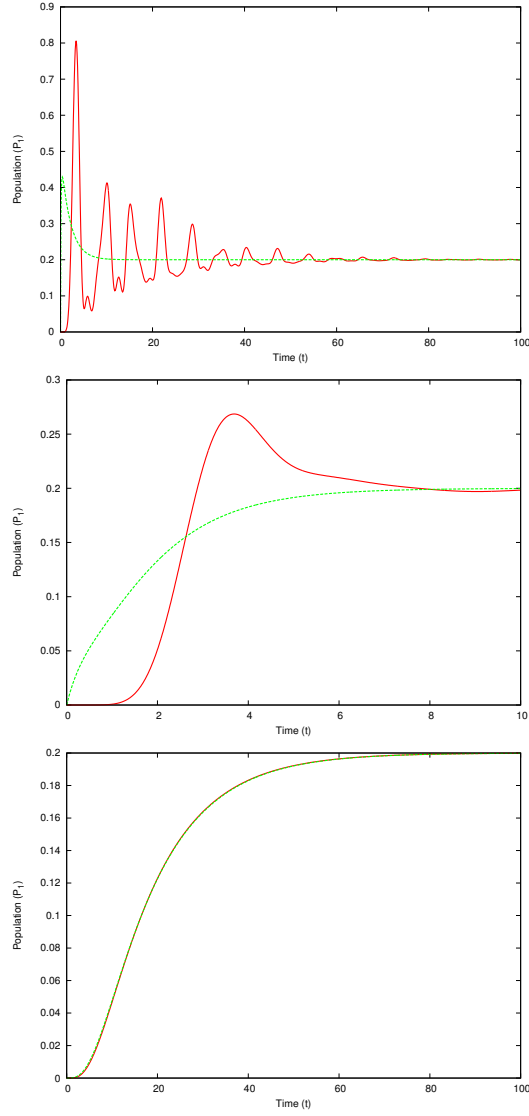


Figure 2.1: Time evolution of P_1 for three different values of dephasing rate: $\Gamma = 0.1$ (top), $\Gamma = 1.0$ (middle), and $\Gamma = 10$ (bottom). The red and dashed-green lines in each panel denote results based on the original quantum dynamics (2.30) and the effective classical equation (2.31), respectively.

Chapter 3

Quantum Energy Transport and the RWA

3.1 Energy Transport and RWA

In this section, we show that our formulation includes the RWA that is a standard method to study quantum open systems. By means of our method, we can clearly explain why the RWA gives unphysical results for energy transport problems.

A system in contact with heat reservoirs is frequently described by the Redfield equation [18–21]. It is derived from the total Hamiltonian:

$$H_{\text{tot}} = H_{\text{S}} + \lambda H_{\text{SB}} + H_{\text{B}}, \quad (3.1)$$

where H_{S} , H_{SB} , and H_{B} denote the system Hamiltonian, the system–bath interaction Hamiltonian, and the bath Hamiltonian respectively. The system–bath coupling λ is assumed to be weak. Here, we assume H_{SB} as the following:

$$H_{\text{SB}} = X \otimes Y, \quad (3.2)$$

where X and Y denote Hermitian operators that operate on the Hilbert space of the system and that of the bath, respectively. Utilizing the second-order perturbation with several approximations, the Redfield equation is obtained in the following form:

$$\frac{d}{dt}\rho = \mathcal{L}^{(\text{Red})}\rho = i[\rho, H_{\text{S}}] + \pi\lambda^2 \sum_{i,j} (\Gamma_{ij} \langle \epsilon_i | X | \epsilon_j \rangle [|\epsilon_i\rangle \langle \epsilon_j| \rho, X] + h.c.), \quad (3.3)$$

where $|\epsilon_i\rangle$ denotes the energy eigenstate of the eigenvalue ϵ_i of H_S and Γ_{ij} denote the Fourier transformations of the reservoir correlation function. The temperature of the reservoir β is given by the Kubo–Martin–Schwinger condition:

$$\Gamma_{ij} = e^{-\beta(\epsilon_i - \epsilon_j)} \Gamma_{ji}. \quad (3.4)$$

The RWA is usually carried out by considering the interaction picture, which results in the following classical master equation [5]:

$$\frac{d}{dt} P_k(t) = 2\pi\lambda^2 \sum_i (\Gamma_{ki} |X_{ik}|^2 P_i(t) - \Gamma_{ik} |X_{ik}|^2 P_k(t)), \quad (3.5)$$

where $P_k(t)$ denotes the probability of observing the energy ϵ_k at time t . The energy-current operators has no sense in the RWA [6]. If we write the Hamiltonian H_S as

$$H = \sum_{k=1}^N H_k, \quad (3.6)$$

the energy current operator from site k to $k+1$ is defined by

$$J_{k,k+1} = i[H_k, H_{k+1}]. \quad (3.7)$$

Let us consider the quantity $\langle E | J_{k,k+1} | E \rangle$ where $|E\rangle$ is an eigenvector of the Hailtonian H_S . From the equality

$$i[H_S, H_k] = J_{k-1,k} - J_{k,k+1}, \quad (3.8)$$

we obtain

$$\langle E | J_{k-1,k} | E \rangle = \langle E | J_{k,k+1} | E \rangle. \quad (3.9)$$

Repeating this to the end of the chain, we find $\langle E | J_{k-1,k} | E \rangle = 0$ for $k = 1, 2, \dots, N-1$. That is, the energy current operators are off-diagonal in the energy representation. Thus, the energy current operators have no physical values in the RWA.

It is easily verified that Eq. (3.5) is equivalent to time evolution by $\mathcal{L}_{PP}^{(\text{Red})}$ with the energy representation. The Redfield equation (3.3) is obtained by means of the second-order perturbation with respect to λ . Hence, for the same level of accuracy, the effective classical Liouvillian (2.24) becomes $\mathcal{L}_{\text{eff}} \simeq \mathcal{L}_{PP}^{(\text{Red})}$. This indicates that the procedure of the RWA represented by Eq. (3.3) through Eq. (3.5) is accounted for in our formulation, and it also indicates that at the same time the observables should be transformed by Eq. (2.28).

3.2 Example

As an example, let us calculate the expectation value of the energy current in the steady state for the following non-equilibrium systems:

$$\begin{cases} \frac{d}{dt}\rho = i[\rho, H] + \gamma(\sigma_1^- \rho \sigma_1^+ - \frac{1}{2}\{\sigma_1^+ \sigma_1^-, \rho\}) + \gamma(\sigma_2^+ \rho \sigma_2^- - \frac{1}{2}\{\sigma_2^- \sigma_2^+, \rho\}) \\ H = |1\rangle\langle 2| + |2\rangle\langle 1| + h(n_1 + n_2). \end{cases} \quad (3.10)$$

where $\sigma_k^+ = |k\rangle\langle 0|$, $\sigma_k^- = |0\rangle\langle k|$, and $|0\rangle$ denotes the vacuum state. Here we are only concerned with the single exciton space, that is, we exclude the state $\sigma_1^+ \sigma_2^+ |0\rangle$. Although we introduce the above quantum master equation a priori here, the RWA can be performed for weak coupling, i.e., small values of γ . The eigenvalues of the Hamiltonian are $\epsilon_0 = 0$, $\epsilon_1 = h - 1$, and $\epsilon_2 = h + 1$. The RWA can be performed if $\epsilon_i - \epsilon_j \gg \gamma$ ($i \neq j$) is satisfied, and it can be realized by assuming a suitable value of h . We define the energy current J as

$$J = -ih(|1\rangle\langle 2| - |2\rangle\langle 1|) \quad (3.11)$$

As in the case of the Redfield equation, for the purpose of simplicity, we ignore the second- and higher-order γ terms.

We first calculate the expectation of the energy current $\langle J \rangle$ in the steady state without using the RWA. The bracket $\langle \rangle$ denotes the statistical average of the observables. The time derivative of an observable A is given by

$$\frac{d}{dt}A = \mathcal{L}^\dagger A = -i[A, H] + \gamma(\sigma_1^+ A \sigma_1^- - \frac{1}{2}\{\sigma_1^+ \sigma_1^-, A\}) + \gamma(\sigma_2^- A \sigma_2^+ - \frac{1}{2}\{\sigma_2^- \sigma_2^+, A\}). \quad (3.12)$$

Using this equation, we can write the time derivatives of the expectation values of observables by

$$\begin{cases} \frac{d}{dt}\langle J \rangle = -2h(\langle n_1 \rangle - \langle n_2 \rangle) - \frac{\gamma}{2}\langle J \rangle \\ \frac{d}{dt}\langle n_1 \rangle = \frac{1}{h}\langle J \rangle - \gamma\langle n_1 \rangle \\ \frac{d}{dt}\langle n_2 \rangle = -\frac{1}{h}\langle J \rangle + \gamma\langle n_2 \rangle. \end{cases} \quad (3.13)$$

Moreover, the completeness relation

$$\sum_{k=0}^2 n_k = 1 \quad (3.14)$$

holds. In the steady state, the left-hand sides of the equations (3.13) vanish. Solving Eqs. (3.13) and (3.14), we obtain the expectation value of the energy current in the steady state:

$$\langle J \rangle \simeq \frac{\gamma h}{3}, \quad (3.15)$$

where the higher order of γ has been omitted.

Next, we compute the energy current J with the RWA. The RWA results in the classical Liouvillian:

$$\mathcal{L}_{\text{eff}} = \frac{\gamma}{2} \begin{pmatrix} -2 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix}, \quad (3.16)$$

where the basis $\{|\epsilon_0\rangle\langle\epsilon_0|, |\epsilon_1\rangle\langle\epsilon_1|, |\epsilon_2\rangle\langle\epsilon_2|\}$ is used in this order. The steady-state solution of the Liouvillian (3.16) is given as

$$\rho^{\text{ss}} = \frac{1}{3}(|\epsilon_0\rangle\langle\epsilon_0| + |\epsilon_1\rangle\langle\epsilon_1| + |\epsilon_2\rangle\langle\epsilon_2|). \quad (3.17)$$

The energy current is expressed in the energy basis as

$$J = i\hbar(|\epsilon_1\rangle\langle\epsilon_2| - |\epsilon_2\rangle\langle\epsilon_1|). \quad (3.18)$$

We note that the expression for J has no P-space components. In conventional approaches, the energy current J is used without any changes, thereby resulting in $\text{Tr}[J\rho^{\text{ss}}] = 0$. This brings to light the necessity of the transformation of J to $\tilde{J}$. From Eqs. (2.28) and (3.12), the transformed current $\tilde{J}$ is given as

$$\tilde{J} \simeq J + \frac{\gamma h}{4}(2|\epsilon_0\rangle\langle\epsilon_0| + |\epsilon_1\rangle\langle\epsilon_1| + |\epsilon_2\rangle\langle\epsilon_2|), \quad (3.19)$$

which reproduces the correct expectation value of the energy current

$$\langle \tilde{J} \rangle = \text{Tr}[\tilde{J}\rho^{\text{ss}}] = \frac{\gamma h}{3}. \quad (3.20)$$

Chapter 4

Quantum Transport Efficiency

4.1 Basic Settings

The system we consider in this chapter is a single exciton hopping on a network of N sites whose Hamiltonian is given by

$$H = \sum_{k,j} H_{k,j} |k\rangle \langle j|, \quad (4.1)$$

where the ket-vector $|k\rangle$ represents the particle being at the site k . A diagonal element of the Hamiltonian $H_{k,k}$ denotes the on-site energy and an off-diagonal element $H_{k,j}$ represents the exchange energy between the site k and site j . We assume that the system is under the influence of its environment, and its time evolution is Markovian. The role of the environment is dephasing and dissipation processes. Dephasing processes conserving the number of exciton is described by the superoperator as

$$\mathcal{L}_{\text{deph}}\rho = \sum_k^N \Gamma_k (n_k \rho n_k - \frac{1}{2} \{n_k, \rho\}), \quad (4.2)$$

while dissipation processes are described as

$$\mathcal{L}_{\text{diss}}\rho = \sum_k^N \mu (\sigma_k^- \rho \sigma_k^+ - \frac{1}{2} \{\sigma_k^+ \sigma_k^-, \rho\}), \quad (4.3)$$

where $n_k = |k\rangle \langle k|$ and the bracket $\{.,.\}$ denotes the anti-commutator. The raising and lowering operators at the k -th site are denoted by σ_k^+ and σ_k^- ,

respectively. To argue the efficiency of transport, we introduce trapping processes that catch the exciton at site l . The trapping process is given as

$$\mathcal{L}_{\text{trap}}\rho = \kappa(\sigma_l^- \rho \sigma_l^+ - \frac{1}{2}\{\sigma_l^+ \sigma_l^-, \rho\}). \quad (4.4)$$

Thus, time evolution of the density matrix is described by the Lindblad equation

$$\frac{d}{dt}\rho = i[\rho, H] + (\mathcal{L}_{\text{deph}} + \mathcal{L}_{\text{diss}} + \mathcal{L}_{\text{trap}})\rho, \quad (4.5)$$

where parameters Γ_k , μ and κ are positive number. The transport efficiency is defined by how often the exciton is trapped at site τ during the time interval t , which is expressed by

$$\zeta(t) = \kappa \int_0^t ds \text{Tr}[n_\tau e^{\mathcal{L}s} \rho(0)], \quad (4.6)$$

where $\mathcal{L}$ is the Liouvillian that dominates the dynamics (4.5). In many studies, infinitely long time interval is assumed so that the exciton fully goes out the system. We also take the long time limit $t = \infty$ and express the transport efficiency $\zeta = \zeta(\infty)$.

4.2 Exact Replacement with Population Dynamics

The reduced equation (2.24) is derived by expanding the original quantum master equation with respect to $1/\Gamma$. Therefore, it is only valid for large values of Γ . In this section, we show that the replacement of quantum dynamics with the classical equation can be carried out for any values of the parameters for quantities such as transport efficiency.

Let us consider the quantum open system that is described by the Markovian quantum master equation:

$$\frac{d}{dt}\rho = \mathcal{L}\rho. \quad (4.7)$$

Let us assume that the quantum master equation has a unique steady state ρ^{ss} . Let us consider the following quantity:

$$\zeta = \int_0^\infty dt \text{Tr}[A e^{\mathcal{L}t} \rho(0)], \quad (4.8)$$

where A denotes a P-space observable that satisfies $\text{Tr}[A\rho^{\text{ss}}] = 0$.

We first show that the time integral in Eq. (4.8) is related to a certain steady-state problem from the analogy of the linear-response theory. For this purpose, we modify the Liouvillian $\mathcal{L}$ to $\mathcal{K}$ as

$$\mathcal{K} = \mathcal{L} + \epsilon\chi, \quad (4.9)$$

where ϵ is the small parameter and the superoperator χ satisfies

$$\chi = \mathcal{P}\chi\mathcal{P}, \quad \chi\rho^{\text{ss}} = \chi\rho_{\text{P}}^{\text{ss}} = \rho(0), \quad (4.10)$$

where $\rho_{\text{P}}^{\text{ss}}$ denotes the P-space components of ρ^{ss} . The steady-state solution η of the modified Liouvillian $\mathcal{K}$ is expressed as

$$\eta = \rho^{\text{ss}} + \epsilon \int_0^\infty dt e^{\mathcal{L}t} \chi \rho^{\text{ss}} + \mathcal{O}(\epsilon^2) = \rho^{\text{ss}} + \epsilon \int_0^\infty dt e^{\mathcal{L}t} \rho(0) + \mathcal{O}(\epsilon^2). \quad (4.11)$$

Thus, ζ can be represented as

$$\zeta = \lim_{\epsilon \rightarrow 0} \epsilon^{-1} \text{Tr}[A\eta] = \lim_{\epsilon \rightarrow 0} \epsilon^{-1} \text{Tr}[A\eta_{\text{P}}], \quad (4.12)$$

where η_{P} represents the P-space components of η .

The steady-state problem is expressed as

$$\begin{pmatrix} \mathcal{L}_{\text{PP}} + \epsilon\chi & \mathcal{L}_{\text{PC}} \\ \mathcal{L}_{\text{CP}} & \mathcal{L}_{\text{CC}} \end{pmatrix} \begin{pmatrix} \eta_{\text{P}} \\ \eta_{\text{C}} \end{pmatrix} = 0. \quad (4.13)$$

Let us transform the above equation by the superoperator $\mathcal{S}$

$$\mathcal{S} = \begin{pmatrix} I & 0 \\ \mathcal{L}_{\text{CC}}^{-1} \mathcal{L}_{\text{CP}} & I \end{pmatrix}. \quad (4.14)$$

From Eqs. (2.14) and (2.15), we obtain the following equation:

$$\mathcal{S}\mathcal{L}\mathcal{S}^{-1}\mathcal{S}\eta = \begin{pmatrix} \mathcal{L}_{\text{eff}} + \epsilon\chi & \mathcal{L}_{\text{PC}} \\ \mathcal{L}_{\text{CC}}^{-1} \mathcal{L}_{\text{CP}} (\mathcal{L}_{\text{eff}} + \epsilon\chi) & \mathcal{L}_{\text{CC}}^{-1} \mathcal{L}_{\text{CP}} \mathcal{L}_{\text{PC}} + \mathcal{L}_{\text{CC}} \end{pmatrix} \begin{pmatrix} \eta_{\text{P}} \\ 0 \end{pmatrix} = 0. \quad (4.15)$$

Thus, η_{P} is the steady-state solution of the superoperator $\mathcal{L}_{\text{eff}} + \epsilon\chi$, and it can be expressed as

$$\eta_{\text{P}} = \rho_{\text{P}}^{\text{ss}} + \epsilon \int_0^\infty dt e^{\mathcal{L}_{\text{eff}}t} \rho(0) + \mathcal{O}(\epsilon^2). \quad (4.16)$$

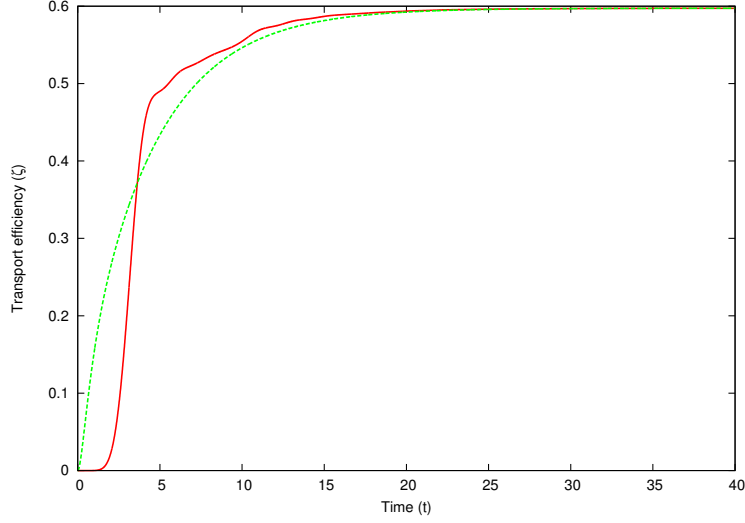


Figure 4.1: Numerical calculation of $\zeta(t)$ based on the original quantum dynamics (red line) and the classical dynamics (green dashed-line). The original quantum evolution asymptotically coincides with the classical replacement in the long-time regime.

Using Eqs. (4.11), (4.12), and (4.16), we obtain the following equation:

$$\zeta = \int_0^\infty dt \text{Tr}[Ae^{\mathcal{L}t}\rho(0)] = \int_0^\infty dt \text{Tr}[Ae^{\mathcal{L}_{\text{eff}}t}\rho(0)]. \quad (4.17)$$

Thus, the time evolution of the quantum system is fully replaced by population dynamics.

To validate the above argument, we numerically calculate the quantum transport efficiency for the system given by the following equation:

$$\frac{d}{dt}\rho = \mathcal{L}\rho = i[\rho, H] + \mathcal{L}_{\text{deph}}\rho + \mathcal{L}_{\text{diss}}\rho + \mathcal{L}_{\text{trap}}\rho, \quad (4.18)$$

where the Hamiltonian H is the tight-binding model given by Eq. (2.29),

and the Lindblad superoperators are given by

$$\begin{cases} \mathcal{L}_{\text{deph}} = \Gamma \sum_{k=1}^N (n_k \rho n_k - \frac{1}{2} \{n_k, \rho\}) \\ \mathcal{L}_{\text{diss}} = \mu \sum_{k=1}^N (\sigma_k^- \rho \sigma_k^+ - \frac{1}{2} \{\sigma_k^+ \sigma_k^-, \rho\}) \\ \mathcal{L}_{\text{trap}} = \kappa (\sigma_1^- \rho \sigma_1^+ - \frac{1}{2} \{\sigma_1^+ \sigma_1^-, \rho\}). \end{cases} \quad (4.19)$$

Let us suppose that the particle is at the N -th site initially. We numerically calculate the time evolution of $\zeta(t)$ with parameters $N = 5$, $\kappa = 1$, $\mu = 0.1$, and $\Gamma = 0.1$ (Fig. 4.1). The classical time evolution based on the Liouvillian $\mathcal{L}_{\text{eff}}$ does not coincide with the original quantum time evolution in the short-time regime; however, the time evolutions converge with the same value in the long-time regime.

We note that the superoperator $\mathcal{L}_{\text{eff}}$ does not ensure the positivity of the density matrix in general. Nevertheless, in the case of the transport efficiency problem, the time evolution can be intuitively interpreted. This is because the superoperator $\mathcal{L}_{\text{eff}}$ is trace-preserving. Therefore, the particle flow can be defined. The only difference with respect to the general classical picture is that negative values of population can be obtained.

4.3 ENAQT in ordered systems

Recently, Kassal and Aspuru-Guzik have pointed out that ENAQT phenomena can occur also in ordered systems. This means that there exists another mechanism of ENAQT different from suppression of Anderson localization [31]. In the three-site ordered chain, there are two regions where ENAQT can be seen. One is the case where both the trapping rate κ and the dissipation rate μ are small. The other is the case where μ is small but κ has a large value. In this section, we study the problem in the replaced classical picture and clarify the reason why ENAQT is observed.

The system we consider here is given by equations (4.18) and (4.19) with $N = 3$. The replaced Liouvillian $\mathcal{L}_{\text{eff}}$ can be analytically calculated for such

a small system and it is given by

$$\mathcal{L}_{\text{eff}} = \begin{pmatrix} 0 & \kappa + \mu & \mu & \mu \\ 0 & -\kappa - \mu - L_{2,1} - L_{3,1} & L_{1,2} & L_{1,3} \\ 0 & L_{2,1} & -\mu - L_{1,2} - L_{3,2} & L_{2,3} \\ 0 & L_{3,1} & L_{3,2} & -\mu - L_{1,3} - L_{2,3} \end{pmatrix}, \quad (4.20)$$

where we represent the Liouvillian with the basis $\{|0\rangle\langle 0|, |1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|\}$ in this order and

$$\begin{cases} L_{1,2} = L_{2,1} = \frac{4(\kappa + 2\mu + 2\Gamma)(\mu + \Gamma)}{(\kappa + 2\mu + 2\Gamma)^2(\mu + \Gamma) + 2\kappa + 8\mu + 8\Gamma} \\ L_{2,3} = L_{3,2} = \frac{2(\kappa + 2\mu + 2\Gamma)^2}{(\kappa + 2\mu + 2\Gamma)^2(\mu + \Gamma) + 2\kappa + 8\mu + 8\Gamma} \\ L_{1,3} = L_{3,1} = \frac{8}{(\kappa + 2\mu + 2\Gamma)^2(\mu + \Gamma) + 2\kappa + 8\mu + 8\Gamma}. \end{cases} \quad (4.21)$$

The replaced Liouvillian $\mathcal{L}_{\text{eff}}$ is a positive map in this case because parameters κ , μ and Γ are non-negative. ENAQT can be seen if the particle is on the central site at the initial time, while it is not observed in the case where the source and trap lie at opposite ends of the chain.

First, we consider the case where κ and μ are small. Figure 4.2 shows that ENAQT occurs when dephasing of $\mathcal{O}(\mu)$ is applied. Let us see this phenomena in the classical picture. Assume that the dissipation rate μ is small and the dephasing rate is $\Gamma = \mathcal{O}(\mu)$. We here focus on the particle movement, therefore, for simplicity, we set $\kappa = 0$. Under these conditions, hopping rates (4.21) become $L_{1,2} = L_{2,3} \simeq \mu + \Gamma$ and $L_{1,3} \simeq (\mu + \Gamma)^{-1}$. Thus, dephasing increases nearest neighbor hopping rates and decreases end-to-end hopping rates. This shows why ENAQT occurs when the source is at the center of the chain and does not if it is at the end.

We next consider the other situation of ENAQT in the ordered system. Figure 4.2 shows that the transport efficiency with the highly large trapping rate is less than those with small trapping rates. In the classical picture, it can be understood that the denominator in equations (4.21) is the function of κ^2 and the particle will not move to the other site in large κ situation. Although the transport efficiency is quite small, ENAQT is also seen in such a situation. Assuming that the dissipation rate μ is small and the trapping rate $\kappa = \mu^{-2}$, hopping rates with $\Gamma = 0$ are given by $L_{1,2} \simeq 4\mu^2$, $L_{2,3} \simeq 2\mu^{-1}$ and $L_{1,3} \simeq 8\mu^3$. ENAQT is observed when dephasing $\Gamma = \mathcal{O}(\mu^{-1})$ exists and

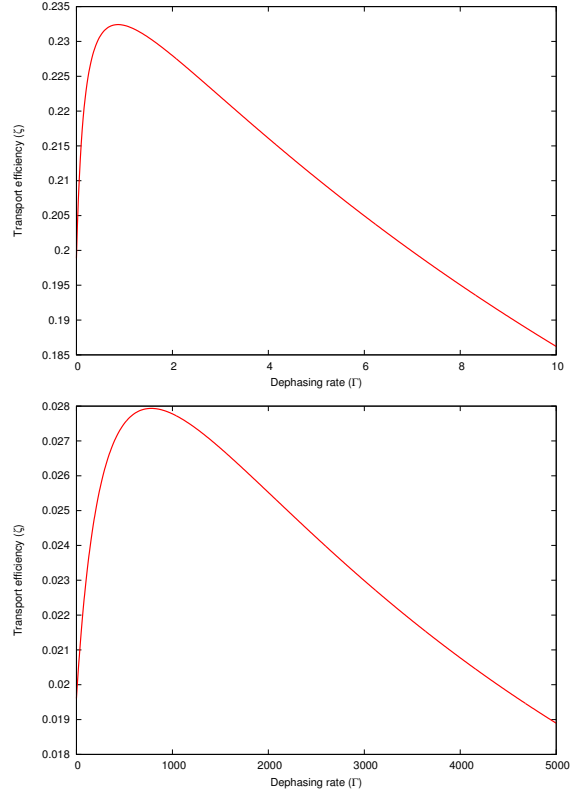


Figure 4.2: ENAQT in the three site system. The particle is initially at the center of the chain. The left panel is in the case where both the trapping rate and the dissipation rate are small ($\kappa = \mu = 0.1$). The right panel is the other situation where the trapping rate is large and the dissipation rate is small ($\kappa = 10^4$ and $\mu = 10^{-2}$).

here we take $\Gamma = \mu^{-1}$. Then, the hopping rates are changed as: $L_{1,2} \simeq 4\mu^2$, $L_{2,3} \simeq 2\mu$ and $L_{1,3} \simeq 8\mu^5$. The role of dephasing in this case is equalization of $L_{1,2}$ and $L_{2,3}$, that is, hopping rates from the central site to both ends become almost the same order with respect to μ due to dephasing. This fact favors the transfer of the particle to the trapping site. However, the dissipation rate μ becomes relatively large. As a result, quite a small improvement of the transport efficiency is observed.

Thus, we can analyze ENAQT phenomena on the basis of the classical picture. Although the three-site system is very small, we expect that the essence of ENAQT phenomena can be understood with such a small system. ENAQT in disordered systems and the effect of the space-dependent dephasing can be explained in the same manner.

Chapter 5

Conclusions

In this thesis, we have presented the formulation of a quantum-to-classical reduction of quantum master equations utilizing the similarity transformation. The main difference between the conventional projection-operator technique and our method is the transformation of observables. The transformation of observables gives a solution of the current vanishing problem in the RWA scheme. We have confirmed this in the simple example. The transformation of observables is natural because a density matrix has a physical meaning only if we compute the statistical average of an observables.

We expect that the solution of the current vanishing problem presents a development in the study of quantum energy transport. In the study of energy transport in many-body systems, a local energy is also an intriguing quantity. The similarity transformation makes it possible to calculate the proper value of the local energy for the RWA-equation.

We also have shown that the exact replacement with the classical master equation can be carried out for the calculation of the quantity like transport efficiency. We have applied the fact for three-site ordered chain. Understanding the transport efficiency is difficult even in classical systems because it is defined as the time integration. However, some intuitive interpretation can be obtained.

Bibliography

- [1] G. S. Engel, T. R. Calhoun, E. L. Read, T-K. Ahn, T. Mančal, Y-C. Chen, R. E. Blankenship and G. R. Fleming, *Nature* **446**, 782 (2007)
- [2] E. Collini, C. Y. Wong, K. E. Wilk, P. M. G. Curmi, P. Brumer and G. D. Scholes, *Nature* **463**, 644 (2010)
- [3] M. B. Plenio and S. F. Huelga, *New J. Phys.* **10**, 113019 (2008)
- [4] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd and A. Aspuru-Guzik, *New J. Phys.* **11** 033003 (2009)
- [5] H-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002)
- [6] H. Wichterich, M. J. Henrich, H-P. Breuer, J. Gemmer, and M. Michel, *Phys. Rev. E* **76**, 031115 (2007)
- [7] M. Esposito, U. Harbola, and S. Mukamel, *Rev. Mod. Phys.* **81**, 1665 (2009)
- [8] T. Yuge, T. Sagawa, A. Sugita, and H. Hayakawa, *Phys. Rev. B* **86**, 235308 (2012)
- [9] G. Lindblad, *Commun. Math. Phys.* **48**, 119 (1976)
- [10] A. Dhar, *Advances in Physics* **57** (5), 457 (2008)
- [11] M. Znidaric, T. Prosen, G. Benetti, G. casati, and D. Rossini, *Phys. Rev. E* **81**, 051135 (2010)
- [12] M. Michel and O. Hess, *Phys. Rev. B* **77**, 104303 (2008)

- [13] T. Prosen, New J. Phys. **10**, 043026 (2008)
- [14] R. Steinigeweg, M. Ogiewa, and J. Gemmer, EPL **87**, 10002 (2009)
- [15] K. Sun, C. Wang, and Q. Chen, EPL **92**, 24002 (2010)
- [16] W. Li and P. Tong, Phys. Rev. E **83**, 031128 (2011)
- [17] K. Saito, Europhys Lett. **61**, 34 (2003)
- [18] K. Saito, S. Takesue, and S. Miyashita, Phys. Rev. E **61**, 2397 (2000)
- [19] Y. Yan, C.-Q. Wu, G. Casati, T. Prosen, and B. Li, Phys. Rev. B **77**, 172411 (2008)
- [20] T. Prosen and B. Žunkovič, New J. Phys. **12**, 025016 (2010)
- [21] J. Wu and M. Berciu, Phys. Rev. E **83**, 214416 (2011)
- [22] S. Attal and Y. Pautrar, Ann. Henri Poincaré **7**, 59 (2006)
- [23] A. Dhahri, J. Phys. A **41**, 275305 (2008)
- [24] N. Kamiya and S. Takesue, J. Phys. Soc. Jpn. **82**, 114002 (2013)
- [25] A. Marais, I. Sinayskiy, A. Kay, F. Petruccione and A. Ekert, New. J. Phys. **15**, 013038 (2013)
- [26] A. Shabani, M. Mohseni, H. Rabitz and S. Lloyd, Phys. Rev. E **86**, 011915 (2012)
- [27] F. Caruso, A. W. Chin, A. Datta, S. F. Huelga and M. B. Plenio, J. Chem. Phys. **131**, 105106 (2009)
- [28] A. W. Chin, A. Datta, F. Caruso, S. F. Huelga and M. B. Plenio, New. J. Phys. **12**, 065002 (2010)
- [29] A. Shabatani, M. Mohseni, H. Rabitz and S. Lloyd, Phys. Rev. E **89**, 042706 (2014)
- [30] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd, and A. Aspuru-Guzik, New J. Phys. **11**, 033003 (2009)
- [31] I. Kassal and A. Aspuru-Guzik, New J. Phys. **14**, 053041 (2012)

- [32] K. M. Pelzer, A. F. Fidler, G. B. Griffin, S. K. Gray, and G. S. Engel, New J. Phys. **15**, 095019 (2013)
- [33] J. Adolphs and T. Renger, Biophys. J. **91**, 2778 (2006)
- [34] L. L. Foldy and S. A. Wouthuysen, Phys. Rev. **78**, 29 (1950)
- [35] S. Okubo, Prog. Theor. Phys. **12**, 603 (1954)
- [36] M. Žnidarič, New J. Phys. **12**, 043001 (2010)
- [37] M. Žnidarič, J. Stat. Mech. **2010**, L05002 (2010)
- [38] D. Manzano, M. Tiersch, A. Asadian, and H. J. Briegel, Phys. Rev. E **86**, 061118 (2012)
- [39] J. J. Mendoza-Arenas, T. Grujic, D. Jaksch, and S. R. Clark, Phys. Rev. E **87**, 235130 (2013)
- [40] S. Hoyer, M. Sarovar, and K. B. Whaley, New J. Phys. **12**, 065041 (2010)
- [41] H. Haken and P. Reineker, Z. Phys. **249**, 253 (1972)