

APPROACHES TO OPEN QUANTUM SYSTEMS: DECOHERENCE, LOCALISATION AND ALL THAT

by

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Abstract

This thesis is mainly concerned with issues in quantum open systems and the foundations of quantum theory.

Chapter I introduces the aim, background and main results which take place in the following chapters. Chapters II and III are used to study and compare the decoherent histories approach, the environment-induced decoherence and the localisation properties of the solutions to the stochastic Schrödinger equation in quantum jump simulation and quantum state diffusion approaches, for a quantum two-level system model. We show, in particular, that there is a close connection between the decoherent histories and the quantum jump simulation, complementing a connection with the quantum state diffusion approach noted earlier by Diósi, Gisin, Halliwell and Percival. In the case of the decoherent histories analysis, the degree of approximate decoherence is discussed in detail. As by-product, by using the von Neumann entropy, we also discuss the predictability and its relation to the upper bounds of degree of decoherence.

In Chapter IV, we give an alternative and elementary derivation of the Hu-Paz-Zhang master equation for quantum Brownian motion in a general environment, which involves tracing the evolution equation

for the Wigner function. We also discuss the master equation in some special cases. This master equation provides a very useful tool to study the decoherence of a quantum system due to the interaction with its environment.

In Chapter V, a derivation of the parameter-based uncertainty relation between position and momentum is given. This uncertainty relation can be regarded as an exact counterpart of the time-energy uncertainty relation.

The final chapter is a rather brief summary of the thesis.

Declaration

The work in this thesis was carried out in the Theoretical Physics Group, Imperial College, London between October 1994 and October 1997 under the supervision of Dr. J. J. Halliwell.

The thesis is based on a series of published papers [*Physical Review*, **D 53**, 2012 (1996); *Physics Letters*, **A 223**, 9 (1996) and *Physica*, **A 248**, 393 (1998)]. In particular, Chapter four in the thesis is based on a collaboration work with Jonathan Halliwell. I would like to thank him for his kind permission to include it into this thesis.

The work presented in this thesis, except where otherwise stated, is original and has not been submitted before for any degree or diploma of this or any other university.

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To
the memory of my mother, Guofeng Han-Yu
and to
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Chapter 1

Introduction

“What sort of things do *you* remember best?” Alice ventured to ask.

“Oh, things that happened the week after next,” the Queen replied in a careless tone.

—*Lewis Carroll*

Through the Looking-Glass

Quantum theory has been so successful that it has been regarded as a universal physical theory. On the one hand, it allows precise calculation of various physical processes and the theoretical calculations agree with empirical data to a remarkable degree. On the other hand, the foundation of quantum theory, at least the Copenhagen interpretation, has made many physicists uneasy even since the birth of the theory.

In the Copenhagen interpretation [1], the measuring devices or classical observers play an integral part in the formulation of the theory. Quantum theory takes classical theory as its limiting case while as an

indispensable part of its own theoretical formulation.

Moreover, the measurement problem in quantum theory has never been fully settled. The von Neumann projection postulate is only an *ad hoc* hypothesis which is imperfectly understood. The measurement process is not described by the Schrödinger equation. One can only talk about the measured results, but not the measuring process itself.

In quantum cosmology, the situation is even worse. Quantum theory of the whole universe must be interpreted without relying on the so-called classical outside observer.

In summary, the traditional Copenhagen interpretation is inadequate, since it relies on an outside classical domain.

In last three decades, several proposals have been made to overcome the weak points of the Copenhagen interpretation. A real breakthrough has occurred in recent years. Two primary paradigms – the environment-induced decoherence approach, proposed by Zurek [2, 3, 4], and the consistent histories approach by Griffiths [5] and later by Omnès [6, 7] and by Gell-Mann and Hartle [8, 9, 10] have been recently developed to solve the fundamental issues in quantum theory, especially, quantum measurement problems and the transition from quantum to classical. The environment-induced decoherence emphasises the division between the system and its environment. The interaction of the

system with its environment is responsible for the decay of the quantum coherence of the system. The decoherent histories approach is designed to provide the most general descriptions for a closed system by using the concept of history – a sequence of events at a succession of times. Both approaches are applicable to open quantum systems.

Another set of viable theories within the framework of quantum mechanics are the various unravellings of master equation as stochastic Schrödinger equations for the single member of the ensemble. Among others, the quantum state diffusion by Gisin and Percival and the quantum jump simulation approaches have been extensively studied in recent years (*e.g.*, see [11, 12, 13, 14, 15]). As phenomenological theories, these stochastic approaches are not only of theoretical interest but also of practical value.

The open quantum system provides a unified framework to exhibit the properties of the various approaches we have mentioned above. The master equation which describes the evolution of the open quantum system plays a central role in the investigations into the decay of quantum coherence due to the interaction with a much larger environment. It does not, however, tell us how an individual member of an ensemble evolves in a dissipative environment. The unravelling of master equation as stochastic Schrödinger equation could provide such a description

within its domain of applicability. Corresponding to the decoherence process in the density operator formalism, in stochastic Schrödinger equation approaches, the solution to the stochastic Schrödinger equation often possesses a very remarkable property – the solution tends to localise at some special states after a localisation time scale. For quantum state diffusion approach, this localisation property has been justified in many different situations [14, 15, 16, 17, 18, 19].

It is worth emphasising that a key point in these approaches is the mutual influence between the system of interest and its environment. This mutual influence is the common sources of the many different phenomena such as dissipation, fluctuation, decoherence, localisation, *etc.*

Analysis of decoherence and localisation properties is usually rather involved. The entanglement of the complicated mathematics and the subtle conceptual issues often tends to make detailed scrutiny of the basic concepts impossible. The some quantum optical models and quantum Brownian motion models, as exactly solvable models, are of great attractiveness due to their simplicity and yet physical meaningfulness.

The purposes of this thesis are following: First, in Chapters II and III, we will employ a widely used quantum open system model — a two level system model as a unified framework to examine the dynamics of

the open quantum system by decoherent histories, environment-induced decoherence and stochastic Schrödinger equations. We mainly consider the decoherence process and the localisation process. The various time scales concerning these processes are discussed. One of main result in this part is an establishment of a close connection between the decoherence histories and quantum jump simulation [20], complementing a connection with quantum state diffusion noted earlier by Diósi, Gisin, Halliwell and Percival [18]. By using this simple model, we have compared the decoherent histories and environment-induced decoherence approaches in some detail. In the case of the approximate decoherence, we provide a detailed analysis of the degree of decoherence of the two-level models, which is important for a real physical process.

Second, we provide, in Chapter IV, an alternative derivation of master equation for quantum Brownian motion model in general environment at arbitrary temperature [21]. This is another typical quantum open system model. Our derivation is physically natural and mathematical simple.

Finally, in Chapter V, we present a derivation of a new uncertainty relation between position and momentum which can be served as a counterpart of the time-energy uncertainty relation [22].

The plan of this thesis is as follows. In Chapter I, we present a

brief introduction of conceptual development of our research subjects. In Chapter II, after a brief review of environment-induced decoherence and decoherent histories approaches, we present a two-level system model and its basic properties. We then study the consistent histories approach and its relation to the environment-induced decoherence, the degree of decoherence and predictability by using von Neumann entropy. In Chapter III, we study the unravelling of master equation and the localisation properties of the solutions to the stochastic Schrödinger equations in both quantum jump simulations and quantum state diffusions. We discuss the quantum Brownian motion and parameter-based uncertainty relation in Chapters IV and V, respectively. We finally conclude the whole thesis in Chapter VI. The proof of a Theorem in Chapter II and an alternative determination of coefficient of master equation of QBM in Chapter V are included in the appendices.

Chapter 2

Decoherence and Predictability

“All right” said the Cat; and this time it vanished quite slowly, beginning with the end of the tail, and ending with the grin, which remained some time after the rest of it had gone.

—*Lewis Carroll*

Alice’s Adventures in Wonderland

The first purpose of this chapter is to examine, by making use of a two-level system, the two rival approaches: environment-induced decoherence and decoherent histories approaches. In particular, the decoherent histories analysis for this two-level model will be used to compare with quantum jump simulation and quantum state diffusion approaches in Chapter 3.

Our second purpose is to investigate the degree of approximate decoherence by using Dowker-Halliwell criterion. We also show a rela-

tionship between the predictability and von Neumann entropy.

This chapter will concentrate on examining the decoherence process in a two-level system, starting with a brief review of both environment-induced decoherence and decoherent histories approaches, which play a central role in the next two chapters.

2.1 Environment-induced decoherence

Decoherence of density matrices (often called the environment-induced decoherence) was initiated by Zurek for the purpose of providing a solution to the measurement problem [2]. The essence of this theory is to single out, through the interaction of the system with its environment, some special states (often called the pointer basis) which remain least affected by the interaction of environment.

It has been noticed that macroscopic objects are impossible to isolate from their surroundings [23, 24]. The constant interaction of the system with the large environment results in a decoherence process (often in a very short time scale) which destroys the all possible superpositions of macroscopically distinct states [4, 24]. One consequence of this decoherence, being described by a density matrix, is that, after a decoherence time scale, the density matrix is approximately diagonal in the pointer basis.

In some idealised models [2], the self-Hamiltonian of the system H_s was completely neglected or was assumed codiagonal with interaction Hamiltonian H_{int} . The eigenstates of an observable Λ which satisfies

$$[H_s + H_{int}, \Lambda] = 0$$

naturally constitute a “pointer basis”.

In realistic physical processes, however, a set of nontrivial observables which simultaneously commute with both the self- and interaction Hamiltonian is not likely to exist. In fact, during the decoherence process, all of the states in Hilbert space will be affected by the interaction with environment, the “pointer basis” are the states that are most stable, so they can be selected by a “predictability sieve” [4, 25, 26].

We should mention that the emergence of classicality is in a central position in both environment-induced decoherence and consistent histories programmes. But it is noticeable that the criteria for classicality are not entirely clear.

It has been argued that the consistent histories approach cannot provide a complete characterisation of classicality without borrowing the concepts from the other formalisms such as environment-induced decoherence [27]. More thorough investigation into this aspect would be important.

Based on the quantum Brownian motion model, Zurek *et al* [26] have characterised the effectiveness of decoherence in terms of a predictability sieve, and identified the maximally predictive states as the most classical, and have shown that coherent states are maximal. It seems that entropy plays important role in these studies.

2.2 Decoherent histories approach

The consistent histories approach was proposed by Griffiths [5] and developed by Omnès [6, 7] and by Gell-Mann and Hartle [8, 9, 10]. The reviews of the theory and some important developments can be found in [28, 29, 30, 31, 32, 33].

A history is defined in general as a sequence of properties of an isolated system occurring at different times. Precisely, suppose that system is given at initial time t_0 by a density matrix ρ and $t_1, t_2, \dots, t_n$ is a sequence of time satisfying

$$t_0 \leq t_1 < t_2 < \dots < t_n$$

We also suppose that, at each time a property of system, represented by a projection operator will be assigned. A typical history is denoted as

$$C_\alpha = P_{\alpha_1}^{(1)}(t_1) \dots P_{\alpha_n}^{(n)}(t_n)$$

where $P_{\alpha_i}^{(i)}(t_i)$ are the projection operators in the Heisenberg picture at times t_i :

$$P_{\alpha_i}^{(i)}(t_i) = e^{\frac{i}{\hbar}(t_i-t_0)H} P_{\alpha_i}^{(i)} e^{-\frac{i}{\hbar}(t_i-t_0)H}, \quad (2.1)$$

here, H is the Hamiltonian of the closed system. These projection operators satisfy exhaustive and exclusive conditions:

$$\sum_{\alpha_i} P_{\alpha_i}^{(i)}(t_i) = I, \quad P_{\alpha_i}^{(i)}(t_i) P_{\beta_i}^{(i)}(t_i) = \delta_{\alpha_i \beta_i} P_{\alpha_i}^{(i)}(t_i). \quad (2.2)$$

The superscript (i) labels the set of projections used at time t_i and α_i denotes the particular alternative.

Like in ordinary probability theory, rather than merely considering single history, one usually considers the whole sample space which contains all possible outcomes.

The main goal of decoherent histories approach is to assign each history a probability without referring to the measurements. A natural way to assign the probability to a history is

$$\begin{aligned} p(C_\alpha) &= \text{Tr}(C_\alpha^\dagger \rho(t_0) C_\alpha) \\ &= \text{Tr} \left(P_{\alpha_n}^{(n)} \dots P_{\alpha_1}^{(1)} \rho(t_0) P_{\alpha_1}^{(1)} \dots P_{\alpha_n}^{(n)} \right) \end{aligned} \quad (2.3)$$

However, one finds that (2.3) generally does not satisfy the usual probability sum rule. Precisely, for two different histories C_α and $C_{\alpha'}$, one would not expect that

$$p(C_\alpha + C_{\alpha'}) = p(C_\alpha) + p(C_{\alpha'})$$

always holds.

The necessary and sufficient condition to guarantee the above equation holds is the real part of decoherence functional $D[\underline{\alpha}, \underline{\alpha}']$ vanishes.¹
i.e.:

$$\text{Re} D[\underline{\alpha}, \underline{\alpha}'] = \text{Re Tr}(C_{\alpha}^{\dagger} \rho(t_0) C_{\alpha'}) = 0 \quad (2.4)$$

for any two different histories C_{α} and $C_{\alpha'}$. The sets of histories satisfying (2.4) are said to be *consistent* (or *weakly decoherent*). Physical mechanisms causing (2.4) to be satisfied typically lead also to the stronger condition

$$D[\underline{\alpha}, \underline{\alpha}'] = 0, \quad \forall \underline{\alpha} \neq \underline{\alpha}' \quad (2.5)$$

which is called *medium decoherence* [9]. (In this thesis, we simply refer it as *decoherence*)

Decoherent histories approach offers a sensible way to assign probability to a sequence of properties of a quantum system without referring to the measurement. It has many appealing features. Some of them are mentioned as follows:

1. Physically interesting histories are seldom exactly decoherent, they satisfy, at best, the so-called approximate decoherence conditions [9, 30].

2. Generally, only coarse-graining histories can be consistent. Obviously, the coarse-graining preserves decoherence but loses information

¹For simplicity we write $C_{\underline{\alpha}}$ as $\underline{\alpha}$.

about the system (initial state).

3. The existence of decoherent sets of histories is closely related to the existence of records, *i.e.* storage of information about the system of interest somewhere in the environment [9, 28].

4. Although the decoherent histories approach was primarily designed for a closed system, the approach is of particular importance for a open system which may be regarded as a subsystem of a large closed system. For the open quantum system, a natural coarse-graining is to focus only on the properties of the distinguished system whilst ignoring the environment. In this case, a natural selection of projections at each time is of form $P_\alpha \otimes I^\mathcal{E}$, where P_α is a projection onto the distinguished subsystem and $I^\mathcal{E}$ denotes the identity projection on the environment. In the Markovian regime, the decoherence functional could be constructed entirely in terms of the reduced density matrix of the system [27]:

$$D[\underline{\alpha}, \underline{\alpha'}] = \text{Tr} \left(P_{\alpha_n}^{(n)} K_{t_{n-1}}^{t_n} [P_{\alpha_{n-1}}^{(n-1)} \dots K_{t_1}^{t_2} [P_{\alpha_1}^{(1)} K_{t_0}^{t_1} [\rho_0] P_{\alpha'_1}^{(1)}] \dots P_{\alpha'_{n-1}}^{(n-1)}] P_{\alpha'_n}^{(n)} \right), \quad (2.6)$$

where the trace is taken over the distinguished system only. The quantity $K_{t_{k-1}}^{t_k}[\cdot]$ is super-propagator for the reduced density operator: $\rho_t = K_0^t[\rho_0]$. This property will be well used in the following discussions in this and next chapters.

5. It has been argued that consistent histories approach can be used to characterise the emergence of classical behaviour from the quantum substrate, a quasi-classical domain is defined as a set of decohering, maximally refined coarse-grained histories that exhibit strong correlations according to some deterministic law [8, 9]

6. Finally, we should mention that the decoherent histories approach is related to another mechanism of transition from quantum to classical which bear the same name – decoherence proposed by Zurek (a brief review of this approach is given in last subsection). The relation between these two approaches have been discussed¹ [27, 34, 35, 36].

2.3 Two-state model

A two-level system can be regarded as, in some sense, the fundamental building block in quantum theory. We consider a two-level atom system, which is radiatively damped by its interaction with the many modes of a radiation field in thermal equilibrium at temperature T . The upper level and lower level are denoted by $|2\rangle$ and $|1\rangle$, respectively. This is a typical example of the so-called system-plus-reservoir models in which quantum mechanics is fully implemented. In the case of our model, the system of interest is a single atom, and the reservoir

¹We will compare those two approaches based on a two-level systems in Section 2.4.2

is represented by a quantised radiation field. Under some conditions, one may derive the master equation for the two-level atom by tracing out over the radiation variables. This master equation describes a Markovian process and consequently takes the standard Lindblad form (in the Schrödinger picture) (*e.g.*, see [12, 37, 38]):

$$\begin{aligned}\dot{\rho} = & - \frac{i}{\hbar}[H, \rho] \\ & + \frac{\gamma}{2}(\bar{n} + 1)(2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a) \\ & + \frac{\gamma}{2}\bar{n}(2a^\dagger \rho a - aa^\dagger \rho - \rho aa^\dagger). \end{aligned} \quad (2.7)$$

Here, the Hamiltonian of the atom is given by

$$H = \frac{\hbar\omega}{2}\sigma_z \quad (2.8)$$

where ω is the renormalised frequency. The Lindblad operators, which model the effects of the environment in this situation, are

$$L_1 = \sqrt{\gamma(\bar{n} + 1)}a, \quad L_2 = \sqrt{\gamma\bar{n}}a^\dagger. \quad (2.9)$$

The transition rate from $|2\rangle \rightarrow |1\rangle$ is described by the term proportional to $(\gamma/2)(\bar{n} + 1)$ which contains both the simulated transitions and spontaneous transitions rates, and the transition rate from $|1\rangle \rightarrow |2\rangle$ is described by the term proportional to $(\gamma/2)\bar{n}$ which gives the rate of absorptive transition caused by taking thermal photons from the

radiation. The damping constant γ is the Einstein A -coefficient, and $\bar{n} = \bar{n}(\omega, T)$ is chosen as

$$\bar{n} = \frac{1}{e^{\hbar\omega/k_B T} - 1}. \quad (2.10)$$

We use σ_x, σ_y and σ_z to denote Pauli matrices and $a, a^\dagger$ atomic lowering and raising operators, which are defined in the usual way

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (2.11)$$

and

$$a = \frac{1}{2}(\sigma_x - i\sigma_y), \quad a^\dagger = \frac{1}{2}(\sigma_x + i\sigma_y). \quad (2.12)$$

The master equation (2.7) has been widely discussed in many places and is of importance in many quantum optical problems [12, 37].

A convenient way to solve the master equation (2.7) is to write down it in the basis $|2\rangle, |1\rangle$:

$$\dot{\rho}_{22} = -\gamma(\bar{n} + 1)\rho_{22} + \gamma\bar{n}\rho_{11}, \quad (2.13)$$

$$\dot{\rho}_{11} = \gamma(\bar{n} + 1)\rho_{22} - \gamma\bar{n}\rho_{11}, \quad (2.14)$$

$$\dot{\rho}_{21} = -\left[\frac{\gamma}{2}(2\bar{n} + 1) + i\omega\right]\rho_{21}, \quad (2.15)$$

$$\dot{\rho}_{12} = -\left[\frac{\gamma}{2}(2\bar{n} + 1) - i\omega\right]\rho_{12}. \quad (2.16)$$

The first two equations are the well-known Einstein rate equations. The general solutions to Eqs.(2.13)-(2.16) are as follows

$$\rho_{22}(t) = \frac{\bar{n}}{\bar{n} + 1}B_1 + B_2e^{-\gamma(2\bar{n}+1)t}, \quad (2.17)$$

$$\rho_{11}(t) = B_1 - B_2 e^{-\gamma(2\bar{n}+1)t}, \quad (2.18)$$

$$\rho_{21}(t) = B_3 e^{-[\frac{\gamma}{2}(2\bar{n}+1)+i\omega]t}, \quad (2.19)$$

$$\rho_{12}(t) = B_4 e^{-[\frac{\gamma}{2}(2\bar{n}+1)-i\omega]t}, \quad (2.20)$$

where B_i ($i = 1, 2, 3, 4$) are arbitrary constants which can be easily determined once the initial condition is given. For the initial density matrix with $\text{Tr}(\rho_0) = 1$ we easily get

$$B_1 = \frac{\bar{n} + 1}{2\bar{n} + 1} \quad (2.21)$$

$$B_2 = \rho_{22}(0) - \frac{\bar{n}}{2\bar{n} + 1} \quad (2.22)$$

$$B_3 = \rho_{21}(0) \quad (2.23)$$

$$B_4 = \rho_{12}(0) \quad (2.24)$$

It immediately follows from the solutions of master equation that the density operator ρ tends to the stationary density operator ρ_s as $t \rightarrow \infty$:

$$\rho \longrightarrow \rho_s = \begin{bmatrix} \frac{\bar{n}}{2\bar{n}+1} & 0 \\ 0 & \frac{\bar{n}+1}{2\bar{n}+1} \end{bmatrix}. \quad (2.25)$$

It is seen from the above that the off-diagonal elements, which represent the quantum coherence between the excited state and the ground state of the atom, vanish in the stationary state. This fact implies that, due to the influence of the random noise, the quantum coherence decays exponentially as time evolves. This is an elementary example of

environment-induced decoherence (*e.g.*, see [2, 3, 4]). Diagonalization occurs in the basis $|2\rangle, |1\rangle$. It has been shown by Joos and Zeh [24] in their seminal paper that the decoherence processes are typically very effective in a wide variety of situations. In the case of our model, from equations (2.15) and (2.16), it follows that the decoherence time scale t_D is given by

$$t_D \sim \frac{1}{\gamma(2\bar{n} + 1)}. \quad (2.26)$$

In particular, when $\hbar\omega \ll k_B T$,

$$t_D \sim \frac{\hbar}{\gamma k_B T}. \quad (2.27)$$

While for $\hbar\omega \gg k_B T$, *i.e.*, at low temperature limit:

$$t_D \sim \frac{1}{\gamma}. \quad (2.28)$$

For the time being, we are mainly concerned with the two types of time scales²: One is the decoherence time – which is time scale on which the off-diagonal elements of the density matrix are suppressed, and the other is the relaxation time – which is time scale on which the system approaches thermal equilibrium. It might be useful to note that these two types of time scales coincide in this two-level model. This is, certainly, a special feature of the two-level model, which is

²Another two time scales – decoherent history time and localisation time are to be discussed in Sections III and IV, respectively.

unlikely shared by other models³. It has been found that, for example, the decoherence time in quantum Brownian motion model is typically much shorter than the relaxation time [19, 39].

It is easily shown that master equation (2.7) is invariant under unitary transformations of the Lindblad operators:

$$a \longmapsto UaU^\dagger, \quad a^\dagger \longmapsto Ua^\dagger U^\dagger, \quad (2.29)$$

where U is a unitary matrix. Correspondingly, the density operator ρ transforms in the same way:

$$\rho \longmapsto U\rho U^\dagger. \quad (2.30)$$

Thus, when $t \rightarrow \infty$

$$\rho \longrightarrow U\rho_s U^\dagger. \quad (2.31)$$

Generally, the density matrix $U\rho_s U^\dagger$ is no longer diagonal. This indicates that environment-induced decoherence does not occur in other bases. This property is useful on comparison between the environment-induced decoherence and decoherent histories approaches.

³It is not difficult to contemplate a two-level model in which those two time scales are different.

2.4 Decoherent histories in the two-level system model

2.4.1 Decoherent history analysis

In what follows we shall make a detailed analysis of the decoherent histories in the two-level model described by the master equation (2.7) which depicts a Markovian process.

First, let us consider the projection operators represented by

$$P_1 = |1\rangle\langle 1| \text{ and } P_2 = |2\rangle\langle 2|. \quad (2.32)$$

Obviously, $\{P_i, i = 1, 2\}$ form a set of complete and exclusive projection operators. Physically, P_1 may represent that the atom emits a photon whereas P_2 may represent that the atom absorbs a photon. Then the decoherence functional at two time points is given by

$$D[\underline{\alpha}, \underline{\alpha}'] = \delta_{\alpha_2 \alpha_2'} \text{Tr} \left(P_{\alpha_2}^2 K_{t_1}^{t_2} \left[P_{\alpha_1}^1 K_0^{t_1} [\rho_0] P_{\alpha_1'}^1 \right] \right). \quad (2.33)$$

It is easily shown that, for any 2×2 matrix A , the matrix $P_i A P_j$ ($i \neq j$) is an upper (or a lower) triangle matrix. From equations (2.15), (2.16) we know that $K_{t_i}^{t_{i+1}}[\cdot]$ propagates the matrix with zero diagonal elements into the matrix with zero diagonal elements. So, for any initial density matrix ρ_0 , the trace in Eq. (2.33) is exactly zero for any different pairs of histories ($\underline{\alpha} \neq \underline{\alpha}'$) and for any interval $t_2 - t_1$. This

demonstrates that the set of histories consisting of projectors (2.32) are exactly decoherent. The generalisation to n time points is straightforward. The exact decoherence for any time interval is slightly surprising. (The density matrix, by contrast, only becomes exactly diagonal as $t \rightarrow \infty$). This exactness is due to the simplicity of the model and we do not expect it to be a generic feature.

Next, consider more general projection operators which correspond to the projection to any direction. With any direction denoted by a unit vector $n = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, we associate a vector $|n\rangle$ which belongs to the Hilbert space of the two-level system,

$$|n\rangle = \cos \frac{\theta}{2} |1\rangle - e^{-i\phi} \sin \frac{\theta}{2} |2\rangle. \quad (2.34)$$

Then one can define the following projection operators on the Hilbert space of the system:

$$P_+ = |n\rangle\langle n|, \quad P_- = |n'\rangle\langle n'|, \quad (2.35)$$

where $|n'\rangle$ is the orthogonal complimentary of $|n\rangle$:

$$|n'\rangle = e^{i\phi} \sin \frac{\theta}{2} |1\rangle + \cos \frac{\theta}{2} |2\rangle. \quad (2.36)$$

We shall show that a set of histories consisting of the projection operators P_+ and P_- are approximately decoherent. To this end, first, note

that for any 2×2 matrix A ,

$$\text{Tr}(P_+AP_-) = \text{Tr}(P_-AP_+) = 0. \quad (2.37)$$

Hence, from (2.17)–(2.20), it can be seen that, after the propagation of $K_{t_i}^{t_{i+1}}[\cdot]$, all of the diagonal elements of matrix $K_{t_1}^{t_2}[P_{\pm}K_{t_0}^{t_1}[\rho_0]P_{\mp}]$ contain an exponential damping factor

$$\text{Damping factor} = e^{-\gamma(2\bar{n}+1)t}. \quad (2.38)$$

Thus, we conclude

$$D[\underline{\alpha}, \underline{\alpha'}] \approx 0, \forall \underline{\alpha} \neq \underline{\alpha'}. \quad (2.39)$$

This proves that the set of histories consisting of P_+, P_- are approximately decoherent if time interval between t_k and t_{k+1} is larger than the characteristic time scale,

$$t_{\text{decoherence}} \sim \frac{1}{\gamma(2\bar{n} + 1)}. \quad (2.40)$$

This is an expected result. We will give a more detailed estimate of the degree of decoherence in the next section.

Note that $t_{\text{decoherence}}$ decreases as the coupling γ is made stronger. From (2.10), it is easy to see that the decoherence is more effective if the temperature of bath, T , increases. Conversely, decreasing temperature will make system spend more time to decohere. The maximum

decoherence time for a set of histories is $1/\gamma$ which corresponds to zero temperature of bath. In this case, the damping is caused by only spontaneous emission, and then the decoherence process is not very effective.

In summary, we find exact decoherence of histories characterised by the projections onto $|1\rangle$ and $|2\rangle$, and approximate decoherence in any other basis.

Finally, we examine the probabilities for two times histories consisting of projections (2.32). These are given by

$$\begin{aligned} p(1, 2) &= \text{Tr} \left(P_1 K_{t_1}^{t_2} [P_2 K_{t_0}^{t_1} [\rho_0] P_2] \right) \\ &= \frac{\bar{n} + 1}{2\bar{n} + 1} (1 - \delta) \rho_{22}(t_1), \end{aligned} \quad (2.41)$$

$$\begin{aligned} p(2, 1) &= \text{Tr} \left(P_2 K_{t_1}^{t_2} [P_1 K_{t_0}^{t_1} [\rho_0] P_1] \right) \\ &= \frac{\bar{n}}{2\bar{n} + 1} (1 - \delta) \rho_{11}(t_1), \end{aligned} \quad (2.42)$$

$$\begin{aligned} p(1, 1) &= \text{Tr} \left(P_1 K_{t_1}^{t_2} [P_1 K_{t_0}^{t_1} [\rho_0] P_1] \right) \\ &= \frac{1}{2\bar{n} + 1} [\bar{n} + (\bar{n} + 1)\delta] \rho_{22}(t_1), \end{aligned} \quad (2.43)$$

$$\begin{aligned} p(2, 2) &= \text{Tr} \left(P_2 K_{t_1}^{t_2} [P_2 K_{t_0}^{t_1} [\rho_0] P_2] \right) \\ &= \frac{1}{2\bar{n} + 1} [(\bar{n} + 1) + \bar{n}\delta] \rho_{11}(t_1). \end{aligned} \quad (2.44)$$

Where

$$\rho_{22}(t_1) = \frac{\bar{n}}{2\bar{n} + 1} + \left[\rho_{22}(0) - \frac{\bar{n}}{2\bar{n} + 1} \right] \delta, \quad (2.45)$$

$$\rho_{11}(t_1) = \frac{\bar{n} + 1}{2\bar{n} + 1} - \left[\rho_{22}(0) - \frac{\bar{n}}{2\bar{n} + 1} \right] \delta, \quad (2.46)$$

and $\delta = \exp\{-\gamma(2\bar{n} + 1)\Delta t\}$ ($\Delta t = t_i - t_{i-1}$, $i = 1, 2$).

As for the n times histories, the calculation for the elementary probabilities will be straightforward. For instance,

$$\begin{aligned} p(1, 1, \dots, 1) &= \text{Tr} \left(P_1 K_{t_{n-1}}^{t_n} [P_1 K_{t_{n-2}}^{t_{n-1}} [P_1 \dots K_{t_1}^{t_2} [P_1 K_{t_1}^{t_2} [\rho_0] P_1] \dots P_1] P_1] \right) \\ &= \frac{1}{(2\bar{n} + 1)^{n-1}} [\bar{n} + (\bar{n} + 1)\delta]^{n-1} \rho_{22}(t_1). \end{aligned} \quad (2.47)$$

Similarly, one may calculate the transition probabilities, *etc.*

2.4.2 Decoherent history vs. environment-induced decoherence

Both decoherent histories and environment-induced decoherence approaches are designed to solve the fundamental problems in quantum theory, in particular, quantum measurement problems and transition from quantum to classical. The comparison on the two approaches is of interest and of importance. Although it is believed that there is a close interrelationship between them, they are by no means equivalent. First of all, they differ in the conceptual aspect [4]. The environment-induced decoherence emphasises the division between the system of interest and its environment. The mutual interaction is responsible for the decay of the quantum coherence. While the decoherent histories approach to

⁵Here we use equal time interval for histories.

quantum theory permits prediction to be made in genuinely closed systems, such as the whole universe. Apart from this conceptual difference, with this two-level system we will be able to see some other interesting differences. One such difference is that, for any direction $|n\rangle$, the sets of histories consisting of the projections $P_+ = |n\rangle\langle n|$ and $P_- = |n'\rangle\langle n'|$ are decoherent (approximately) for any initial state. However, we have seen from Section 2.3 that the density matrix tends to become diagonal only in a particular basis $|1\rangle, |2\rangle$. Another intriguing difference is the time scales in two formulations. As was shown in the previous section, the histories consisting of the projection onto two levels $|1\rangle$ and $|2\rangle$ are exactly decoherent for any time, moreover, it is independent of the initial density matrices. Whereas environment-induced decoherence in the same basis $|1\rangle, |2\rangle$ could only occur after a certain time, which is dependent on the initial state. From the above we see that those two formalisms differ enormously in this two-level model.

It should be noted that the differences exhibited here may not be of generality. It is likely that these differences are purely due to the simplicity of the model or due to the approximations employed in the derivation of master equation (such as Born-Markov approximations). However, at any rate, we have shown, within the domain of applicability of the model presented here, the differences between these two

formalisms are significant. Moreover, our discussions here could serve as the useful hints for the further studies on more realistic models.

2.5 Degree of decoherence and predictability

In this section we will explicitly estimate the degree of decoherence. We show that the degree of decoherence is determined by the largest and the smallest eigenvalues of the projection operators and density matrix at a certain time (See below Section 2.5.1). By using von Neumann entropy, we also discuss the predictability and its relation to the upper bounds of degree of decoherence.

2.5.1 Approximate decoherence

Physically, one would not expect the decoherence takes place exactly. Therefore the investigation of the approximate decoherence is of importance. In practical problems, one can, at best, only expect that probability sum rules are satisfied up to order ϵ , for some constant $\epsilon < 1$. Namely, the interference terms do not have to be exactly zero, but **smaller** than probabilities by a factor of ϵ . One simple inequality, called Dowker-Halliwell criterion, which turns out to be very useful to

the study of the degree of decoherence, is [30, 40]:

$$|D[\underline{\alpha}.\underline{\alpha'}]|^2 \leq \epsilon^2 D[\underline{\alpha}.\underline{\alpha}] D[\underline{\alpha'}.\underline{\alpha'}]. \quad (2.48)$$

(The condition for using this inequality can be found in [30]) We say that a system decoheres to order ϵ if the decoherence functional satisfies (2.48). As shown in [30], such a condition implies that the most probability sum rules will then be satisfied to order ϵ .

The degree of decoherence, based on this two-level mode will be studied in some detail.

To begin with, we establish the following trace inequality which is useful to our studies of the approximate decoherence.

Theorem: Suppose that M and N are two $n \times n$ positive definite matrices. Let P and Q be two $n \times n$ Hermitian matrices satisfying

$$QP = PQ = 0. \quad (2.49)$$

Then

$$|\text{Tr}(MPNQ)|^2 \leq \epsilon^2 \text{Tr}(MPNP) \text{Tr}(MQNQ) \quad (2.50)$$

where $\epsilon = \min\{\epsilon^M, \epsilon^N\}$, here $\epsilon^M = (\lambda_{\max}^M - \lambda_{\min}^M)/(\lambda_{\max}^M + \lambda_{\min}^M)$, $\epsilon^N = (\lambda_{\max}^N - \lambda_{\min}^N)/(\lambda_{\max}^N + \lambda_{\min}^N)$, $\lambda_{\max}^M, \lambda_{\min}^M$ and $\lambda_{\max}^N, \lambda_{\min}^N$ are the maximal and the minimal eigenvalues of M and N , respectively.

Remark: In fact, the condition that both M and N are the positive definite matrices could be generalised to that one is positive definite,

say M , while another N is positive semidefinite. In this case, $\epsilon = \epsilon^M$. It is hoped that the above theorem is also useful in some other cases. The generalisation of the theorem, with some necessary changes, to the operators with bounded spectrum in an infinite Hilbert space is straightforward. The theorem is proved in the Appendix 1.

This theorem is very simple and useful. In what follows we will apply the above theorem to the two-level model.

For a general initial state represented by ρ_0 (pure or mixed state), the decoherence functional of two time points may be written as

$$D[\underline{\alpha}, \underline{\alpha'}] = \text{Tr} \left(P_{\pm} K_{t_1}^{t_2} \left[P_{-} K_0^{t_1} [\rho_0] P_{+} \right] \right). \quad (2.51)$$

We now write

$$A = K_0^{t_1} [\rho_0], \quad (2.52)$$

$$B = \tilde{K}_{t_1}^{t_2} [P_{\pm}]. \quad (2.53)$$

Then Eq. (2.51) may be rewritten, in the new notation, as

$$D[\underline{\alpha}, \underline{\alpha'}] = \text{Tr} (B P_{-} A P_{+}). \quad (2.54)$$

Note that $\tilde{K}$ in (2.53) is the super-propagator for the projection operators

$$P(t) = \tilde{K}_0^t [P(0)]. \quad (2.55)$$

The evolution equation for the projection operators is given by

$$\begin{aligned}\dot{P} &= \frac{i}{\hbar}[H, P] \\ &+ \frac{\gamma}{2}(\bar{n} + 1)(2a^\dagger P a - a^\dagger a P - P a^\dagger a) \\ &+ \frac{\gamma}{2}\bar{n}(2a P a^\dagger - a a^\dagger P - a a^\dagger P),\end{aligned}\quad (2.56)$$

where $H, a, a^\dagger$ are defined as before. Note that the evolution equation for the projection operator P is different from that for the density operator ρ (2.7). This reflects the difference between the Schrödinger and Heisenberg pictures in the density operator formalism. The explicit form of Eq. (2.56) may be written

$$\dot{P}_{22} = \gamma(\bar{n} + 1)(P_{11} - P_{22}), \quad (2.57)$$

$$\dot{P}_{11} = \gamma\bar{n}(P_{22} - P_{11}), \quad (2.58)$$

$$\dot{P}_{21} = -[\frac{\gamma}{2}(2\bar{n} + 1) - i\omega]P_{21}, \quad (2.59)$$

$$\dot{P}_{12} = -[\frac{\gamma}{2}(2\bar{n} + 1) + i\omega]P_{12}. \quad (2.60)$$

The general solutions to the above equations are

$$P_{22}(t) = C_1 + C_2 e^{-\gamma(2\bar{n}+1)t}, \quad (2.61)$$

$$P_{11}(t) = C_1 - \frac{\bar{n}}{\bar{n} + 1} C_2 e^{-\gamma(2\bar{n}+1)t}, \quad (2.62)$$

$$P_{21}(t) = C_3 e^{-[\frac{\gamma}{2}(2\bar{n}+1) - i\omega]t}, \quad (2.63)$$

$$P_{12}(t) = C_4 e^{-[\frac{\gamma}{2}(2\bar{n}+1) + i\omega]t}, \quad (2.64)$$

where C_i ($i = 1, 2, 3, 4$) are arbitrary constants. For given initial values, these constants can be expressed as

$$C_1 = \frac{\bar{n}}{2\bar{n}+1}P_{22}(0) + \frac{\bar{n}+1}{2\bar{n}+1}P_{11}(0), \quad (2.65)$$

$$C_2 = \frac{\bar{n}+1}{2\bar{n}+1}(P_{22}(0) - P_{11}(0)), \quad (2.66)$$

$$C_3 = P_{21}(0), \quad (2.67)$$

$$C_4 = P_{12}(0). \quad (2.68)$$

From the definitions (2.52) and (2.53), it is easy to see that in general, both A and B could be positive definite matrices, and since P_- and P_+ are projection operators, so the condition (2.49) is automatically satisfied. Using the theorem above, we immediately arrive at

$$|\text{Tr}(BP_+AP_-)|^2 \leq \epsilon^2 \text{Tr}(BP_+AP_+) \text{Tr}(BP_-AP_-). \quad (2.69)$$

That is,

$$|D[\underline{\alpha}, \underline{\alpha'}]|^2 \leq \epsilon^2 D[\underline{\alpha}, \underline{\alpha}])D[\underline{\alpha'}, \underline{\alpha'}]. \quad (2.70)$$

where $\epsilon = \min\{\epsilon^A, \epsilon^B\}$,

$$\epsilon^A = |\lambda_1^A - \lambda_2^A|, \quad (2.71)$$

$$\epsilon^B = \frac{|\lambda_1^B - \lambda_2^B|}{\lambda_1^B + \lambda_2^B}. \quad (2.72)$$

Here λ_i^A ($i = 1, 2$) and λ_i^B ($i = 1, 2$) are two eigenvalues of A and B , respectively. (Note that $\lambda_1^A + \lambda_2^A = 1$) From Eqs. (2.71) and (2.72), it

is easily seen that the degree of decoherence may depend on both the projection operators we use and the initial state of the system. This is also an expected result. For the two-level system, ϵ^A and ϵ^B can be calculated exactly. Consider, first, the eigenvalues of A . Since Eq. (2.7) preserves the trace, ϵ^A can be written as

$$\epsilon^A = \sqrt{1 - 4\lambda_1^A \lambda_2^A} = \sqrt{1 - 4 \det A}. \quad (2.73)$$

The determinant of A can be explicitly evaluated from the general solutions (2.17, 2.18, 2.19, 2.20),

$$\begin{aligned} \det A = & \frac{\bar{n}(\bar{n}+1)}{(2\bar{n}+1)^2} + \left[\frac{\bar{n}}{2\bar{n}+1} \right] \rho_{11}(0) + \frac{\bar{n}+1}{2\bar{n}+1} \rho_{22}(0) \\ & - \left[\frac{2\bar{n}(\bar{n}+1)}{(2\bar{n}+1)^2} - \rho_{21}(0)\rho_{12}(0) \right] \delta \\ & + \left[\rho_{22}(0) - \frac{\bar{n}}{2\bar{n}+1} \right] \left[\rho_{11}(0) - \frac{\bar{n}+1}{2\bar{n}+1} \right] \delta^2, \end{aligned} \quad (2.74)$$

where $\delta = \exp\{-\gamma(2\bar{n}+1)t_1\}$. In order that a set of histories are to be decoherent, one expects that δ should be small.

Similarly, ϵ^B can be expressed as

$$\epsilon^B = \sqrt{1 - \frac{4 \det B}{(\text{Tr} B)^2}}. \quad (2.75)$$

From (2.61)–(2.64), $\text{Tr} B$ and $\det B$ can be easily obtained:

$$\text{Tr} B = 2C_1 + \frac{1}{\bar{n}+1} C_2 \delta_1, \quad (2.76)$$

$$\det B = C_1^2 + \left[\frac{1}{\bar{n}+1} C_1 C_2 - C_3 C_4 \right] \delta_1 - \frac{\bar{n}}{\bar{n}+1} C_2^2 \delta_1^2, \quad (2.77)$$

where $\delta_1 = \exp\{-\gamma(2\bar{n} + 1)(t_2 - t_1)\}$.

The above discussions show explicitly how the degree of decoherence is related to the projection operators, the initial states and the temperature of bath, as well as the time spacing interval, in accordance with our general expectations.

It may be helpful to consider some special cases in which the simpler expressions for ϵ^A and ϵ^B may be obtained. In the long time limit, the density matrix will tend to the stationary density matrix. Then we may get a much simpler expression for ϵ^A :

$$\epsilon^A \sim \frac{1}{2\bar{n} + 1}. \quad (2.78)$$

As mentioned before, for the decoherent histories, δ and δ_1 should be small. If we only keep the terms up to the first order of δ_1 , then ϵ^B becomes

$$\epsilon^B \sim \left[\frac{C_3 C_4 \delta_1}{C_1^2 + \frac{1}{\bar{n}+1} C_1 C_2 \delta_1} \right]^{1/2}. \quad (2.79)$$

Similarly, the expression for ϵ^A can be readily obtained from Eq. (2.74).

It is clearly seen from the above expressions that the degree of decoherence improves as the bath temperature increases. We also see that the projections with the smaller off-diagonal elements will give a better degree of decoherence. For a given system with the initial state, then the matter for investigation is to determine which histories, i.e., which

string of projections, will lead to the decoherence condition being satisfied. Therefore, we see that ϵ^B serves as the main criterion for the degree of decoherence.

2.5.2 von Neumann entropy and predictability

It is also of interest to compute the von Neumann entropy of $\rho(t)$ [4, 26]. One interesting result we find here is the correlation between the initial density matrix, von Neumann entropy and the upper bounds of the degree of decoherence. We will also discuss the preferred states by using von Neumann entropy rather than linear entropy, in this two-level model.

In the case of system-plus-reservoir model, the pure states of the system, due to the interaction with environment, will typically deteriorate into the mixtures with the different rates. The rate at which pure initial states evolve into the mixtures reflects the stability of those pure states which are continuously monitored by the environment. The von Neumann entropy provides a convenient measure of the loss of predictability:

$$S = -\text{Tr}(\rho \ln \rho), \quad (2.80)$$

By definition, the more predictable state (pure state) may have less increase of the entropy in a fixed time period. This characterisation

process of predictability is called the *predictability sieve* (coined by Zurek [4]) which has been studied recently in quantum Brownian motion model by using the linear entropy [4, 26, 41]. We will see that two-level system serves as a very nice toy model to employ this “predictability sieve” by directly using the von Neumann entropy.

For the purpose of the evaluating the entropy, we choose a special basis in which ρ is diagonal. Let λ_1 and λ_2 be the eigenvalues of ρ , then Eq. (2.80) reduces to

$$S = - \sum_{i=1}^2 \lambda_i \ln \lambda_i . \quad (2.81)$$

Obviously, λ_1 and λ_2 can be expressed as

$$\lambda_1 = \frac{1 + \epsilon^A}{2}, \quad \lambda_2 = \frac{1 - \epsilon^A}{2} . \quad (2.82)$$

Hence, Eq. (2.81) can be rewritten as

$$S = - \left[\frac{(1 + \epsilon^A)}{2} \ln \frac{(1 + \epsilon^A)}{2} + \frac{(1 - \epsilon^A)}{2} \ln \frac{(1 - \epsilon^A)}{2} \right] . \quad (2.83)$$

A trivial observation shows that the von Neumann entropy $S(\epsilon^A)$ is a monotonically decreasing function of ϵ^A . Here, we find an interesting relation between the predictability of initial state and ϵ^A , which is an upper bound of the degree of decoherence. Namely, the von Neumann entropy provides a restriction on the upper bound of the degree of decoherence. Precisely, the initial density matrix which leads to larger

entropy production may give smaller ϵ^A . This relation between the predictability and the degree of the decoherence is a physically expected result. To obtain the higher degree of the decoherence one would expect that the environment has stronger influence on the system of interest, such as increasing the temperature of the bath. Then the predictability of the state, correspondingly, decreases.

It is useful to point out here that the actual degree of decoherence could be much smaller than the upper bound ϵ^A , since it is often typically undercut by the lesser upper bound ϵ^B . Moreover, the matter for investigation in histories approach is to determine which histories will satisfy the given degree of decoherence. In contrast, our goal here is merely to see how the initial states are related to the upper bounds of the degree of decoherence, hence, we do not take any particular set of histories into account.

Next, by using von Neumann entropy we shall find the most predictable states, those states will, by definition, generate least entropy production for a given time interval. Since the entropy S (2.83) is the monotonically decreasing function of ϵ^A , it is equivalent to find the states which give rise to the largest ϵ^A . From (2.73) and (2.74) it is

easily seen that

$$|\alpha\rangle = e^{i\phi} \sqrt{\frac{\bar{n}+1}{2\bar{n}+1}}|1\rangle \pm \sqrt{\frac{\bar{n}}{2\bar{n}+1}}|2\rangle \quad (2.84)$$

minimise the von Neumann entropy, and therefore are the preferred states. This is slightly surprising from both decoherent histories and environment-induced decoherence points of view. At first sight, one might expect that $|1\rangle$ and $|2\rangle$ would be the preferred states, since this basis plays a very special role in both formalisms. However, from equations (2.15) and (2.16) it is easy to see that the pure states $|1\rangle$ and $|2\rangle$ will immediately deteriorate into the mixed states. Namely, those two states are most vulnerable to the influence of the environment. This explains why the basis $|1\rangle$ and $|2\rangle$ are not the preferred states.

Also, we see from the above discussions that the states, which diagonalize the density matrix, are not necessarily same as the preferred states that are sorted by the Zurek's predictability sieve.

2.6 Discussion

In this chapter, we have shown that there are a number of sets of decoherent histories in this two-level model. Clearly, these decoherent histories are not equally important from physical point of view. Among those, the most natural one is that which consist of the projections onto

$|1\rangle$ and $|2\rangle$. We have proven that this set of histories give the best degree of decoherence. Note that the density matrix in the basis $|1\rangle$ and $|2\rangle$ will become diagonal after a typically short time.

The approximate decoherence is of basic importance in practical physical process. By using this two-level system model we can clearly see what determines the degree of decoherence. For a given set of histories, the only adjustable parameters are the temperature of bath, the time-spacing interval and the initial state of the system, in accordance with our general expectations.

We have studied the predictability of the pure states in this two-level model. The von Neumann entropy in this situation serves as predictability sieve to sort out the preferred states which yield the smallest entropy production. As byproduct, we also see an interesting relation between the upper bound of degree of decoherence and the initial density operators through the von Neumann entropy.

Finally, there are several special features of our model which are worth pointing out explicitly. First, the Hamiltonian of the system is diagonal in the basis $|1\rangle, |2\rangle$. We see that the evolution equations for the diagonal elements and the off-diagonal elements of the density matrix are decoupled in this situation. One consequence of this is the exactness of decoherence histories of the projections onto $|1\rangle, |2\rangle$. An

immediate generalisation of our model is to consider the Hamiltonian that does not enjoy this property. One such example is that, in addition to a thermal radiation field, the two-level atom is applied a coherent driving field. Notice that, in this situation, the evolution equations for the diagonal and off-diagonal elements of density matrix are no longer decoupled. The effect of making this change is that, instead of decoherence, the quantum coherence could be generated due to the influence of the coherent driving field [12]. Another special feature is that the decoherence time and relaxation time scales coincide. This is perhaps a typical feature of the two level-models. In the quantum Brownian motion model, the decoherence time is much shorter than relaxation time [19, 39]. At last, let us note that the coarse-graining in our two-level system is made by using projection operators on the system whilst ignoring the environment. It would be interesting to consider the general n -dimensional model in which the effect of a further coarse-graining on the degree of decoherence can be discussed.

Chapter 3

Stochastic Localisation Processes

Alice laughed. “There’s no use trying,” she said: “One *can’t* believe the impossible things.”

“I dare say you haven’t had much practice,” said the Queen. “When I was your age, I always did it for half hour a day. Why, sometime I’ve believed as many as six impossible things before breakfast....”

—*Lewis Carroll*
Through the Looking-Glass

3.1 Unravelling of master equation

It is well known that the master equation provides an ensemble description of a quantum system. The unravelling of master equation as the stochastic Schrödinger equation for the state vector, complementing the ensemble description, provide many insights into the foundation of quantum theory, especially in quantum measurement and the use-

ful tools to study various practical problems in the quantum optics (*e.g.*, see [16, 17]). In this chapter we will study the localisation in the two different unravellings of the master equation – quantum jump simulation and quantum state diffusion approaches. The former use the discrete random variables whereas the latter use the continuous random variables.

3.1.1 Quantum jump simulation

In the measurement schemes, such as direct photo-detection, the master equation, which models the measurement process, in some sense describes the lack of information of the systems. Namely, it describes the measurement process in which the results of measurement are not extracted. The quantum jump simulations, by contrast, mimic that ~~which~~ may be observed in a single run of the experiment. The state of system in this situation is represented by a wave function. The whole physical process under consideration is the combinations of continuous evolutions and abrupt jumps which are characterised by the discrete random variables. Therefore, the wave function of an individual system is usually governed by a stochastic differential equation. The stochastic unravellings are said to be equivalent to the master equations if the former after the stochastic average could reproduce the latter. The al-

ternative description by a single wave function is not confined in the measurement processes. In general, any master equation with Lindblad form [42] can be unravelled into the stochastic Schrödinger equation¹.

For the master equation (2.7), the stochastic Schrödinger equation takes the following form:

$$\begin{aligned}
 |d\psi\rangle &= -\frac{i}{\hbar} H|\psi\rangle dt \\
 &+ \sum_{i=1}^2 \left(\frac{L_i}{\sqrt{\langle N_i \rangle}} - 1 \right) |\psi\rangle dW_i \\
 &+ \sum_{i=1}^2 \left(\frac{\langle N_i \rangle}{2} - \frac{N_i}{2} \right) |\psi\rangle dt.
 \end{aligned} \tag{3.1}$$

Here $L_1 = \sqrt{\gamma(\bar{n}+1)}a$, $L_2 = \sqrt{\gamma\bar{n}}a^\dagger$ are the Lindblad operators representing the influence of the environment and $N_i = L_i^\dagger L_i$ ($i = 1, 2$). $\langle N_i \rangle = \langle \psi | N_i | \psi \rangle$ represents quantum average and M represents the ensemble average. The real random variables dW_i ($i = 1, 2$) satisfy

$$dW_i dW_j = \delta_{ij} dW_i, \tag{3.2}$$

$$M(dW_i) = \langle N_i \rangle dt \quad (i = 1, 2). \tag{3.3}$$

Under condition (3.2), it is easy to see that dW_i only take two values: 0 and 1. The master equation (2.7) can be recovered from the stochastic Schrödinger equation (3.1) in the sense that if $|\psi\rangle$ is the solution to Eq. (3.1) then $\rho = M|\psi\rangle\langle\psi|$ satisfies master equation (2.7).

¹Very recently, Diósi, Gisin and Strunz have described a nonlinear non-Markovian version of quantum state diffusion theory. See [43, 44].

In what follows we shall discuss the ‘localisation’ properties of the single jump trajectories. Here, by ‘localisation’ we mean that the quantum state vector generated by the stochastic Schrödinger equation will converge to some fixed states in the mean square .

More precisely, let A be an operator (not necessarily Hermitian), then we define the quantum mean square deviation as

$$\sigma(A, A) = \langle A^\dagger A \rangle - \langle A^\dagger \rangle \langle A \rangle. \quad (3.4)$$

If the solution of the stochastic Schrödinger equation (3.1) satisfies

$$M \frac{d}{dt} \sigma(A, A) \leq 0, \quad (3.5)$$

namely, the dispersion of the operator A tends to decrease as time evolves. Then we say that the solution localises at the eigenstates of the operator A (A is sometimes called the collapse operator).

For the stochastic Schrödinger equation for the quantum jump simulation in two-level system, the collapse operator is σ_z . Then quantum mean square deviation in this case is

$$(\Delta \sigma_z)^2 = 1 - \langle \sigma_z \rangle^2. \quad (3.6)$$

In order to prove the localisation, we should first derive the evolution equation of the expectation value of σ_z by using the following formula:

$$d\langle A \rangle = \langle \psi | A | d\psi \rangle + \langle d\psi | A | \psi \rangle + \langle d\psi | A | d\psi \rangle, \quad (3.7)$$

where A is an operator. From (3.1), it is straightforward to arrive at the following equation

$$\begin{aligned} d\langle\sigma_z\rangle &= (1 - \langle\sigma_z\rangle)dW_1 - (1 + \langle\sigma_z\rangle)dW_2 \\ &+ [\langle\sigma_z\rangle\langle N_1 + N_2\rangle + \langle N_1 - N_2\rangle] dt. \end{aligned} \quad (3.8)$$

Notice that

$$d(\Delta\sigma_z)^2 = -2\langle\sigma_z\rangle d\langle\sigma_z\rangle - (d\langle\sigma_z\rangle)^2. \quad (3.9)$$

Then, inserting Eq. (3.8) into the above equation, taking the ensemble means and remembering (3.3), we obtain

$$\begin{aligned} M \frac{d}{dt}(\Delta\sigma_z)^2 &= -\frac{1}{2}\gamma(\bar{n} + 1)(1 - \langle\sigma_z\rangle)^2(1 + \langle\sigma_z\rangle) \\ &\quad - \frac{1}{2}\gamma\bar{n}(1 + \langle\sigma_z\rangle)^2(1 - \langle\sigma_z\rangle). \end{aligned} \quad (3.10)$$

The right-hand side of Eq. (3.10) is non-positive, and that it vanishes if and only if $|\psi\rangle$ is $|2\rangle$ or $|1\rangle$. Hence we conclude that the solution to the stochastic Schrödinger equation (3.1) will localise at $|2\rangle$ or $|1\rangle$ after a certain time. That is, any initial state (which will be a superposition of $|1\rangle$ and $|2\rangle$) will tend to a solution in which the atom undergoes stochastic jumps between $|1\rangle$ and $|2\rangle$.

Let us now estimate this localisation time. From (3.10), a few manipulations directly give

$$M \frac{d}{dt}(\Delta\sigma_z)^2 \leq -\gamma(2\bar{n} + 1)(\Delta\sigma_z)^2. \quad (3.11)$$

So the localisation rate $t_{\text{localization}}$ is

$$t_{\text{localization}} \sim \frac{1}{\gamma(2\bar{n} + 1)}, \quad (3.12)$$

which agrees with the decoherence time scale (2.26). Note that this is the minimum localisation time. The actual time for localisation might be larger than this time.

In some sense, that the localisation in quantum jump simulation chooses the basis $|1\rangle, |2\rangle$ appears to be natural, since they correspond to the trajectories that would actually be observed in an individual experiment. As expected, the set of histories consisting of projection onto the basis give the best degree of decoherence. In addition, we have seen that the density matrix becomes diagonal in this basis. Here, we have demonstrated a close connection between the different approaches. This is the main result in the paper. The connection we have established here bridges the two different approaches—decoherent histories and quantum jump simulations. The former is regarded as a fundamental theory with a wide range of applicability, whilst the latter is mainly seen as a tool with great practical values, in particular, in the computational aspects.

Finally, let us compute the evolution of the populations of the two

levels:

$$d|\langle 1|\psi\rangle|^2 = \frac{1}{2}(\langle\sigma_z\rangle - 1)dW_1 + \frac{1}{2}(1 + \langle\sigma_z\rangle)dW_2 - \frac{1}{2}[\langle\sigma_z\rangle\langle N_1 + N_2\rangle + \langle N_1 - N_2\rangle]dt, \quad (3.13)$$

$$d|\langle 2|\psi\rangle|^2 = \frac{1}{2}(1 - \langle\sigma_z\rangle)dW_1 - \frac{1}{2}(1 + \langle\sigma_z\rangle)dW_2 + \frac{1}{2}[\langle\sigma_z\rangle\langle N_1 + N_2\rangle + \langle N_1 - N_2\rangle]dt. \quad (3.14)$$

Then it follows that from the above equations,

$$|\langle 1|\psi\rangle|^2 \longrightarrow \frac{\bar{n} + 1}{2\bar{n} + 1}, \quad (3.15)$$

$$|\langle 2|\psi\rangle|^2 \longrightarrow \frac{\bar{n}}{2\bar{n} + 1}. \quad (3.16)$$

That is to say, after a few localisation time scales (3.12), the average populations of the first and second levels will become constant. This result is completely in tune with that by using density matrix formalism.

3.1.2 Quantum state diffusion

In this subsection, we will illustrate the localisation process in another unravelling of the master equation – the quantum state diffusion approach, which was introduced by Gisin and Percival [11] to describe the quantum open system by using a stochastic Schrödinger equation² for the normalised pure state vector of an individual system of the

²This stochastic differential equation is often called the Langevin-Ito equation. For details, see *e.g.* C. W. Gardiner [45].

ensemble. Similar to the quantum jump simulation, a solution of the Langevin-Ito equation for the diffusion of a pure quantum state in state space represents a single member of an ensemble whose density operator satisfies the corresponding master equation.

Generally, if the master equation takes the standard Lindblad form [42]:

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \sum_i (L_i \rho L_i^\dagger - \frac{1}{2} L_i^\dagger L_i \rho - \frac{1}{2} \rho L_i^\dagger L_i) \quad (3.17)$$

Then, correspondingly, the Langevin-Ito stochastic equation can be written as

$$\begin{aligned} |d\psi\rangle &= -\frac{i}{\hbar} H |\psi\rangle dt \\ &+ \sum_i (\langle L_i^\dagger \rangle L_i - \frac{1}{2} L_i^\dagger L_i - \frac{1}{2} \langle L_i^\dagger \rangle \langle L_i \rangle) |\psi\rangle dt \\ &+ \sum_i (L_i - \langle L_i \rangle) |\psi\rangle d\xi_i, \end{aligned} \quad (3.18)$$

where H is a Hamiltonian (of the open system) and L_i are Lindblad operators, as before, $\langle L_i \rangle = \langle \psi | L_i | \psi \rangle$. The complex Wiener processes $d\xi_i$ satisfy

$$M(d\xi_i) = 0, M(d\xi_i d\xi_j) = 0, M(d\xi_i^* d\xi_j) = \delta_{ij} dt, \quad (3.19)$$

where M denotes a mean over the ensemble. The first term in the above equation is unitary evolution with interaction of the environment. The first summation term is called drift term, while the second summation is called fluctuation term.

Quantum state diffusion reproduces the master equation in the mean:

$$\rho = M|\psi\rangle\langle\psi|, \quad (3.20)$$

where $|\psi\rangle$ satisfy the quantum state diffusion equation (3.18), then it can be shown that ρ satisfies the master equation (3.17).

In order to show the localisation properties of the Langevin-Ito equation we now consider the simplest case which is assumed that bath temperature is zero ($\bar{n} = 0$). In this case the master equation (2.7) reduces to

$$\begin{aligned} \dot{\rho} = & - \frac{i}{\hbar}[H, \rho] \\ & + \frac{\gamma}{2}(2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a), \end{aligned} \quad (3.21)$$

Then the corresponding Langevin-Ito equation is given by

$$\begin{aligned} |d\psi\rangle = & -\frac{i}{\hbar}H|\psi\rangle dt \\ & + \frac{\gamma}{2}(2\langle a^\dagger\rangle a - a^\dagger a - \langle a^\dagger\rangle\langle a\rangle)|\psi\rangle dt \\ & + \sqrt{\gamma}(a - \langle a\rangle)|\psi\rangle d\xi, \end{aligned} \quad (3.22)$$

where $d\xi$ is the complex Wiener process satisfying

$$M(d\xi) = 0, \quad M(d\xi d\xi) = 0, \quad M(d\xi^* d\xi) = dt, \quad (3.23)$$

where M denotes a mean over probability distribution.

The evolution of the quantum average of operators can be calculated by using the following formula:

$$\begin{aligned}
 d\langle G \rangle &= \frac{i}{\hbar} \langle [H, G] \rangle dt \\
 &\quad - \frac{1}{2} \sum_i \langle L_i^\dagger [L_i, G] + [G, L_i^\dagger] L_i \rangle dt \\
 &\quad + \sum_i (\sigma(G^\dagger, L_i) d\xi_i + \sigma(L_i, G) d\xi_i^*), \quad (3.24)
 \end{aligned}$$

where

$$\sigma(A, B) = \langle A^\dagger B \rangle - \langle A^\dagger \rangle \langle B \rangle \quad (3.25)$$

Using Eq. (3.24), it is straightforward to get the following equations:

$$\begin{aligned}
 d\langle \sigma_x \rangle &= \left[-\frac{\omega}{\hbar} \langle \sigma_y \rangle - \frac{\gamma^2}{2} \langle \sigma_x \rangle \right] dt \\
 &\quad + \frac{\sqrt{\gamma}}{2} [1 + \langle \sigma_z \rangle - \langle \sigma_x \rangle^2 + i \langle \sigma_x \rangle \langle \sigma_y \rangle] d\xi \\
 &\quad + \frac{\sqrt{\gamma}}{2} [1 + \langle \sigma_z \rangle - \langle \sigma_x \rangle^2 - i \langle \sigma_x \rangle \langle \sigma_y \rangle] d\xi^*, \quad (3.26)
 \end{aligned}$$

$$\begin{aligned}
 d\langle \sigma_y \rangle &= \left[-\frac{\omega}{\hbar} \langle \sigma_x \rangle - \frac{\gamma^2}{2} \langle \sigma_y \rangle \right] dt \\
 &\quad + \frac{\sqrt{\gamma}}{2} [-i(1 + \langle \sigma_z \rangle) + i \langle \sigma_y \rangle^2 - \langle \sigma_x \rangle \langle \sigma_y \rangle] d\xi \\
 &\quad + \frac{\sqrt{\gamma}}{2} [i(1 + \langle \sigma_z \rangle) - i \langle \sigma_y \rangle^2 - \langle \sigma_x \rangle \langle \sigma_y \rangle] d\xi^* \quad (3.27)
 \end{aligned}$$

$$\begin{aligned}
 d\langle \sigma_z \rangle &= -[\langle \sigma_z \rangle \gamma + \gamma] dt \\
 &\quad - \frac{\sqrt{\gamma}}{2} (1 + \langle \sigma_z \rangle) (\langle \sigma_x \rangle - i \langle \sigma_y \rangle) d\xi \\
 &\quad - \frac{\sqrt{\gamma}}{2} (1 + \langle \sigma_z \rangle) (\langle \sigma_x \rangle + i \langle \sigma_y \rangle) d\xi^*. \quad (3.28)
 \end{aligned}$$

Moreover, we need to calculate the higher order moments. For any

Hermitian operator A we have from (3.4),

$$\begin{aligned} d(\Delta A)^2 &= d(\langle A^2 \rangle - \langle A \rangle^2) \\ &= d\langle A^2 \rangle - 2\langle A \rangle d\langle A \rangle - (d\langle A \rangle)^2. \end{aligned} \quad (3.29)$$

Then we easily obtain

$$\begin{aligned} M \frac{d}{dt} (\Delta \sigma_x)^2 &= 2\omega \langle \sigma_x \rangle \langle \sigma_y \rangle + \gamma \langle \sigma_x \rangle^2 \\ &\quad - \frac{\gamma}{2} (\Delta \sigma_x)^4 - \gamma (\Delta \sigma_x)^2 \langle \sigma_z \rangle \\ &\quad - \frac{\gamma}{2} \langle \sigma_z \rangle^2 - \frac{\gamma}{2} (\langle \sigma_x \rangle \langle \sigma_y \rangle)^2, \end{aligned} \quad (3.30)$$

$$\begin{aligned} M \frac{d}{dt} (\Delta \sigma_y)^2 &= -2\omega \langle \sigma_x \rangle \langle \sigma_y \rangle + \gamma \langle \sigma_y \rangle^2 \\ &\quad - \frac{\gamma}{2} (\Delta \sigma_y)^4 - \gamma (\Delta \sigma_y)^2 \langle \sigma_z \rangle \\ &\quad - \frac{\gamma}{2} \langle \sigma_z \rangle^2 - \frac{\gamma}{2} (\langle \sigma_x \rangle \langle \sigma_y \rangle)^2. \end{aligned} \quad (3.31)$$

Now, we are in the position to consider the localisation of solutions to Eq. (3.22). Using master equation, it is very easy to see that the atom will soon collapse into the lower state $|1\rangle$ and keeps there forever. Here we shall demonstrate that any solution to Langevin-Ito equation (3.22) will localise at the lower state after a localisation time. The collapse operator in this case is

$$A = \sigma_x + i\sigma_y. \quad (3.32)$$

Then by using (3.4) we get

$$\sigma(A, A) = (\Delta \sigma_x)^2 + (\Delta \sigma_y)^2 + 2\langle \sigma_z \rangle. \quad (3.33)$$

Hence we have

$$\begin{aligned}
 M \frac{d}{dt} \sigma(A, A) &= \gamma \langle \sigma_x \rangle^2 + \gamma \langle \sigma_y \rangle^2 - \frac{\gamma}{2} (\Delta \sigma_x)^4 \\
 &\quad - \frac{\gamma}{2} (\Delta \sigma_y)^4 - \gamma (\Delta \sigma_x)^2 \langle \sigma_z \rangle - \gamma (\Delta \sigma_y)^2 \langle \sigma_z \rangle \\
 &\quad - \gamma \langle \sigma_z \rangle^2 - 2\gamma (\langle \sigma_z \rangle + 1) - \gamma (\langle \sigma_x \rangle \langle \sigma_y \rangle)^2. \quad (3.34)
 \end{aligned}$$

In order to prove that the left-hand side of Eq. (3.34) is non-positive, let us denote

$$(\Delta \sigma_x)^2 = 1 + X, \quad (3.35)$$

$$(\Delta \sigma_y)^2 = 1 + Y, \quad (3.36)$$

$$\langle \sigma_z \rangle = -1 + Z. \quad (3.37)$$

Substituting equations (3.35), (3.36) and (3.37) into Eq. (3.34) we have

$$M \frac{d}{dt} \sigma(A^\dagger, A) = \gamma \left[-R^2 - X - Y - 2Z - \frac{1}{2}(Y - Z)^2 - \frac{1}{2}(X - Z)^2 \right], \quad (3.38)$$

where $R = \langle \sigma_x \rangle \langle \sigma_y \rangle$. Note that

$$X + Y + 2Z = \sigma(A, A) \geq 0. \quad (3.39)$$

Then we show that

$$M \frac{d}{dt} \sigma(A^\dagger, A) \leq 0 \quad (3.40)$$

and the equality holds if and only if

$$X = Y = Z = 0. \quad (3.41)$$

That is, the average in the left hand sides of equations (3.35), (3.36), and (3.37) is taken over the ground state $|1\rangle$. This proves that the solution to Eq. (3.22) will localise at the ground state when the evolution time is larger than the localisation time.

Finally, let us estimate the localisation rate of the quantum state evolution. Using Eq. (3.38) and Eq. (3.39), we immediately obtain

$$M \frac{d}{dt} \sigma(A, A) \leq -\gamma (\sigma(A, A))^2. \quad (3.42)$$

So the localisation rate $t_{\text{localization}}$ is

$$t_{\text{localization}} \sim \frac{1}{\gamma}. \quad (3.43)$$

In summary, we have shown the localisation process in both quantum jump simulation and quantum state diffusion. Those localisations have been extensively discussed in the quantum state diffusion approaches. Here we have seen that the similar localisation process could also occur in the quantum jump simulation. It should be noted that, in the case of the zero-temperature of our two-level model, for any initial state of the system, the atom will eventually localise at the ground state. Therefore, the system will always evolve from a pure state into the pure state. In this sense we say that the decoherence and localisation are basically trivial in this case. However, the above demonstration of localisation can still be regarded as a useful example for showing that

quantum state diffusion picture provides a consistent description with the density matrix formalism and decoherence approach.

It is interesting to compare the master equation formulation with their stochastic unravellings. Clearly, the master equations provide a fundamental description of the quantum open systems. But numerical simulation of the many-freedom problems seems rather awkward due to occupying the large memory of computer. Moreover, it cannot provide a description for an individual system. The quantum trajectories approaches—the unravelling of master equation as the stochastic Schrödinger equation could do this job and have advantages over master equation in computational aspect [11, 46]. For this two-level model, the merit of stochastic unravellings is mainly in conceptual aspects. Generally, the localisation process is very difficult to show analytically, if not impossible.

Obviously, the unravelling of master equation is not unique. Quantum jump simulations and quantum state diffusions are only two well-known examples, which lie in our interests in this paper. These stochastic unravellings are often connected with the certain measurement schemes. For instance, the quantum jump simulation can be associated with the direct photo-detection, and quantum state diffusion corresponds to the heterodyne detection. In a quantum jump process, quantum jump sim-

ulation may be a natural candidate for description of the process. The quantum state diffusion by nature is continuous diffusion process. However, if the transition is so fast that the “diffusion” from one level to the other level of atom can be regarded as an instantaneous process, then quantum state diffusion could also give rise to the “jump” process [13, 16]. It should be noted that the applicability of quantum jump simulation and quantum state diffusion are different. The preference of these stochastic approaches are largely dependent on the physical models employed and the problems to be solved. In general, the relation between those two approaches is by no means obvious. Undoubtedly, the researching into this relation would be of importance and of interest [47].

3.2 Discussion

In this chapter, based on the two-level system models presented in the last chapter, we have studied quantum jump simulation and quantum state diffusion. We have demonstrated the localisation in both quantum jump simulations and quantum state diffusion approaches. Here we conclude with a summary and a few remarks.

On combining the results in the last chapter, in which we have shown that the most natural set of histories is that which consist of

the projections onto $|1\rangle$ and $|2\rangle$. We have proven that this set of histories give the best degree of decoherence. Note that the density matrix in the basis $|1\rangle$ and $|2\rangle$ will become diagonal after a typically short time. Remarkably, we have shown, in this chapter, that the solutions to the stochastic Schrödinger equation in the quantum jump simulation will localise at $|1\rangle$ or $|2\rangle$ after certain time which is basically same as the decoherence time. Also, we have shown the localisation process in quantum state diffusion in the case of zero temperature. Our results have demonstrated a close connection between the decoherent histories and quantum jump simulation approaches, knowing that the two approaches have totally different origins³.

In addition, we have found that the environment-induced decoherence, decoherent histories and the localisation process are more effective as the bath temperature increases. Physically, this is an expected result as the bath at a higher temperature would have stronger influence on the system. These results are in agreement with former studies on the quantum Brownian models [19] as well as on the quantum optical models [35].

It is important to notice that, as phenomenological theories, both quantum state diffusion and quantum jump simulation must be used

³This connection has been independently proved by T. Brun [48]. For a recent review, see M. Plenio and P. Knight [49].

under some conditions (*e.g.*, see [13]). The comparison between different approaches therefore must be made in caution since the correspondence between them is by no means mathematically one-to-one correspondence. Rather, we emphasise that, underlying the quantum open system, the mutual influence between the system and its environment is the common theoretical base of all of those approaches and both decoherence and localisation are nothing more than the different manifestations of a single entity.

The environment-induced decoherence, decoherent histories as well as various stochastic Schrödinger equations have provided many important insights into the understanding of fundamental problems in quantum theory. The investigation into the similarity and difference between the different approaches is of importance. The more thorough studies in this aspect would be useful.

Chapter 4

Quantum Brownian motion

“... there is a pleasure in recognising the old things from a new point of view.”

—*Richard Feynman*

An Abstract from “Space-Time Approach to Non-Relativistic Quantum Mechanics”

In the previous two chapters, the quantum two-level system, being taken as a typical quantum open system, has been studied in some details. As we emphasised before, analysis of the decoherence is rather mathematical involved, and it is often very difficult, if not impossible, to find an exact solutions of the problems. For a deepening understanding, however, the exact soluble models are always useful. Besides two-level systems, quantum Brownian motion(QBM) model is another widely used model in quantum decoherence, quantum dissipation, statistical physics in general *etc* [50, 51, 52, 53]. In the following sections we will provide an alternative derivation of the master equation of QBM.

4.1 Introduction

Quantum Brownian motion (QBM) models provide a paradigm of open quantum systems that has been very useful in quantum measurement theory [54], quantum optics [12] and decoherence [9, 30, 55]. One of the advantages of the QBM models is that they are reasonably simple, yet sufficiently complex to manifest many important features of realistic physical processes.

Central to the study of QBM is the master equation for the reduced density operator of the Brownian particle, derived by tracing out the environment in the evolution equation for the combined system plus environment. A variety of such derivations have been given [56, 57, 58, 59]. The most general is that of Hu, Paz and Zhang [60, 61], who used path integral techniques and in particular, the Feynman-Vernon influence functional.

The purpose of this chapter is to provide an alternative and elementary derivation of the Hu-Paz-Zhang master equation for QBM, by tracing the evolution equation for the Wigner function of the whole system.

This chapter is planned as follows. In Section 4.2, the quantum Brownian motion model is presented and a derivation of Fokker-Planck

equation governing the evolution of Wigner functions of the system of interest is given. In Sections 4.3 and 4.4, the determination of coefficients of the master equation for the general case and particular case are given¹, respectively.

4.2 Master equation for quantum Brownian motion

The system we considered is a harmonic oscillator with mass M and bare frequency Ω , in interaction with a thermal bath consisting of a set of harmonic oscillators with mass m_n and natural frequency ω_n . The Hamiltonian of the system plus environment is given by

$$H = \frac{p^2}{2M} + \frac{1}{2}M\Omega^2 q^2 + \sum_n \left(\frac{p_n^2}{2m_n} + \frac{1}{2}m_n\omega_n^2 q_n^2 \right) + q \sum_n C_n q_n, \quad (4.1)$$

where q, p and q_n, p_n are the coordinates and momenta of the Brownian particle and oscillators, respectively, and C_n are coupling constants.

The state of the combined system (4.1) is most completely described by a density matrix $\rho(q, q_i; q', q'_i, t)$ where q_i denotes $(q_1, \dots, q_N)$, and ρ evolves according to

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho]. \quad (4.2)$$

¹Another method of determining the coefficients of the master equation by using the Laplace transform will be given in Appendix 2.

The state of the Brownian particle is described the reduced density matrix, defined by tracing over the environment,

$$\rho_r(q, q', t) = \int \prod_n (dq_n dq'_n \delta(q_n - q'_n)) \rho(q, q_i; q', q'_i, t). \quad (4.3)$$

The equation of time evolution for the reduced density matrix is called the master equation. For a general environment, Hu, Paz, and Zhang [60] derived the following master equation by using path integral techniques:

$$\begin{aligned} i\hbar \frac{\partial \rho_r}{\partial t} = & -\frac{\hbar^2}{2M} \left(\frac{\partial^2 \rho_r}{\partial q^2} - \frac{\partial^2 \rho_r}{\partial q'^2} \right) + \frac{1}{2} M \Omega^2 (q^2 - q'^2) \rho_r \\ & + \frac{1}{2} M \delta \Omega^2(t) (q^2 - q'^2) \rho_r \\ & - i\hbar \Gamma(t) (q - q') \left(\frac{\partial \rho_r}{\partial q} - \frac{\partial \rho_r}{\partial q'} \right) \\ & - iM \Gamma(t) h(t) (q - q')^2 \rho_r \\ & + \hbar \Gamma(t) f(t) (q - q') \left(\frac{\partial \rho_r}{\partial q} + \frac{\partial \rho_r}{\partial q'} \right). \end{aligned} \quad (4.4)$$

The explicit form of the coefficients of the above equation will be given later on. The coefficient $\delta \Omega^2(t)$ is the frequency shift term, the coefficients $\Gamma(t)$ is the “quantum dissipative” term, and the coefficients $\Gamma(t)h(t), \Gamma(t)f(t)$ are “quantum diffusion” terms. Generally, these coefficients are time dependent and of quite complicated behaviour.

We find it convenient to use the Wigner function of the reduced

density matrix²

$$\tilde{W}(q, p, t) = \frac{1}{2\pi} \int du e^{iup/\hbar} \rho_r \left(q - \frac{u}{2}, q + \frac{u}{2}, t \right). \quad (4.5)$$

Taking the Wigner transform of (4.4), we obtain³

$$\begin{aligned} \frac{\partial \tilde{W}}{\partial t} = & - \frac{1}{M} p \frac{\partial \tilde{W}}{\partial q} + M[\Omega^2 + \delta\Omega^2(t)] q \frac{\partial \tilde{W}}{\partial p} \\ & + 2\Gamma(t) \frac{\partial(p\tilde{W})}{\partial p} + \hbar M\Gamma(t)h(t) \frac{\partial^2 \tilde{W}}{\partial p^2} \\ & + \hbar\Gamma(t)f(t) \frac{\partial^2 \tilde{W}}{\partial q \partial p}. \end{aligned} \quad (4.6)$$

The inverse transformation of (4.5) is given by

$$\rho_r(q, q', t) = \int dp e^{-ip(q-q')/\hbar} \tilde{W} \left(\frac{q+q'}{2}, p, t \right). \quad (4.7)$$

Our strategy for deriving the master equation (4.4) is to derive the Fokker-Planck type equation (4.6) from the Wigner equation for the total system. The master equation can be obtained from the Wigner equation for the system by using the transformation (4.7).

We shall make the following two assumptions:

- (1) The system and the environment are initially uncorrelated, *ie.* the initial Wigner function factors

$$W_0(q, p; q_i, p_i) = W_0^s(q, p) W_0^b(q_i, p_i), \quad (4.8)$$

²For detail discussions of Wigner functions, *e.g.*, see [62].

³We believe that Eq.(2.48) in Ref. [60] contains some incorrect numerical factors.

where W_0^s and W_0^b are the Wigner functions of the system and the bath, respectively, at $t = 0$.

(2) The heat bath is initially in a thermal equilibrium state at temperature $T = (k_B\beta)^{-1}$. This means that the initial Wigner function of bath is of Gaussian form,

$$\begin{aligned} W_0^b &= \prod_n W_{n0}^b \\ &= \prod_n N_n \exp\left\{-\frac{2}{\omega_n \hbar} \tanh\left(\frac{1}{2}\hbar\omega_n\beta\right) H_n\right\}, \end{aligned} \quad (4.9)$$

where H_n is the Hamiltonian of the n -th oscillator in the bath,

$$H_n = \frac{p_n^2}{2m_n} + \frac{1}{2}m_n\omega_n^2 q_n^2. \quad (4.10)$$

In addition, one easily see that the initial moments of the bath are

$$\langle q_n(0) \rangle = \langle p_n(0) \rangle = 0, \quad (4.11)$$

$$\langle q_n(0)q_m(0) \rangle = 0 \text{ (if } m \neq n), \quad (4.12)$$

$$\langle p_n(0)p_m(0) \rangle = 0 \text{ (if } m \neq n), \quad (4.13)$$

$$\langle q_n(0)p_m(0) + p_m(0)q_n(0) \rangle = 0, \quad (4.14)$$

and

$$\begin{aligned} \langle q_n^2(0) \rangle &= \frac{\hbar}{2m_n\omega_n} \coth\left(\frac{1}{2}\hbar\omega_n\beta\right), \\ \langle p_n^2(0) \rangle &= \frac{1}{2}\hbar m_n\omega_n \coth\left(\frac{1}{2}\hbar\omega_n\beta\right). \end{aligned} \quad (4.15)$$

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For the QBM problem described by (4.1) and (4.2), the Wigner function of the combined system plus environment satisfies

$$\begin{aligned} \frac{\partial W}{\partial t} = & - \frac{p}{M} \frac{\partial W}{\partial q} + M\Omega^2 q \frac{\partial W}{\partial p} \\ & + \sum_n \left(-\frac{p_n}{m_n} \frac{\partial W}{\partial q_n} + m_n \omega_n^2 q_n \frac{\partial W}{\partial p_n} \right) \\ & + \sum_n C_n \left(q_n \frac{\partial W}{\partial p} + q \frac{\partial W}{\partial p_n} \right). \end{aligned} \quad (4.16)$$

By integrating over the bath variables on the both sides of the above equation, one obtains

$$\frac{\partial \tilde{W}}{\partial t} = -\frac{p}{M} \frac{\partial \tilde{W}}{\partial q} + M\Omega^2 q \frac{\partial \tilde{W}}{\partial p} + \sum_n C_n \int \prod_i dq_i dp_i q_n \frac{\partial W}{\partial p}, \quad (4.17)$$

where $\tilde{W}(q, p)$ is the reduced Wigner function⁴

$$\tilde{W}(q, p) = \int_{-\infty}^{+\infty} \prod_i dq_i dp_i W(q, p; q_i, p_i). \quad (4.18)$$

The first two terms on the right-hand side of the Eq. (4.17) give rise to the standard evolution equation of the system. The last term contains all the information about the behaviour of the system in the presence of interaction with environment.

In what follows, we shall demonstrate that the quantity

$$G(q, p) = \sum_n C_n \int \prod_i dq_i dp_i q_n W \quad (4.19)$$

⁴This definition is equivalent to Eqs. (4.3) and (4.5)

appearing (differentiated with respect to p) in (4.17) can be expressed in terms of $\tilde{W}$ and its derivatives. To this end, we first perform Fourier transform of $G(q, p)$

$$\begin{aligned} G(k, k') &= \int dq dp e^{ikq + ik'p} G(q, p) \\ &= \sum_n C_n \int dq dp \prod_i dq_i dp_i q_n e^{ikq + ik'p} W(q, p; q_i, p_i) \end{aligned} \quad (4.20)$$

It is well known that $q(t), p(t)$ and $q_n(t), p_n(t)$ are related to the classical evolution of their initial values $q(0), p(0)$ and $q_n(0), p_n(0)$ through a canonical transformation:

$$\mathbf{z}(t) = U(t)\mathbf{z}(0), \quad (4.21)$$

where

$$\mathbf{z}(t) = (q(t), q_1(t) \dots q_N(t); p(t), p_1(t), \dots p_N(t)).$$

Since the Hamiltonian (4.1) is quadratic, the Eq. (4.16) has the same form as the classical Liouville equation, so the solution of Eq. (4.16) is of the form,

$$W_t(\mathbf{z}) = W_0(U^{-1}(t)\mathbf{z}). \quad (4.22)$$

Changing the integration variables into their initial values by this canonical transformation, we obtain

$$G(k, k') = \int dq(0) dp(0) \prod_i dq_i(0) dp_i(0)$$

$$\begin{aligned}
& \times \left[f q(0) + g p(0) + \sum_n (f_n q_n(0) + g_n p_n(0)) \right] \\
& \times \exp \left[i k \left(\alpha q(0) + \beta p(0) \right) + \sum_n (a_n q_n(0) + b_n p_n(0)) \right] \\
& \times \exp \left[i k' M \left(\dot{\alpha} q(0) + \dot{\beta} p(0) + \sum_n (\dot{a}_n q_n(0) + \dot{b}_n p_n(0)) \right) \right] \\
& \times W_0^s(q(0), p(0)) W_0^b(q_i(0), p_i(0)) .
\end{aligned} \tag{4.23}$$

Here the coefficients $f, g, f_n, g_n, \alpha, \beta, a_n, b_n$ are time dependent. Their explicit values are not required.

Similarly, the Fourier transform of the reduced Wigner function is

$$\begin{aligned}
\tilde{W}(k, k') &= \int dq dp e^{ikq + ik'p} \tilde{W}(q, p) \\
&= \int dq(0) dp(0) \prod_i dq_i(0) dp_i(0) \\
& \times \exp \left[i k \left(\alpha q(0) + \beta p(0) \right) + \sum_n (a_n q_n(0) + b_n p_n(0)) \right] \\
& \times \exp \left[i k' M \left(\dot{\alpha} q(0) + \dot{\beta} p(0) + \sum_n (\dot{a}_n q_n(0) + \dot{b}_n p_n(0)) \right) \right] \\
& \times W_0^s(q(0), p(0)) W_0^b(q_i(0), p_i(0)) .
\end{aligned} \tag{4.24}$$

Now compare $G(k, k')$ and $\tilde{W}(k, k')$. They differ by the terms linear in $q(0), p(0), q_n(0), p_n(0)$ in the preexponential factor in $G(k, k')$. Consider the factors $f_n q_n(0)$ and $g_n p_n(0)$ in $G(k, k')$. Since they multiply $W_0^b(q_i(0), p_i(0))$, and since $W_0^b(q_i(0), p_i(0))$ is Gaussian in $q_n(0), p_n(0)$, the terms $f_n q_n(0) W_0^b$ and $g_n p_n(0) W_0^b$ may be replaced by terms of the form $\partial W_0^b / \partial q_n(0), \partial W_0^b / \partial p_n(0)$ up to time dependent factors. An in-

tegration by parts then may be performed, and these factors are then effectively replaced by multiplicative factors of k, k' .

Similarly, the factors $f q(0), g p(0)$ in the prefactor in $G(k, k')$ may be replaced by $\partial/\partial k, \partial/\partial k'$ (plus some more factors of k and k'). Hence, it is readily seen that $G(k, k')$ is a linear combination of terms of the form $k, k', \partial/\partial k, \partial/\partial k'$ operating on $\tilde{W}(k, k')$, with time dependent coefficients.

Inverting the Fourier transform, it follows that

$$G = A(t)q\tilde{W} + B(t)p\tilde{W} + C(t)\frac{\partial\tilde{W}}{\partial q} + D(t)\frac{\partial\tilde{W}}{\partial p}. \quad (4.25)$$

for some coefficients $A(t), B(t), C(t), D(t)$ to be determined. This result immediately leads to the general form Wigner equation :

$$\begin{aligned} \frac{\partial\tilde{W}}{\partial t} = & - \frac{p}{M} \frac{\partial\tilde{W}}{\partial q} + M\Omega^2 q \frac{\partial\tilde{W}}{\partial p} + A(t)q \frac{\partial\tilde{W}}{\partial p} \\ & + B(t) \frac{\partial(p\tilde{W})}{\partial p} + C(t) \frac{\partial^2\tilde{W}}{\partial p \partial q} + D(t) \frac{\partial^2\tilde{W}}{\partial p^2}. \end{aligned} \quad (4.26)$$

4.3 Determination of coefficients (general case)

Having found the functional form of the Wigner equation (4.26) of the Brownian particle, the next step is to determine the coefficients in the equation. Undoubtedly, there is more than one way to do this. Here we shall choose a way which is both mathematically simple and physically

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heuristic. Towards this direction, let us consider the time evolution of the expectation values of the system variables: q, p, q^2, p^2 and $\frac{1}{2}(pq+qp)$.

By using Eq. (4.16), we have

$$\frac{d}{dt}\langle q \rangle = \frac{1}{M}\langle p \rangle, \quad (4.27)$$

$$\frac{d}{dt}\langle p \rangle = -M\Omega^2\langle q \rangle - \sum_n C_n\langle q_n \rangle, \quad (4.28)$$

$$\frac{d}{dt}\langle q^2 \rangle = \frac{1}{M}\langle pq + qp \rangle, \quad (4.29)$$

$$\frac{d}{dt}\langle p^2 \rangle = -M\Omega^2\langle pq + qp \rangle - 2\sum_n C_n\langle pq_n \rangle, \quad (4.30)$$

$$\frac{d}{dt}\langle pq + qp \rangle = \frac{2}{M}\langle p^2 \rangle - 2M\Omega^2\langle q^2 \rangle - 2\sum_n C_n\langle qq_n \rangle. \quad (4.31)$$

Similarly, using Eq. (4.26) yields

$$\frac{d}{dt}\langle q \rangle = \frac{1}{M}\langle p \rangle, \quad (4.32)$$

$$\frac{d}{dt}\langle p \rangle = -(M\Omega^2 + A)\langle q \rangle - B\langle p \rangle, \quad (4.33)$$

$$\frac{d}{dt}\langle q^2 \rangle = \frac{1}{M}\langle pq + qp \rangle, \quad (4.34)$$

$$\frac{d}{dt}\langle p^2 \rangle = -(M\Omega^2 + A)\langle pq + qp \rangle - 2B\langle p^2 \rangle + 2D, \quad (4.35)$$

$$\begin{aligned} \frac{d}{dt}\langle pq + qp \rangle &= \frac{2}{M}\langle p^2 \rangle - 2(M\Omega^2 + A)\langle q^2 \rangle \\ &\quad - B\langle pq + qp \rangle + 2C. \end{aligned} \quad (4.36)$$

Since the evolution equations of the expectation values are confined to the system variables, the above two sets of equations must be identical.

Now by comparing (4.28) with (4.33) we see that

$$\sum_n C_n \langle q_n \rangle = A \langle q \rangle + B \langle p \rangle . \quad (4.37)$$

Similarly, by comparing (4.31) with (4.36), (4.30) with (4.35), respectively, we get

$$\sum_n C_n \langle qq_n \rangle = A \langle q^2 \rangle + \frac{B}{2} \langle qp + pq \rangle - C , \quad (4.38)$$

$$\sum_n C_n \langle pq_n \rangle = \frac{A}{2} \langle pq + qp \rangle + B \langle p^2 \rangle - D . \quad (4.39)$$

The coefficients A, B, C, D may now be determined from (4.37)-(4.39) by regarding the expectation values $\langle q \rangle, \langle q_n q \rangle$ etc. as expectation values of Heisenberg picture operators, and by solving the operator equation of motion. For simplicity, we still use ordinary notation to represent an operator without adding a hat on it.

The solution to the equation of motion may be written

$$q_n(t) = \alpha_n q(t) + \beta_n p(t) + \sum_m (a_{nm} q_m(0) + b_{nm} p_m(0)) , \quad (4.40)$$

$$q(t) = \alpha q(0) + \beta p(0) + \sum_n (a_n q_n(0) + b_n p_n(0)) , \quad (4.41)$$

for some time-dependent coefficients $\alpha_n, \beta_n, a_{nm}, b_{nm}, \alpha, \beta, a_n, b_n$. Note that $q_n(t)$ has been expressed in terms of the final, not initial values of q, p . By substituting Eq. (4.40) into Eq. (4.37), keeping (4.11) in mind, and comparing the two sides of the resulting equation, we have

$$A = \sum_n C_n \alpha_n , \quad B = \sum_n C_n \beta_n . \quad (4.42)$$

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Similarly, substituting (4.40) and (4.41) into (4.38) and (4.39), respectively, we get

$$C = - \sum_{mn} C_n (a_{nm} a_m \langle q_m^2(0) \rangle + b_{nm} b_m \langle p_m^2(0) \rangle), \quad (4.43)$$

$$D = -M \sum_{mn} C_n (a_{nm} \dot{a}_m \langle q_m^2(0) \rangle + b_{nm} \dot{b}_m \langle p_m^2(0) \rangle). \quad (4.44)$$

Here we have made use of $p = M\dot{q}$. The coefficients A, B, C, D are therefore completely determined by solving the equation of motion.

We now do this explicitly.

We have

$$\ddot{q}(t) + \Omega^2 q(t) = -\frac{1}{M} \sum_n C_n q_n(t), \quad (4.45)$$

$$\ddot{q}_n(t) + \omega_n^2 q_n(t) = -\frac{C_n}{m_n} q(t). \quad (4.46)$$

The solution to Eq.(4.46) is as follows:

$$\begin{aligned} q_n(t) = & q_n(0) \cos(\omega_n t) + \frac{p_n(0)}{m_n} \frac{\sin(\omega_n t)}{\omega_n} \\ & - C_n \int_0^t ds \frac{\sin[\omega_n(t-s)]}{\omega_n} \frac{q(s)}{m_n}. \end{aligned} \quad (4.47)$$

Combining (4.45) and (4.47) gives

$$\ddot{q}(t) + \Omega^2 q(t) + \frac{2}{M} \int_0^t d\tau \eta(t-s) q(s) = \frac{f(t)}{M}, \quad (4.48)$$

where

$$f(t) = - \sum_n C_n \left(q_n(0) \cos(\omega_n t) + \frac{p_n(0)}{m_n} \frac{\sin(\omega_n t)}{\omega_n} \right). \quad (4.49)$$

The kernel $\eta(s)$ is defined as

$$\eta(s) = \frac{d}{ds}\gamma(s), \quad (4.50)$$

where

$$\gamma(s) = \int_0^{+\infty} d\omega \frac{I(\omega)}{\omega} \cos(\omega s). \quad (4.51)$$

Here $I(\omega)$ is the spectral density of the environment:

$$I(\omega) = \sum_n \delta(\omega - \omega_n) \frac{C_n^2}{2m_n\omega_n}. \quad (4.52)$$

In order to get the expressions (4.40) and (4.41), we solve equation (4.48) with the following two different initial conditions:

$$q(s=0) = q(0), \quad \dot{q}(s=0) = \frac{p(0)}{M}. \quad (4.53)$$

and

$$q(s=t) = q(t), \quad \dot{q}(s=t) = \frac{p(t)}{M}. \quad (4.54)$$

where t is any given time point. In doing so, we consider the elementary functions $u_i(s)$ ($i = 1, 2$) introduced by Hu, Paz and Zhang [60] which satisfy the following homogeneous integro-differential equation

$$\ddot{\Sigma}(s) + \Omega^2 \Sigma(s) + \frac{2}{M} \int_0^s d\lambda \eta(s-\lambda) \Sigma(\lambda) = 0 \quad (4.55)$$

with the boundary conditions:

$$u_1(s=0) = 1, \quad u_1(s=t) = 0, \quad (4.56)$$

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and

$$u_2(s = 0) = 0, \quad u_2(s = t) = 1. \quad (4.57)$$

The solution to equation (4.55) with the initial condition (4.53) is obtained as the linear combination of u_1, u_2 ,

$$w(s) = \left(u_1(s) - \frac{\dot{u}_1(0)}{\dot{u}_2(0)} u_2(s) \right) q(0) + \frac{u_2(s)}{\dot{u}_2(0)} \frac{p(0)}{M}. \quad (4.58)$$

The solution to equation (4.48) with the homogeneous initial conditions can be formally written as

$$\tilde{w}(s) = \frac{1}{M} \int_0^t d\tau G_1(s, \tau) f(\tau). \quad (4.59)$$

Where Green function $G_1(s, \tau)$ satisfies

$$\frac{d^2}{ds^2} G_1(s, \tau) + \Omega^2 G_1(s, \tau) + \frac{2}{M} \int_0^s d\lambda \eta(s - \lambda) G_1(\lambda, \tau) = \delta(s - \tau) \quad (4.60)$$

with

$$G_1(s = 0, \tau) = 0, \quad \frac{d}{ds} G_1(s = 0, \tau) = 0. \quad (4.61)$$

Then the solution to the equation (4.48) with initial condition (4.53) reads

$$q(s) = w(s) + \tilde{w}(s), \quad (4.62)$$

explicitly,

$$q(s) = \left(u_1(s) - \frac{\dot{u}_1(0)}{\dot{u}_2(0)} u_2(s) \right) q(0) + \frac{u_2(s)}{\dot{u}_2(0)} p(0)$$

$$\begin{aligned}
& - \sum_n \frac{C_n}{M} \int_0^t d\tau G_1(s, \tau) \cos(\omega_n \tau) q_n(0) \\
& - \sum_n \frac{C_n}{M} \int_0^t d\tau G_1(s, \tau) \frac{\sin(\omega_n \tau)}{\omega_n} \frac{p_n(0)}{m_n}. \quad (4.63)
\end{aligned}$$

It can be shown that the solution to the homogeneous equation (4.55) with the initial conditions (4.54) is

$$u(s) = \left(u_2(s) - \frac{\dot{u}_2(t)}{\dot{u}_1(t)} u_1(s) \right) q(t) + \frac{u_1(s)}{\dot{u}_1(t)} \frac{p(t)}{M}, \quad (4.64)$$

and

$$\tilde{u}(s) = \frac{1}{M} \int_0^t d\tau G_2(s, \tau) f(\tau) \quad (4.65)$$

is the solution to the inhomogeneous equation (4.48) with the homogeneous initial conditions

$$\tilde{u}(t) = 0, \quad \dot{\tilde{u}}(t) = 0. \quad (4.66)$$

The equation for Green function $G_2(s, \tau)$ is analogous.

Hence, we get the solution to Eq. (4.48) with the initial conditions (4.54)

$$\begin{aligned}
q(s) &= u(s) + \tilde{u}(s) \\
&= \left(u_2(s) - \frac{\dot{u}_2(t)}{\dot{u}_1(t)} u_1(s) \right) q(t) + \frac{u_1(s)}{\dot{u}_1(t)} \frac{p(t)}{M} \\
&\quad - \sum_n \frac{C_n}{M} \int_0^t d\tau G_2(s, \tau) \cos(\omega_n \tau) q_n(0) \\
&\quad - \sum_n \frac{C_n}{M} \int_0^t d\tau G_2(s, \tau) \frac{\sin(\omega_n \tau)}{\omega_n} \frac{p_n(0)}{m_n}. \quad (4.67)
\end{aligned}$$

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Substituting (4.67) into (4.47), one obtains

$$\begin{aligned}
 q_n(t) = & -\frac{C_n}{m_n \omega_n} \int_0^t ds \sin[\omega_n(t-s)] \left(u_2(s) - \frac{\dot{u}_2(t)}{\dot{u}_1(t)} u_1(s) \right) q(t) \\
 & -\frac{C_n}{m_n \omega_n} \int_0^t ds \sin[\omega_n(t-s)] \frac{u_1(s)}{\dot{u}_1(t)} \frac{p(t)}{M} \\
 & + q_n(0) \cos(\omega_n t) + \frac{p_n(0)}{m_n} \frac{\sin(\omega_n t)}{\omega_n} \\
 & + \frac{1}{M} \sum_m \frac{C_n C_m}{m_n \omega_n} \int_0^t ds \int_0^t d\tau \sin[\omega_n(t-s)] \\
 & \times G_2(s, \tau) \cos(\omega_m \tau) q_m(0) \\
 & + \frac{1}{M} \sum_m \frac{C_n C_m}{m_n \omega_n} \int_0^t ds \int_0^t d\tau \sin[\omega_n(t-s)] \\
 & \times G_2(s, \tau) \frac{\sin(\omega_m \tau)}{m_m \omega_m} p_m(0). \tag{4.68}
 \end{aligned}$$

By using (4.42) we immediately arrive at

$$\begin{aligned}
 A(t) = & -\sum_n \frac{C_n^2}{m_n \omega_n} \int_0^t ds \sin[\omega_n(t-s)] \\
 & \times \left(u_2(s) - \frac{\dot{u}_2(t)}{\dot{u}_1(t)} u_1(s) \right), \tag{4.69}
 \end{aligned}$$

$$B(t) = -\frac{1}{M} \sum_n \frac{C_n^2}{m_n \omega_n} \int_0^t ds \sin[\omega_n(t-s)] \frac{u_1(s)}{\dot{u}_1(t)}. \tag{4.70}$$

Furthermore, A, B can be written as

$$A(t) = 2 \int_0^t ds \eta(t-s) u_2(s) - 2 \frac{\dot{u}_2(t)}{\dot{u}_1(t)} \int_0^t ds \eta(t-s) u_1(s), \tag{4.71}$$

$$B(t) = \frac{2}{M \dot{u}_1(t)} \int_0^t ds \eta(t-s) u_1(s). \tag{4.72}$$

From (4.63), the momentum of the Brownian particle is then

$$p(t) = M \dot{q}(t)$$

$$\begin{aligned}
&= \left(\dot{u}_1(t) - \frac{\dot{u}_1(0)}{\dot{u}_2(0)} \dot{u}_2(t) \right) M q(0) + \frac{\dot{u}_2(t)}{\dot{u}_2(0)} p(0) \\
&\quad - \sum_n \int_0^t d\tau G'_1(t, \tau) \cos(\omega_n \tau) q_n(0) \\
&\quad - \sum_n \int_0^t d\tau G'_1(t, \tau) \frac{\sin(\omega_n \tau)}{\omega_n} \frac{p_n(0)}{m_n}. \tag{4.73}
\end{aligned}$$

Here “prime” stands for derivative with respect to the first variable of $G_1(s, \tau)$.

With these results (see equations (4.43), (4.44)), It can be easily shown that

$$\begin{aligned}
C(t) &= \frac{\hbar}{M} \int_0^t d\lambda G_1(t, \lambda) \nu(t - \lambda) \\
&\quad + \frac{2\hbar}{M^2} \int_0^t ds \int_0^t d\tau \int_0^t d\lambda \eta(t - s) \\
&\quad \times G_1(t, \lambda) G_2(s, \tau) \nu(\tau - \lambda), \tag{4.74}
\end{aligned}$$

and

$$\begin{aligned}
D(t) &= \hbar \int_0^t d\lambda G'_1(t, \lambda) \nu(t - \lambda) \\
&\quad + \frac{2\hbar}{M} \int_0^t ds \int_0^t d\tau \int_0^t d\lambda \eta(t - s) \\
&\quad \times G'_1(t, \lambda) G_2(s, \tau) \nu(\tau - \lambda). \tag{4.75}
\end{aligned}$$

where $\nu(s)$ is defined as

$$\nu(s) = \int_0^{+\infty} d\omega I(\omega) \coth\left(\frac{1}{2}\hbar\omega\beta\right) \cos(\omega s). \tag{4.76}$$

It is seen that the coefficients $A(t), B(t), C(t), D(t)$ are dependent only on the kernels $\eta(s)$ and $\nu(s)$ and the initial state of the bath, not depen-

dent on the initial state of the system. Once the spectral density of the environment is given, in principle, the elementary functions $u_i (i = 1, 2)$ and Green functions $G_i (i = 1, 2)$ can be solved from equations (4.55), (4.60), etc. Then the coefficients of master equation can be determined.

4.4 Particular cases

In this section, we will consider some special cases. Let us at first treat a special case in which we assume that the interaction between the system and environment is weak, so the C_n are small. In this case, the coefficients are of simple forms, and the determination of these coefficients is very simple and straightforward. We shall work out these coefficients directly using the method in the last section, rather than the general formulae.

The solution to Eq. (4.46) may be written as

$$\begin{aligned}
 q_n(t) = & q_n(0) \cos(\omega_n t) + \frac{p_n(0)}{m_n} \frac{\sin(\omega_n t)}{\omega_n} \\
 & - \frac{C_n}{m_n} \int_0^t dt' \frac{\sin[\omega_n(t-t')]}{\omega_n} \cos[\Omega(t'-t)] q(t) \\
 & - \frac{C_n}{m_n} \int_0^t dt' \frac{\sin[\omega_n(t-t')]}{\omega_n} \frac{\sin[\Omega(t'-t)]}{\Omega} \frac{p(t)}{M} \\
 & + O(C_n^2).
 \end{aligned} \tag{4.77}$$

Using Eq. (4.37) and ignoring terms with higher than the second order

of C_n , we get

$$\begin{aligned} \sum_n C_n \langle q_n(t) \rangle &= \left\{ \sum_n -\frac{C_n^2}{m_n} \int_0^t dt' \frac{\sin[\omega_n(t-t')]}{\omega_n} \cos[\Omega(t'-t)] \right\} \langle q(t) \rangle \\ &+ \left\{ \frac{1}{M} \sum_n -\frac{C_n^2}{m_n} \int_0^t dt' \frac{\sin[\omega(t-t')]}{\omega_n} \right. \\ &\quad \left. \times \frac{\sin[\Omega(t'-t)]}{\Omega} \right\} \langle p(t) \rangle . \end{aligned} \quad (4.78)$$

Then we immediately get

$$A(t) = 2 \int_0^t ds \eta(s) \cos(\Omega s) , \quad (4.79)$$

$$B(t) = -\frac{2}{M\Omega} \int_0^t ds \eta(s) \sin(\Omega s) . \quad (4.80)$$

We next evaluate $\sum_n C_n \langle q(t) q_n(t) \rangle$ and $\sum_n C_n \langle p(t) q_n(t) \rangle$. After a few manipulations, we arrive at the expressions

$$C(t) = -\sum_n C_n \left\{ \langle q(t) q_n(0) \rangle \cos(\omega_n t) + \langle q(t) p_n(0) \rangle \frac{\sin(\omega_n t)}{m_n \omega_n} \right\} , \quad (4.81)$$

and

$$D(t) = -\sum_n C_n \left\{ \langle p(t) q_n(0) \rangle \cos(\omega_n t) + \langle p(t) p_n(0) \rangle \frac{\sin(\omega_n t)}{m_n \omega_n} \right\} . \quad (4.82)$$

To calculate $C(t)$ and $D(t)$, we need to expand $q(t)$ up to the second order of C_n :

$$\begin{aligned} q(t) &= q(0) \cos(\Omega t) + \frac{p(0)}{M} \frac{\sin(\Omega t)}{\Omega} \\ &- \sum_n \frac{C_n}{M} \int_0^t ds \frac{\sin[\Omega(t-s)]}{\Omega} \cos(\omega_n s) q_n(0) \\ &- \sum_n \frac{C_n}{M} \int_0^t ds \frac{\sin[\Omega(t-s)]}{\Omega} \frac{\sin(\omega_n s)}{\omega_n} \frac{p_n(0)}{m_n} \\ &+ O(C_n^2) . \end{aligned} \quad (4.83)$$

The expansion of $p(t)$ is easily obtained from that of $q(t)$,

$$p(t) = M\dot{q}(t). \quad (4.84)$$

With these results it is easy to compute $C(t)$ and $D(t)$:

$$C(t) = \frac{\hbar}{M\Omega} \int_0^t ds \nu(s) \sin(\Omega s), \quad (4.85)$$

$$D(t) = \hbar \int_0^t ds \nu(s) \cos(\Omega s). \quad (4.86)$$

This simple example exhibits the time dependency of the coefficients of the master equation in a general environment. Eqs. (4.79), (4.80), (4.85), (4.86) are in agreement with Hu, Paz and Zhang [60].

As another example, we briefly discuss the purely Ohmic case in the Fokker-Planck limit (a particular form of high temperature limit), which has been extensively discussed in the literature [56, 53]. In this case one has

$$\eta(s - s') = M\gamma\delta'(s - s') \quad (4.87)$$

$$\nu(s - s') = \frac{2M\gamma k_B T}{\hbar} \delta(s - s') \quad (4.88)$$

Then the equation (4.55) reduces to

$$\ddot{u}(s) + \Omega_{\text{ren}}^2 u(s) + \gamma \dot{u}(s) = -2\gamma\delta(s)u(0) \quad (4.89)$$

where $\Omega_{\text{ren}}^2 = \Omega^2 - 2\gamma\delta(0)$. After solving this equation, a few calculations give

$$A(t) = -2M\gamma\delta(0), \quad (4.90)$$

$$B(t) = 2\gamma, \quad (4.91)$$

$$C(t) = 0, \quad (4.92)$$

$$D(t) = 2M\gamma k_B T. \quad (4.93)$$

Then the Wigner equation reads:

$$\frac{\partial \tilde{W}}{\partial t} = -\frac{p}{M} \frac{\partial \tilde{W}}{\partial q} + M\Omega_{\text{ren}}^2 q \frac{\partial \tilde{W}}{\partial p} + 2\gamma \frac{\partial(p\tilde{W})}{\partial p} + 2M\gamma k_B T \frac{\partial^2 \tilde{W}}{\partial p^2}. \quad (4.94)$$

In this regime, the coefficients of this Wigner equation are constants.

4.5 Discussion

We have shown how to derive the Hu-Paz-Zhang master equation by tracing the evolution equation for the Wigner function of the whole system. Although actually quite lengthy, we referred to it earlier as “elementary” because it is conceptually so. The length comes largely from the simple but tedious job of solving the classical equation of motion for prescribed boundary conditions, Eqs. (4.45)-(4.76).

Our evolution equation, Eq. (4.26), is in general non-Markovian, because the time-dependent coefficients depend on a fiducial moment of time, namely the initial time at which the Wigner function is assumed to factor. Generally, one would expect a non-Markovian evolution equation at a particular moment of time t to involve the integral of the Wigner function over times to the past of t . The possibility that

this non-Markovian equation can be written in the simpler, superficially “memoryless” form (4.26) was first emphasised by Shibata *et al.* [63, 64, 65].

Finally, we have a remark on the relevant work by Anglin and Habib [66], who also consider the derivation of the Wigner equation Eq. (4.6) by tracing the Wigner equation for the whole system. Their approach is very similar to our derivation of Eq. (4.26) in section 4.2. They also emphasised that, at least as far as solving equations goes, the derivation is an essentially classical calculation. They do not, however, give explicitly the detailed derivation of the coefficients, as we do in section 4.3.

Chapter 5

Parameter-based Uncertainty Relations

“I *have* tasted eggs, certainly,” said Alice, who was a very truthful child; “but little girls eat eggs quite as much as serpents do, you know.”

“I don’t believe it,” said the Pigeon; “but if you do, why then they’re a kind of serpent, that’s all I can say.”

—*Lewis Carroll*

Alice’s Adventures in Wonderland

5.1 Introduction

In [67] Mandelstam and Tamm prove the following uncertainty relation between the time and energy:

$$|\langle \psi(0) | \psi(t) \rangle|^2 \geq \cos^2 \left(\frac{\Delta \hat{H} t}{\hbar} \right), \text{ for } 0 \leq t \leq \frac{\pi \hbar}{2 \Delta \hat{H}} \quad (5.1)$$

where $\Delta H = \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}$. Since then the parameter based uncertainty relation and related problems have been extensively studied in

various contexts [68, 69, 70, 71, 72, 73, 74, 75, 76, 77]. For an excellent review, *e.g.*, see [74].

The parameter-based uncertainty relations between position and momentum has been considered in [71, 73]. A particular interesting case can be formulated as follows: For a given state represented by $|\psi(x)\rangle$, we use δx to denote the distance for the translation of $|\psi(x)\rangle$ to an orthogonal state and $\Delta\hat{P}$ to denote the momentum uncertainty in the state $|\psi(x)\rangle$, then

$$\delta x \Delta\hat{P} \geq \frac{h}{4} \quad (5.2)$$

where h is Planck constant without being divided by 2π . The interpretation of (5.2) may be as follows: The distance for displaced observer who ‘see’ the quantum state is completely different from that the undisplaced observer does is not less than $\Delta\hat{P}/\hbar$. Note that this uncertainty relation is on the same footing as that between time and energy (see [70]).

In this chapter we shall provide a new derivation for the inequality (5.2), we also prove that the right hand side of the above inequality (5.2) can not be improved, namely, $h/4$ is the greatest lower bound. Our derivation is analogous to that in [76] for the time-energy uncertainty relation.

5.2 Derivation of uncertainty relation

In the following, for simplicity, we only consider the wave functions with one spatial dimension in the position space. Also, we assume that the system is not in an eigenstate of the momentum operator $\hat{P}$.

In order to get the shortest distance for the translation to an orthogonal state we introduce a formal quantity that will play a central role in our derivation. This quantity is known as the correlation amplitude.

To begin with, let us consider a system in a state described by the wave function $|\psi(x)\rangle$ (with a slight abuse of notation), we use the notation $|\psi(x - a)\rangle$ to stand for the displaced state. The correlation amplitude associated with these two states is defined as

$$C(a) = \langle \psi(x) | \psi(x - a) \rangle \quad (5.3)$$

The modulus of $C(a)$ provides a quantitative measure of the “resemblance” between the states which are localised around different places, or equivalently, the state remains unchanged but the observer is displaced, then the above “between the states” should be replaced by “between the observers”.

Our aim now is to find the smallest D which satisfies

$$C(D) = \langle \psi(x) | \psi(x - D) \rangle = 0. \quad (5.4)$$

It is convenient to use $|C(a)|^2$. Taking the derivative with respect to the parameter a then we get the following equation,

$$\frac{d}{da}|C(a)|^2 = 2\text{Re} \left[\langle \psi(x-a) | \psi(x) \rangle \langle \psi(x) | \frac{d}{da} \psi(x-a) \rangle \right] \quad (5.5)$$

Let $|\psi(x-a)\rangle$ be the state displaced through the distance a :

$$|\psi(x-a)\rangle = e^{-\frac{i}{\hbar}\hat{P}a}|\psi(x)\rangle \quad (5.6)$$

It follows easily that

$$\frac{d}{da}|\psi(x-a)\rangle = -\frac{i}{\hbar}\hat{P}|\psi(x-a)\rangle \quad (5.7)$$

For any Hermitian operator $\hat{A}$, the following formula holds¹ [76, 78]:

$$\hat{A}|\psi(x)\rangle = \langle \hat{A} \rangle |\psi(x)\rangle + \Delta \hat{A} |\psi_{\perp}(x)\rangle \quad (5.8)$$

where

$$\langle \hat{A} \rangle = \langle \psi(x) | \hat{A} | \psi(x) \rangle$$

$$\Delta \hat{A} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

and $|\psi(x)\rangle$ and $|\psi_{\perp}(x)\rangle$ satisfy

$$\langle \psi(x) | \psi_{\perp}(x) \rangle = 0$$

Using (5.7) and (5.8), we obtain

$$\frac{d}{da}|\psi(x-a)\rangle = -\frac{i}{\hbar}[\langle \hat{P} \rangle |\psi(x-a)\rangle + \Delta \hat{P} |\psi_{\perp}(x-a)\rangle] \quad (5.9)$$

¹Note the decomposition on the right hand side of equality is not unique.

Where $\hat{P}$ is the momentum operator. It then immediately follows that

$$\frac{d}{da}|C(a)|^2 = -\frac{2\Delta\hat{P}}{\hbar}\text{Re}[i\langle\psi(x-a)|\psi(x)\rangle\langle\psi(x)|\psi_{\perp}(x-a)\rangle] \quad (5.10)$$

In order to get the desired minimum distance, we wish to make the function $|C(a)|^2$ decrease to zero as fast as possible. For given $\Delta\hat{P}$ and $|C(a)|$, we have to find the maximum value of $|\langle\psi(x)|\psi_{\perp}(x-a)\rangle|$

Next consider the expansion of the initial state $|\psi(x)\rangle$

$$\begin{aligned} |\psi(x)\rangle &= \langle\psi(x-a)|\psi(x)\rangle|\psi(x-a)\rangle \\ &\quad + \langle\psi_{\perp}(x-a)|\psi(x)\rangle|\psi_{\perp}(x-a)\rangle \\ &\quad + \lambda|\psi_{\perp\perp}(x-a)\rangle \end{aligned} \quad (5.11)$$

where $\langle\psi(x-a)|\psi_{\perp}(x-a)\rangle = 0$ and $\langle\psi_{\perp}(x-a)|\psi_{\perp\perp}(x-a)\rangle = 0$. This leads to the following equation

$$1 = |\langle\psi(x-a)|\psi(x)\rangle|^2 + |\langle\psi_{\perp}(x-a)|\psi(x)\rangle|^2 + |\lambda|^2 \quad (5.12)$$

That is

$$|\langle\psi_{\perp}(x-a)|\psi(x)\rangle| = \sqrt{1 - |C(a)|^2 - |\lambda|^2} \quad (5.13)$$

Obviously, $|\langle\psi_{\perp}(x-a)|\psi(x)\rangle|$ attains its maximum when $\lambda = 0$. Thus, the maximal possible value of the rate of change of $|C(a)|^2$ is given by

$$\frac{2\Delta\hat{P}}{\hbar}|C(a)|\sqrt{1 - |C(a)|^2} \quad (5.14)$$

Now we consider the following equation:

$$\frac{d}{da}|C(a)|^2 = -\frac{2\Delta\hat{P}}{\hbar}|C(a)|\sqrt{1-|C(a)|^2} \quad (5.15)$$

Let us introduce a new parameter θ , and let $\sin\theta = |C(a)|$, then Eq.(5.15) reads

$$\dot{\theta} = \frac{\Delta\hat{P}}{\hbar} \quad (5.16)$$

$\dot{\theta}$ denotes the derivative with respect to the parameter a . $\theta = \pi$ and $\pi/2$ correspond to the orthogonal state and the initial state, respectively. It follows that

$$D = \frac{h}{4\Delta\hat{P}} \quad (5.17)$$

Where D is the shortest distance to an orthogonal state. Suppose we have a physical system whose momentum uncertainty is $\Delta\hat{P}$. Let us denote the distance for the translation to an orthogonal state by δx , then Δx is not less than $h/4\Delta\hat{P}$, namely

$$\delta x \Delta\hat{P} \geq \frac{h}{4} \quad (5.18)$$

This completes the proof of (5.2). So far we have worked exclusively in one-space for simplicity, but everything we have done can be generalised to three-space.

In summary, let us emphasise that the usual position-momentum uncertainty relation is on a quite different footing from that for time and

energy. In some sense, the uncertainty relation (5.18) can be regarded as an exact counterpart of the time-energy uncertainty relation.

Next, we want to prove that $\hbar/4$ on the right hand side of (5.18) can not be improved. Namely, the uncertainty relation (5.18) is a basis law. For this purpose, we consider a simple example. Suppose a physical system whose state is represented by the wave function:

$$\psi_n(x) = \begin{cases} N \sin x & \text{if } -2n\pi \leq x \leq 2n\pi \\ N e^{-(x-2n\pi)^2} \sin x & \text{if } 2n\pi < x < +\infty \\ N e^{-(x+2n\pi)^2} \sin x & \text{if } -\infty < x < -2n\pi \end{cases} \quad (5.19)$$

where N is the normalisation constant. We use δx and $\Delta \hat{x}$ to denote the distance of the translation to an orthogonal state and the uncertainty of the position operator $\hat{x}$, respectively. It is easy to see that δx goes to $\pi/2$ as $n \rightarrow \infty$, but $\Delta \hat{x}$ goes to the infinite. This example shows that the uncertainty relation (5.18) is of quite different nature from the usual uncertainty relation between the position and momentum. It is easy to see that $\Delta \hat{P}$ goes to $\hbar$, then $\delta x \Delta \hat{P}$ goes to $\frac{\hbar}{4}$. This indicates that $D = \hbar/4$ is not only a lower bound but also the greatest lower bound or the infimum.

5.3 Summary

The time and space coordinate are not symmetric in the non-relativistic quantum theory. The time enters into the theory as a parameter while

the position as an observable. This difference also reflects in the uncertainty relations which had been a cornerstone in the development of quantum theory from the very beginning. Namely, the uncertainty relation for position and momentum and that for time and energy are not on the same footing.

In this chapter we have shown that the existence of a uncertainty relations for position and momentum which is of the same form as time-energy uncertainty relation is possible. Although physical interpretation for those two kinds of uncertainty relations could be different, they are indeed of the same mathematical form [79].

Chapter 6

General Conclusion

The central themes of thesis are the investigation of various approaches in connection to the quantum open systems and the foundations of quantum theory.

We have discussed, based on a two-level system model, decoherent histories approach, environment-induced decoherence and stochastic localisation of quantum jump simulation and quantum state diffusion.

We furnished a new derivation of master equation of QBM in general environment, which is a typical quantum open system and is of particular importance in the recent advance of decoherence programmes.

In the last part of the thesis we have described a parameter-based uncertainty relations for position and momentum.

We conclude the thesis with a remark. Recent advances in quantum open system theory have opened up a brand new avenue of ex-

ploring the issues in quantum theory. Among others, the environment-induced decoherence, decoherent histories, as well as various stochastic Schrödinger equations have provided many important insights into the solution to fundamental problems in quantum theory. However, the power, depth and width of the new theories are far beyond fully explored and understood. It is very likely that what we have done so far is merely one touch on the trunk of an elephant by a blind man, it is still far to grasp the whole picture of the animal.

Appendix A

Proof of theorem

In this Appendix, we shall give a proof of Theorem in Chapter II. Since both M and N are positive definite matrices, therefore, one of them, say, N can be decomposed as

$$N = S^\dagger S, \quad (\text{A.1})$$

where S is an $n \times n$ matrix. After an arrangement, the right-hand side of Eq. (2.50) becomes

$$|\text{Tr}(MPS^\dagger SQ)| = |\text{Tr}(SQMPS^\dagger)|. \quad (\text{A.2})$$

Suppose x_m are an orthonormal basis in n dimensional space V . Then

$$|\text{Tr}(MPNQ)| = \left| \sum_m x_m^T (SQMPS^\dagger) x_m \right|, \quad (\text{A.3})$$

where x_m^T is the transpose of x_m . Now, we set

$$y_m = QS^\dagger x_m, \quad (\text{A.4})$$

$$z_m = PS^\dagger x_m. \quad (\text{A.5})$$

Then the trace in Eq. (A.3) may be rewritten as

$$\text{Tr}(MPNQ) = \sum_m y_m^T M z_m. \quad (\text{A.6})$$

Since y_m, z_m are orthogonal vectors and M is a positive definite matrix, then it is not difficult to arrive at the following inequality (see [80])

$$| (y_m^T M z_m) | \leq \epsilon^M (y_m^T M y_m)^{1/2} (z_m^T M z_m)^{1/2}, \quad (\text{A.7})$$

where $\epsilon^M = (\lambda_{\max}^M - \lambda_{\min}^M) / (\lambda_{\max}^M + \lambda_{\min}^M)$, $\lambda_{\max}^M$ and $\lambda_{\min}^M$ are the largest and the smallest eigenvalues of M , respectively. Combining (A.7) with Cauchy's inequality,

$$(\sum_m a_m b_m)^2 \leq \sum_m a_m^2 \sum_m b_m^2, \quad (\text{A.8})$$

then (A.3) becomes

$$\begin{aligned} |\text{Tr}(MPNQ)| &= \left| \sum_m x_m^T (SQMPS^\dagger) x_m \right| \\ &\leq \sum_m |y_m^T M z_m| \\ &\leq \epsilon^M (\sum_m y_m^T M y_m)^{1/2} (\sum_m z_m^T M z_m)^{1/2}. \end{aligned} \quad (\text{A.9})$$

It is easy to identify that

$$\text{Tr}(MPNP) = \sum_m y_m^T M y_m, \quad (\text{A.10})$$

$$\text{Tr}(MQNQ) = \sum_m z_m^T M z_m. \quad (\text{A.11})$$

This proves that

$$|\text{Tr}(MPNQ)| \leq \epsilon^M [\text{Tr}(MPNP)]^{1/2} [\text{Tr}(MQNQ)]^{1/2}. \quad (\text{A.12})$$

Since M and N are in the completely symmetric position, so the similar result is true for ϵ^N . Then it completes the proof of the theorem. $\square$

Appendix B

Coefficients in master equation of QBM

In this appendix, we will provide an alternative method of determining the coefficients $A(t)$, $B(t)$, $C(t)$ and $D(t)$ in the master equation of QBM in the general case (see Chapter IV). Our method solely relies on the Laplace transform which is particularly convenient in some cases.

To begin with, we consider the operator equations of motion of the system described by (4.1) in the Heisenberg representation (from now on, we choose $\hbar = 1$, $M = 1$):

$$\ddot{q}(t) + \Omega^2 q(t) = - \sum_n C_n q_n(t), \quad (\text{B.1})$$

$$\ddot{q}_n(t) + \omega_n^2 q_n(t) = - \frac{C_n}{m_n} q(t). \quad (\text{B.2})$$

We apply the Laplace transform to Eqs (B.1) and (B.2):

$$s^2 \mathcal{L}[q(t)] - sq(0) - p(0) + \Omega^2 \mathcal{L}[q(t)] = - \sum_n C_n \mathcal{L}[q_n(t)], \quad (\text{B.3})$$

$$s^2 \mathcal{L}[q_n(t)] - s q_n(0) - \frac{p_n(0)}{m_n} + \omega_n^2 \mathcal{L}[q_n(t)] = -\frac{C_n}{m_n} \mathcal{L}[q(t)], \quad (\text{B.4})$$

where $\mathcal{L}[\cdot]$ stands for the Laplace transform of the argument. Substituting Eq (B.3) into (B.4), it becomes

$$\begin{aligned} \left[s^2 + \Omega^2 - \sum_n \frac{C_n^2}{(s^2 + \omega_n^2)m_n} \right] \mathcal{L}[q(t)] = & - \sum_n \frac{C_n^2}{s^2 + \omega_n^2} q_n(0) \\ & - \sum_n \frac{C_n}{s^2 + \omega_n^2} \frac{p_n(0)}{m_n} \\ & + s q(0) + p(0) \end{aligned} \quad (\text{B.5})$$

Now we define two functions $\phi(\lambda)$ and $\psi(\lambda)$ as follows

$$\phi(\lambda) = \mathcal{L}^{-1} \left[s \left(s^2 + \Omega^2 - \sum_n \frac{C_n^2}{s^2 + \omega_n^2} \right)^{-1} \right] \quad (\text{B.6})$$

$$\psi(\lambda) = \mathcal{L}^{-1} \left[\left(s^2 + \Omega^2 - \sum_n \frac{C_n^2}{s^2 + \omega_n^2} \right)^{-1} \right] \quad (\text{B.7})$$

where $\mathcal{L}^{-1}$ is the inverse Laplace transform. It is easy to see that $\psi'(\lambda) = \phi(\lambda)$. Moreover, both $\psi(\lambda)$ and $\phi(\lambda)$ satisfy an integro-differential equation:

$$\ddot{\Sigma}(s) + \Omega^2 \Sigma(s) + 2 \int_0^s d\lambda \eta(s - \lambda) \Sigma(\lambda) = 0 \quad (\text{B.8})$$

with the initial conditions

$$\phi(0) = 1, \quad \dot{\phi}(0) = 0, \quad (\text{B.9})$$

$$\psi(0) = 0, \quad \dot{\psi}(0) = 1. \quad (\text{B.10})$$

Noting here that ϕ, ψ are different from the elementary functions $u_1(s)$ and $u_2(s)$ defined in Chapter 4 which satisfy the boundary conditions:

$$u_1(s=0) = 1, \quad u_1(s=t) = 0, \quad (\text{B.11})$$

and

$$u_2(s=0) = 0, \quad u_2(s=t) = 1. \quad (\text{B.12})$$

However, the two sets of functions are equivalent in sense of that they can be represented each other. For the sake of convenience, we explicitly write down these two sets of relations:

$$u_1(\lambda) = \phi(\lambda) - \phi(t) \frac{\psi(\lambda)}{\psi(t)}, \quad (\text{B.13})$$

$$u_2(\lambda) = \frac{\psi(\lambda)}{\psi(t)} \quad (\text{B.14})$$

and

$$\phi(\lambda) = u_1(\lambda) + \frac{\dot{u}_2(t)}{\dot{u}_2(0)} u_2(\lambda), \quad (\text{B.15})$$

$$\psi(\lambda) = \frac{\dot{u}_2(\lambda)}{\dot{u}_2(0)}, \quad (\text{B.16})$$

where t is any given time point.

Next we consider the expression for $q(t)$ in terms of the initial values. To do this, we simply apply the inverse Laplace transform to (B.5). Then it is straitforward to have the following:

$$q(t) = \phi(t)q(0) + \psi(t)p(0) \quad (\text{B.17})$$

$$\begin{aligned}
& - \sum_n C_n \int_0^t ds \psi(s) \cos[\omega_n(t-s)] q_n(0) \\
& - \sum_n C_n \int_0^t ds \psi(s) \frac{\sin[\omega_n(t-s)]}{\omega_n} \frac{p_n(0)}{m_n}.
\end{aligned}$$

Since we have assumed that the bath is initially in a thermal equilibrium state, then the expectation values $\langle q_n(0) \rangle = \langle p_n(0) \rangle = 0$. On combining this and Eq. (B.17), one has

$$\langle q(t) \rangle = \phi(t) \langle q(0) \rangle + \psi(t) \langle p(0) \rangle, \quad (\text{B.18})$$

$$\langle p(t) \rangle = (\dot{u}_1(t) + \phi(t) \dot{u}_2(t)) \langle q(0) \rangle + \psi(t) \dot{u}_2(t) \langle p(0) \rangle. \quad (\text{B.19})$$

Similarly, using Eqs. (B.3) and (B.4), it is easy to show

$$\sum_n C_n \langle q_n(t) \rangle = 2 \int_0^t ds \eta(t-s) \phi(s) \langle q(0) \rangle + 2 \int_0^t ds \eta(t-s) \psi(s) \langle p(0) \rangle. \quad (\text{B.20})$$

Using (B.18) and (B.19) to eliminate $\langle q(0) \rangle$ and $\langle p(0) \rangle$ in Eq. (B.20), it becomes

$$\begin{aligned}
\sum_n C_n \langle q_n(t) \rangle &= 2 \left[\int_0^t ds \eta(t-s) u_2(s) - \frac{\dot{u}_2(t)}{\dot{u}_1(t)} \int_0^t ds \eta(t-s) u_1(s) \right] \langle q(t) \rangle \\
&\quad - 2 \frac{1}{\dot{u}_1(0)} \int_0^t ds \eta(t-s) u_1(s) \langle p(t) \rangle.
\end{aligned} \quad (\text{B.21})$$

On comparing the two sides of both Eqs. (B.21) and (4.37), we thus obtain

$$A(t) = d_2(t) - 2\Gamma(t) \dot{u}_2(t), \quad (\text{B.22})$$

$$B(t) = 2\Gamma(t), \quad (\text{B.23})$$

where

$$\Gamma(t) = \frac{d_1(t)}{2\dot{u}_1(t)}, \quad (\text{B.24})$$

$$d_i(t) = 2 \int_0^t ds \eta(t-s) u_i(s), \quad (i = 1, 2). \quad (\text{B.25})$$

In order to determine the coefficients $C(t)$ and $D(t)$, we need to calculate the higher order expectations:

$$\begin{aligned} \langle q^2(t) \rangle &= \phi^2(t) \langle q^2(0) \rangle + 2\phi(t)\psi(t) \langle \frac{p(0)q(0) + q(0)p(0)}{2} \rangle \\ &\quad + \psi^2(t) \langle p^2(0) \rangle + E \end{aligned} \quad (\text{B.26})$$

$$\begin{aligned} \langle p^2(t) \rangle &= \dot{\phi}^2(t) \langle q^2(0) \rangle + 2\dot{\phi}(t)\psi(t) \langle \frac{p(0)q(0) + q(0)p(0)}{2} \rangle \\ &\quad + \phi^2(t) \langle p^2(0) \rangle + F, \end{aligned} \quad (\text{B.27})$$

$$\begin{aligned} \langle \frac{p(t)q(t) + q(t)p(t)}{2} \rangle &= \dot{\phi}(t)\dot{\phi}(t) \langle q^2(0) \rangle \\ &\quad + \dot{\phi}(t)\psi(t) + \phi^2(t) \langle \frac{p(0)q(0) + q(0)p(0)}{2} \rangle \\ &\quad + \phi(t)\psi(t) \langle p^2(0) \rangle + \frac{1}{2}\dot{E} \end{aligned} \quad (\text{B.28})$$

where

$$E = \sum_n \alpha_n^2(t) \langle q_n^2(0) \rangle + \sum_N \beta_N^2(t) \langle p_N^2(0) \rangle \quad (\text{B.29})$$

$$F = \sum_n \dot{\alpha}_n^2(t) \langle q_n^2(0) \rangle + \sum_N \dot{\beta}_N^2(t) \langle p_N^2(0) \rangle \quad (\text{B.30})$$

and

$$\alpha_n(t) = -C_n \int_0^t ds \psi(s) \cos \omega_n(t-s) \quad (\text{B.31})$$

$$\beta_n(t) = -C_n \int_0^t ds \psi(s) \frac{\sin \omega_n(t-s)}{\omega_n}. \quad (\text{B.32})$$

According to the equations (4.35),(4.46), we finally obtain the expression for the coefficients $C(t)$ and $D(t)$:

$$C(t) = \frac{1}{2}\ddot{E} + (\Omega^2 + A(t))E + \frac{1}{2}B(t)\dot{E} - F \quad (\text{B.33})$$

$$D(t) = \frac{1}{2}\dot{F} + \frac{1}{2}(\Omega^2 + A(t))\dot{E} + B(t)F. \quad (\text{B.34})$$

For the special case (such as high temperature limit), the function ψ and ϕ are very easy to calculate, then the coefficients are then determined immediately.

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