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Open quantum systems

Open quantum systems, density matrix theory and quantum Markov processes

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Abstract

In this Bachelor thesis project, the Lindblad master equation is derived, both as the most general way of modeling interaction with an environment that lacks memory, and through microscopic derivations focused on assumptions about the way the system interacts with its environment (weak-coupling, Born-Markov and rotating wave approximations). It is then applied to a two-level system (qubit).

Contents

Chapter 1

Introduction

1.1 General framework

Quantum mechanics governs the physics of microscopical systems. There are a number of differences between quantum mechanics and classical mechanics. In classical mechanics, predictions about systems are deterministic - a system with a given initial state will always evolve in the same way. In quantum mechanics, however, predictions are probablistic. Quantum mechanics can only give probabilities for various outcomes - if an experiment is performed many times in a row, the result will eventually converge to the distribution predicted by theory[2].

Real quantum systems are subject to interaction with an uncontrollable environment. These systems are known as open quantum systems. When modeling open quantum systems, the system and environment are considered together. A wavefunction describing the full environment will typically contain a large amount of information due to the environment having many degrees of freedom, which makes solving the Schrödinger equation computationally expensive. It is also often hard to devise detailed models of the interactions between the system and environment. Therefore, one often derives equations for the dynamics of the system only; in the case of an environment that lacks memory, the Lindblad master equation is used[2].

The Lindblad master equation is different from the Schrödinger equation in multiple ways; first of all, it describes time evolution of a density matrix rather than a wavefunction. A density matrix corresponds to a statistical ensemble of wavefunctions; for example, wavefunction A with a probability of 25% and wavefunction B with a probability of 75%. This is known as a mixed state[2]. The mixed state arises when computing the partial trace over the environment, isolating the system state from redundant information about the environment. Due to the interaction with the environment, the system will no longer evolve in time according to the Schrödinger equation. The interaction with the environment will express itself as a perturbed system Hamiltonian as well as dissipation through Lindblad operators[2].

In the case of an open system modeled by the Lindblad master equation, the dissipation of the environment is described by Lindblad operator. The time evolution with Lindblad operators occurs through drift and jump processes[4].

1.2 The tensor product; observables

The state of a quantum system is a vector in a Hilbert space. In an open quantum system, the full system is the system of interest considered together with its environment. This is a vector in the tensor product of the system and environment Hilbert spaces[3]. The tensor product is a vector space in which each pair of basis vectors $(|\alpha\rangle, |\beta\rangle)$ from the two Hilbert spaces form a new basis vector $|\alpha\beta\rangle$. Observables for the system are represented by the operator tensor product $O_S \otimes I_B$, while observables for the environment are represented by the tensor product $I_S \otimes O_B$. The interaction with the environment will lead to the system developing entanglement with the environment.

1.3 The partial trace; origin of the mixed states

Consider the observable $O_S \otimes I_B$. If the composite system state is $\sum_{\alpha,\beta} c_{\alpha\beta} |\alpha\beta\rangle$, where α are taken to be the eigenvectors of O_S, the expectation value will be

$$\langle O_S \rangle = \sum_{\alpha,\beta} O_\alpha |c_{\alpha\beta}|^2 . \tag{1.1}$$

When deducing equations for the time evolution of the open system, the environment is typically traced out. This means replacing the wavefunction in the tensor product space with a statistical ensemble of wavefunctions in the system Hilbert space:

$$\left\{ |\alpha\rangle \text{ with probability } p_\alpha = \sum_\beta |c_{\alpha\beta}|^2 \right\}. \tag{1.2}$$

The expectation value is then written as:

$$\langle O_S \rangle = \sum_\alpha p_a \langle \alpha | O_S | \alpha \rangle . \tag{1.3}$$

A statistical ensemble is also known as a mixed state. Mixed states have a representation known as density matrices:

$$\rho = \sum p_\alpha |\alpha\rangle \langle\alpha| . \tag{1.4}$$

This representation is useful when deriving so-called master equations for the time evolution of the reduced system.

1.4 Equations for open systems

An open quantum system is a quantum system that is coupled to an environment. When quantum systems are composed they form a tensor product. This tensor product will evolve in time according to the Schrödinger equation:

$$\partial_t \psi(t) = -iH(t)\psi(t). \tag{1.5}$$

Integration of the time evolution gives

$$\psi(t) = \left(\mathrm{T}_\leftarrow \exp\left[-i \int_0^t H(s) ds \right] \right) \psi(0). \tag{1.6}$$

This motivates the introduction of a time evolution operator $U(t, t_0) = \mathrm{T}_\leftarrow \exp\left[-i \int_{t_0}^t H(s) ds \right]$, where $\mathrm{T}_\leftarrow$ is the time-ordering operator. If the Hamiltonian is independent of time, that is, if $H(t) = H_0$, then the time evolution operator becomes $U(t, t_0) = \exp\left[-iH_0(t - t_0)\right]$. The time evolution of the system+environment density matrix ρ is given by the von Neumann equation[2]

$$\partial_t \rho = [-iH, \rho] . \tag{1.7}$$

Integration of this equation yields

$$\rho(t) = \rho(0) - i \int_0^t [H, \rho(s)] \, ds, \tag{1.8}$$

which is commonly used in microscopic derivations. Taking the partial trace over the environment:

$$\mathrm{tr}_B \partial_t \rho = \mathrm{tr}_B [-iH, \rho] , \tag{1.9}$$

implying

$$\partial_t \rho_S = \partial_t \mathrm{tr}_B \rho = \mathrm{tr}_B [-iH, \rho] . \tag{1.10}$$

To eliminate the dependence on the state of the environment, it is usually assumed to reside in a reference state ρ_B. The environment could for example be a heat bath in a thermal equilibrium[2]:

$$\partial_t \rho_S = \mathrm{tr}_B [-iH, \rho_S(t) \otimes \rho_B] . \tag{1.11}$$

1.5 The Lindblad master equation

The Lindblad master equation is stated as:

$$\partial_t \rho = -i\left[H, \rho\right] + \sum_i \gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\left\{ L_i^\dagger L_i, \rho \right\} \right). \tag{1.12}$$

This governs the time evolution of a density matrix ρ subject to the perturbed system Hamiltonian H and dissipation through the Lindblad operators L_i. Mathematically the Lindblad master equation arises as the most general generator of the quantum dynamical semigroup. Physically it may arise as the equation describing the dynamics of a system subject to weak coupling to a reservoir where the inverse frequency difference τ_S is much smaller than the system relaxation time (time scale over which the system density matrix changes apprechiably); $\tau_S << \tau_R$ and the time τ_B over which the environment correlation functions decay; $\tau_B << \tau_R$, the environment time scale[2].

Chapter 2

Open quantum systems

An open quantum system is a system that is in contact with an environment (see Figure 2.1). It is found that an initial pure quantum state (that is, a vector in the state space) evolves into a statistical ensemble, or mixed quantum state. A mixed quantum state is described by a density matrix; an operator that acts on the system Hilbert space[1]. Time evolution of a mixed state is, in the case of a closed system, governed by the von Neumann equation. In the case of an open system where the environment lacks memeory, time evolution of the mixed state is governed by the Lindblad master equation[2].

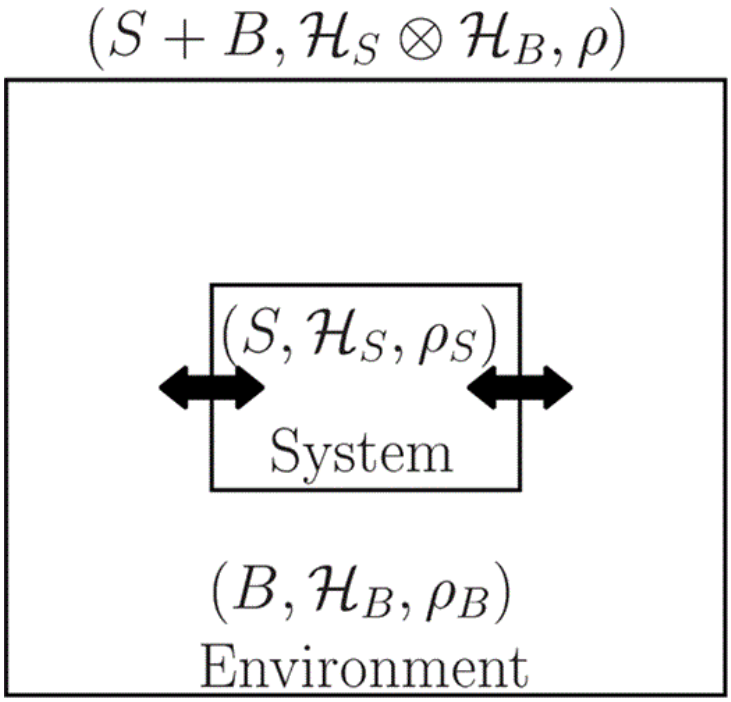


Figure 2.1: Total system formed from system and environment; figure courtesy of [2].

2.1 Mixed states and density matrix theory

Consider a statistical ensemble (mixed state) of (pure) states $\{|\psi_i\rangle\}_{i=0}^{N}$ each with probability p_i. This we represent using a density matrix, which is a matrix ρ that can be expressed as the sum:

$$\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| . \tag{2.1}$$

where the p_i express probabilities for the various states $|\psi_i\rangle$, and thus fulfil $p_i > 0$ and $\sum_i p_i = 1$[3]. This representation is not unique; in fact, for density matrices that represent mixed states, there are many ways of expressing it in terms of pure states [2]. The time evolution of a density matrix is unique, decided by the von Neumann equation. Many computations on density matrices are performed using the trace operation. The trace of a Hermitian matrix O on a Hilbert space $\mathcal{H}$ with orthonormal basis $\{|\psi_i\rangle\}_{i=0}^{N}$ is defined as the sum:

$$\operatorname{Tr} O = \sum_i \langle \psi_i | O | \psi_i \rangle . \tag{2.2}$$

Sometimes, we may consider a Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ that is a tensor product of the Hilbert spaces $\mathcal{H}_A$, with ON-basis $\left\{ \left| \psi_i^A \right\rangle \right\}_{i=0}^N$, and $\mathcal{H}_B$, with ON-basis $\left\{ \left| \psi_i^B \right\rangle \right\}_{i=0}^M$. The partial trace with regards to $\mathcal{H}_B$ is then defined as:

$$\operatorname{Tr}_B O = \sum_i \left\langle \psi_i^B | O | \psi_i^B \right\rangle . \tag{2.3}$$

which is an operator acting on $\mathcal{H}_A$. The value $\left\langle \psi_i^B | O | \psi_i^B \right\rangle$ is defined as the sum:
$\sum_k \left\langle \psi_k^A \psi_i^B | O | \psi_k^A \psi_i^B \right\rangle \left| \psi_k^A \right\rangle \left\langle \psi_k^A \right|$. A consequence of this definition is that $\operatorname{Tr} O = \operatorname{Tr}_A \operatorname{Tr}_B O$.
We list a number of properties of density matrices[3]:

1. Trace equals to one.
$$\operatorname{Tr} \rho = 1. \tag{2.4}$$
2. It is positive semi-definite.
$$\rho \geq 0. \tag{2.5}$$
3. It is Hermitian.
$$\rho^\dagger = \rho. \tag{2.6}$$

How do we show these properties? We have

$$\operatorname{Tr} \rho = \sum_i \langle \psi_i | \left(\sum_j p_j | \psi_j \rangle \langle \psi_j | \right) | \psi_i \rangle = \sum_i \sum_j p_j \langle \psi_i | \psi_j \rangle \langle \psi_j | \psi_i \rangle = \sum_i p_i = 1. \tag{2.7}$$

showing the first property. We have

$$\langle q | \rho | q \rangle = \sum_i p_i \langle q | \psi_i \rangle \langle \psi_i | q \rangle = \sum_i p_i | \langle q | \psi_i \rangle |^2 \geq 0. \tag{2.8}$$

showing the second property. The third property follows from the second, as all matrices are diagonalizable over $\mathbb{C}$, and positivity ensures real eigenvalues. Diagonalizability with real eigenvalues implies that a matrix is Hermitian. Any matrix that fullfils properties 1 and 2 will be a density matrix, as it can be written as a spectral decomposition according to $\rho = \sum \lambda_i | \epsilon_i \rangle \langle \epsilon_i |$where $|\epsilon_i| = 1$, and $\operatorname{Tr} \rho = \sum \lambda_i = 1$. Should any of the λ_i fail to be greater than or equal to zero, ρ would not be a positive matrix. Expectation values of observables are expressed in terms of the trace of the observable when multiplied by the density matrix. The expectation value of an observable A for a state represented by the density matrix ρ is given by

$$\langle A \rangle = \operatorname{Tr} (A\rho) . \tag{2.9}$$

We have

$$\begin{aligned} \langle A \rangle &= \sum_i p_i \langle A \rangle_i = \sum_i p_i \langle \psi_i | A | \psi_i \rangle = \sum_i p_i \langle \psi_i | AI | \psi_i \rangle = \\ &= \sum_{i,j} p_i \langle \psi_i | A | \psi_j \rangle \langle \psi_j | \psi_i \rangle = \sum_j \left\langle \psi_j \middle| A \left(\sum_i p_i | \psi_i \rangle \langle \psi_i | \right) \middle| \psi_j \right\rangle = \operatorname{Tr} (A\rho) . \end{aligned} \tag{2.10}$$

How does a density matrix evolve in time? We have, by the product rule:

$$\partial_t \rho = \sum_i \partial_t p_i | \psi_i \rangle \langle \psi_i | = \sum_i p_i \left(| \psi_i \rangle \langle \partial_t \psi_i | + | \partial_t \psi_i \rangle \langle \psi_i | \right) . \tag{2.11}$$

The Shrödinger equation in theoretical units gives $\partial_t \psi = -iH\psi$, insertion into 2.11 yields:

$$\partial_t \rho = \sum_i p_i \left(\sum_i p_i \left(| \psi_i \rangle \langle -iH\psi_i | + | -iH\psi_i \rangle \langle \psi_i | \right) \right) = i\rho H - iH\rho = [-iH, \rho] . \tag{2.12}$$

This is known as the von Neumann equation.
Convex linear combinations of density matrices, that is, linear combinations $\sum p_i \rho_i$ where $p_i > 0$ and $\sum p_i = 1$ form new density matrices.
The quantity $\operatorname{Tr} \rho^2$ is known as the purity of the density matrix ρ. The purity ranges between $1/N$ and 1, where N is the dimension of the Hilbert space, and is 1 if and only if ρ is a pure state[2]. Purity is preserved under time evolution according to the von Neumann equation[3]. (That is, unitary time evolution.)

2.2 The Bloch sphere

Consider a two-level system; that is, a system with a Hilbert space spanned by two basis vectors which we denote by $|0\rangle$ and $|1\rangle$. A density matrix for this system will have size 2×2. A basis for the space of matrices acting on a two-dimensional Hilbert space is given by the identity together with the Pauli matrices σ_x, σ_y and σ_z, defined as[6]:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.13}$$

Let $\rho = a\left(I + n_x\sigma_x + n_y\sigma_y + n_z\sigma_y\right)$. The trace of a density matrix should be unity, giving

$$\mathrm{Tr}\,\rho = 2a = 1. \tag{2.14}$$

The purity can be expressed as

$$\begin{aligned} \mathrm{Tr}\rho^2 =& \frac{1}{4}\mathrm{Tr}\left(I + n_x^2\sigma_x^2 + n_y^2\sigma_y^2 + n_z^2\sigma_z^2\right) = \frac{1}{4}\mathrm{Tr}\left(I + n_x^2 I + n_y^2 I + n_z^2 I\right) \\ =& \frac{1}{2}\left(1 + |\bar{n}|^2\right). \end{aligned} \tag{2.15}$$

This should range between $1/N$ and 1[3], which implies that

$$\begin{aligned} \mathrm{Tr}\rho^2 \leq 1 \implies \frac{1}{2}\left(1 + |\bar{n}|^2\right) \leq 1 \implies \\ \implies |\bar{n}|^2 \leq 1. \end{aligned} \tag{2.16}$$

In other words, $\bar{n}$ will be a vector within the unit sphere. If $\bar{n}$ is on the surface of the unit sphere, the density matrix represents a pure state, otherwise it represents a mixed state[6]. Points on the surface of this sphere can be expressed in terms of spherical coordinates:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = e^{i\phi_0}\left(\cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\phi}|1\rangle\right). \tag{2.17}$$

the phase factor $e^{i\phi_0}$ has no effect on the physics on the system, and so can be ignored. This yields the Bloch sphere representation of the ket vector, where θ varies between 0 and π, and ϕ varies between 0 and 2π.

2.3 The interaction picture

When studying the dynamics of a quantum system, we typically want to see how a set of observables evolve in time. There are multiple ways of considering the time evolution of a system. One is the Schrödinger picture, in which the wavefunction has some prescribed initial state and evolves in time according to the Schrödinger equation. An alternative to the Schrödinger picture is the Heissenberg picture, in which the observables evolve in time and the wavefunction is constant. For composite quantum systems, there is a third way known as the interaction picture. In the interaction picture, the full system Hamiltonian is separated into the self-Hamiltonians H_S and H_B acting on the individual systems and the (schrödinger picture) interaction Hamiltonian $\hat{H}_{int}(t)$[2]:

$$H(t) = H_S \otimes I_B + I_S \otimes H_B + \hat{H}_{int}(t) = H_0 + \hat{H}_{int}(t). \tag{2.18}$$

The density matrix evolves in time according to the interaction Hamiltonian, while observables evolve according to the self-Hamiltonians. We derive the interaction picture density matrix and interaction picture observables from the Schrödinger picture. This is accomplished by assuming the expectation values of observables to be the same over time.

2.3.1 Time evolution operators

Definition 2.3.1. Time evolution operator. The time evolution operator corresponding to a system with the hamiltonian $H(t)$ is defined as[2]

$$U(t_1, t_0) = T_{\leftarrow}\exp\left[-i\int_{t_0}^{t_1} \mathrm{d}s H(s)\right]. \tag{2.19}$$

where the $T_{\leftarrow}$ is the time-ordering operator. In the case of a time-independent hamiltonian, we obtain:

$$U(t_1, t_0) = \exp\left[-iH(t_1 - t_0)\right]. \tag{2.20}$$

2.3.2 Schrödinger picture

In the Schrödinger picture, we have an initial density matrix $\rho(0)$ that evolves in time according to a time evolution operator $U(t)$[2]:

$$\rho(t) = U(t)\,\rho(0)\,U^{\dagger}(t). \tag{2.21}$$

The expectation value of an observable $A(t)$ may be computed according to[2]

$$\langle A(t)\rangle = \mathrm{Tr}\left[A(t)\,\rho(t)\right]. \tag{2.22}$$

Expressing the time evolution of the density matrix in terms of the Hamiltonian yields the von Neumann equation:

$$\partial_t \rho(t) = \left[-iH(t), \rho(t)\right]. \tag{2.23}$$

2.3.3 Heissenberg picture

In the Heissenberg picture, the density matrix ρ_H is fixed and the operators evolve in time according[2]:

$$\langle A(t)\,\rho(t)\rangle = \left\langle A(t)\,U(t)\,\rho(0)\,U^{\dagger}(t)\right\rangle = \left\langle U^{\dagger}(t)\,A(t)\,U(t)\,\rho(0)\right\rangle = \langle A_H(t)\,\rho_H\rangle. \tag{2.24}$$

Expressing the time evolution of the operator in terms of the Hamiltonian yields

$$\partial_t A_H(t) = \partial_t\left(U^{\dagger}(t)\,A(t)\,U(t)\right) = \left(-iH(t)U(t)\right)^{\dagger} A(t)U(t) - U^{\dagger}(t)\,A\left(-iH(t)U(t)\right) = \left[-iH(t), A_H(t)\right]. \tag{2.25}$$

2.3.4 Interaction picture

We have the full system Hamiltonian

$$H(t) = H_0 + \hat{H}_{int}(t). \tag{2.26}$$

Time evolution operators are introduced according to[2]

$$U(t) = \mathrm{T}_{\leftarrow} \exp\left[-i\int_{t_0}^{t} H(s)\mathrm{d}s\right], \tag{2.27}$$

$$U_0 = \exp\left[-iH_0 t\right], \tag{2.28}$$

$$U_I(t) = U_0^{\dagger} U(t). \tag{2.29}$$

Here, $U(t)$ is the time evolution for the full Hamiltonian, while U_0 the time evolution due to the self-Hamiltonians. The U_I operators can be interpreted as letting the system evolve according to the full Hamiltonian while reversing the time evolution caused by the self-Hamiltonians, yielding interaction time evolution operators. Now consider an expectation value first expressed with Schrödinger picture density matrix $\rho(t)$ and operator $A(t)$:

$$\begin{aligned}
\langle A(t)\rangle =& \mathrm{Tr}\left[A(t)\,\rho(t)\right] = \mathrm{Tr}\left[A(t)\,U(t)\rho(0)U^{\dagger}(t)\right] = \\
=& \mathrm{Tr}\left[A(t)\,U_0 U_I(t)\rho(0)\left(U_0 U_I(t)\right)^{\dagger}\right] = \\
=& \mathrm{Tr}\left[U_0^{\dagger} A(t)\,U_0 U_I(t)\rho(0)U_I(t)^{\dagger}\right] = \\
=& \mathrm{Tr}\left[A_I(t)\,\rho_I(t)\right].
\end{aligned} \tag{2.30}$$

$$\begin{aligned}
\partial_t U_I(t) =& \partial_t U_0^{\dagger} U(t) = \left(-iH_0 U_0\right)^{\dagger} U(t) + U_0^{\dagger}\left(-iH(t)\,U(t)\right) = \\
=& iU_0^{\dagger} H_0 U_0 U_I(t) - iU_0^{\dagger}\left(H_0 + \hat{H}_{int}(t)\right) U_0 U_I(t) = \\
=& -iU_0^{\dagger}\hat{H}_{int}(t)\,U_0 U_I(t).
\end{aligned} \tag{2.31}$$

Introducing the interaction picture interaction Hamiltonian $H_{int} = U_0^\dagger \hat{H}_{int}(t) U_0$ allows writing this relation in a more succint form

$$\partial_t U_I(t) = -iH_{int}(t) U_I(t). \tag{2.32}$$

The time evolution of the density matrix can therefore be written as

$$\partial_t \rho_I(t) = [-iH_{int}(t), \rho_I(t)]. \tag{2.33}$$

And the time evolution of observables can be written as

$$\begin{aligned}\partial_t A_I(t) =& \partial_t \left(U_0^\dagger A(t) U_0\right) = \dot{U_0^\dagger} A(t) U_0 + U_0^\dagger A(t) \dot{U_0^\dagger} = \\ =& iH_0 U_0^\dagger A(t) U_0 - iU_0^\dagger A(t) U_0 H_0 = \\ =& [iH_0, A_I(t)].\end{aligned} \tag{2.34}$$

Chapter 3

The Lindblad master equation

3.1 Statement of the Lindblad master equation: general theorems

The Lindblad master equation describes the Markovian time evolution of an open quantum systems; that is, time evolution of an open system that interacts with an environment which lacks memory[3].

Definition 3.1.1. The Lindblad master equation (diagonal form)

$$\partial_t \rho = -i\left[H, \rho\right] + \sum_i \gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\left\{ L_i^\dagger L_i, \rho \right\} \right). \tag{3.1}$$

where $\gamma_i > 0$.

Here H is the Hamiltonian (not necessarily the same as the closed-system Hamiltonian), and L_i is the Lindblad operator. The Lindblad operator L_i both contributes to the continous time evolution of the system with the $\left\{ L_i^\dagger L_i, \rho \right\}$ term (the drift part), and introduces discontinous time evolution with the $L_i \rho L_i^\dagger$ term (the jump part).[3] In the limiting case $\gamma_i = 0 \, \forall i$, the von Neumann equation is obtained. There are multiple ways in which the Lindblad master equation can be obtained. It is the most general way to express Markovian time evolution of an open system. Microscopic derivations under suitable assumptions also result in the Lindblad master equation, with the Lindblad operators expressed in terms of the interaction Hamiltonian[2].
When deriving the Lindblad master equation, it is common to end up with a form that is not already diagonalized.

Definition 3.1.2. The Lindblad master equation (first standard form)

$$\partial_t \rho = -i\left[H, \rho\right] + \sum_{n,m} h_{nm} \left(A_n \rho A_m^\dagger - \frac{1}{2}\left\{ A_m^\dagger L_n, \rho \right\} \right). \tag{3.2}$$

where h_{nm} is a positive semidefinite matrix[2].
The following theorem can be used to obtain the Lindblad master equation in diagonal form:

Teorem 3.1.3. *The Lindblad master equation in the diagonal form can be obtained through diagonalization of the first standard form, a transformation which is always possible.*

The Lindblad equation fulfils the following invariance properties:

Teorem 3.1.4. *The Lindblad master equation is invariant under the unitary transformation v[2]*

$$\sqrt{\gamma_i} L_i \to \sqrt{\gamma_i'} L_i' = \sum_j v_{ij} \sqrt{\gamma_j} L_j. \tag{3.3}$$

and also under the inhomogeneous transformation[2]

$$L_i \to L_i' = L_i + a_i I, \tag{3.4}$$

$$H \to H' = H + \frac{1}{2i} \sum_j \gamma_j \left(a_j^* L_j - a_j L_j^\dagger \right) + bI. \tag{3.5}$$

The second transformation may be used to obtain traceless Lindblad operators. Finally, the Lindblad master equation is capable of fully describing the Markovian dynamics of all open quantum systems, stated as:

Teorem 3.1.5. *The Lindblad master equation is the most general generator of the quantum dynamical semigroup.[2]*

3.2 Interpretation of the Lindblad operators

What effect do the Lindblad operators have on the dynamics of the system? We know that they, together with a perturbation to the system Hamiltonian, model the interaction of the open system with the environment. To illustrate the various ways in which a Lindblad operator can act on a density matrix, we consider the case of a two-dimensional system Hilbert space (one example of such a system is a qubit). The Lindblad operator L is chosen to be traceless.
The Lindblad master equation describes how the density matrix evolves in time

$$\partial_t \rho = -i\left[H,\rho\right] + \gamma L\rho L^\dagger - \frac{\gamma}{2}L^\dagger L\rho - \frac{\gamma}{2}\rho L^\dagger L. \tag{3.6}$$

Consider the time evolution over a short time step δt[4]:

$$\begin{aligned}\rho\left(t+\delta t\right) =& \rho\left(t\right) + \delta t\cdot\partial_t\rho\left(t\right) = \rho\left(t\right) - i\delta t\left[H,\rho\right] - \frac{\gamma}{2}\delta t L^\dagger L\rho - \frac{\gamma}{2}\delta t\rho L^\dagger L + \gamma\delta t L\rho L^\dagger = \\ =& -i\delta t\left[H,\rho\right] + M_0\rho M_0^\dagger + M_1\rho M_1^\dagger.\end{aligned} \tag{3.7}$$

where we have introduced the self-adjoint operators

$$M_0 = I - \frac{\gamma\delta t}{2}L^\dagger L. \tag{3.8}$$

and

$$M_1 = \sqrt{\gamma\delta t}L. \tag{3.9}$$

the drift and jump part, respectively. What do these operators do to a pure state $|\psi\rangle\langle\psi|$? We see that

$$M_1\left|\psi\right\rangle\left\langle\psi\right|M_1^\dagger = \left(\sqrt{\gamma\delta t}\right)^2\left\langle\psi\left|L^\dagger L\right|\psi\right\rangle\frac{\left|L\psi\right\rangle\left\langle L\psi\right|}{\left\langle\psi\left|L^\dagger L\right|\psi\right\rangle}. \tag{3.10}$$

which represents a jump to a pure state with probability $\gamma\left\langle\psi\left|L^\dagger L\right|\psi\right\rangle\delta t$. With probability $1-\gamma\left\langle\psi\left|L^\dagger L\right|\psi\right\rangle\delta t$, the system remains in the drift branch:

$$\begin{aligned}M_0\left|\psi\right\rangle\left\langle\psi\right|M_0^\dagger =& \left|\left(I-\frac{\gamma\delta t}{2}L^\dagger L\right)\psi\right\rangle\left\langle\left(I-\gamma\delta t/2L^\dagger L\right)\psi\right| = \\ =& \left|\psi\right\rangle\left\langle\psi\right| - \frac{\gamma\delta t}{2}\left|L^\dagger L\psi\right\rangle\left\langle\psi\right| - \frac{\gamma\delta t}{2}\left|\psi\right\rangle\left\langle L^\dagger L\psi\right| + \mathcal{O}\left(\delta t^2\right).\end{aligned} \tag{3.11}$$

The difference between the jump and the drift part is the behavior as $\delta t\to 0$. The drift part will tend towards the previous state, while the probability of the jump part tends towards zero[4]. Instead of thinking in terms of density matrices, we can think in terms of quantum trajectories traced by an initial pure state, as it either drifts or jumps. A large number of simulated quantum trajectories will approach the same solution as the density matrix, but can enhance computational efficiency if the dimension of the Hilbert space is large. We will now illustrate how the choice of eigenvectors affect the behavior of the quantum trajectories.

3.2.1 Degenerate eigenvectors: emission or absorption

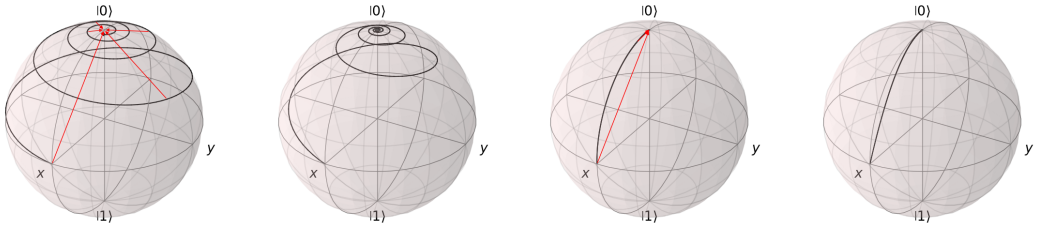
We choose the trace of L to be zero: $\operatorname{Tr}L = \lambda_1+\lambda_2 = 0$. In terms of possible eigenvalues, this means we can either have $\lambda_1=\lambda_2=0$ or $\lambda_1=-\lambda_2$. In the first case, the non-trivial case means the eigenspace for $\lambda=0$ is degenerate, corresponding to a raising or lowering operator:

Teorem 3.2.1. *In the case of two non-orthogonal eigenvectors for the Lindblad operator, it can be expressed according to*

$$L = \sqrt{\gamma}\left|a\right\rangle\left\langle b\right| \tag{3.12}$$

where $|a\rangle$ is an eigenvector with the eigenvalue 0 and $|b\rangle$ is a power vector.[4]

In this case, both the drift and jump branch evolve the state towards $|a\rangle$.



(a) (b) (c) (d)

Figure 3.1: Decay of qubit with initial superposition state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$; drift/jump parts and density matrix evolution illustrated with $H = -\sigma_z$ ((a) and (b)), and $H = 0$ ((c) and (d)).

3.2.2 Non-degenerate orthogonal eigenvectors: dephasing/balanced phase jump

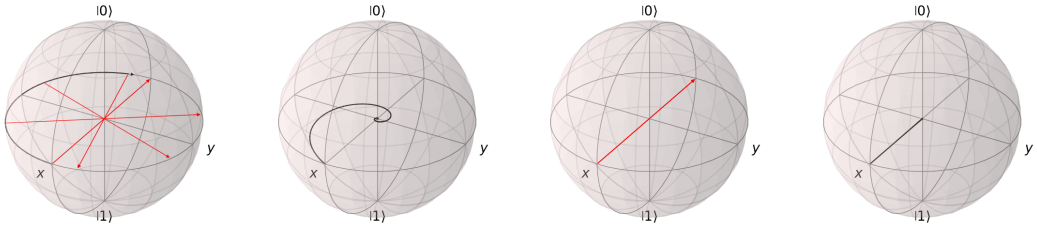
Consider the case where we have two eigenvectors of L that are orthogonal; in this case L may be expressed as:

Teorem 3.2.2. *In the case of two orthogonal eigenvectors for the Lindblad operator, it can be expressed according to*

$$L = \sqrt{\gamma}\left(|a\rangle\langle a| - |b\rangle\langle b|\right). \tag{3.13}$$

where $|a\rangle$ and $|b\rangle$ are eigenvectors with the eigenvalues $\pm\sqrt{\gamma}$.[4]

In this case, an initally coherent superposition of $|a\rangle$ and $|b\rangle$ will over time evolve to have a completely random phase relationship.



(a) (b) (c) (d)

Figure 3.2: Dephasing of qubit with initial superposition state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$; drift/jump parts and density matrix evolution illustrated with $H = -\sigma_z$ ((a) and (b)), and $H = 0$ ((c) and (d)).

3.2.3 Non-degenerate non-orthogonal eigenvectors: dephasing/unbalanced phase jump

Consider the case where we have two eigenvectors of L that are not orthogonal; in this case we have the following expression for L:

Teorem 3.2.3. *In the case of two non-orthogonal eigenvectors for the Lindblad operator, it can be expressed according to*

$$L = \frac{\sqrt{\gamma}}{\sqrt{1-\alpha^2}}\left(|a\rangle\langle a| - |b\rangle\langle b| - \alpha e^{i\beta}|a\rangle\langle b| + \alpha e^{-i\beta}|b\rangle\langle a|\right). \tag{3.14}$$

where $\langle a|b\rangle = \alpha e^{i\beta}$, $|a\rangle$ and $|b\rangle$ are eigenvectors with the eigenvalues $\pm\sqrt{\gamma}$[4]

Proof. Let

$$L = L_{aa}|a\rangle\langle a| + L_{ba}|b\rangle\langle a| + L_{ab}|a\rangle\langle b| + L_{bb}|b\rangle\langle b|. \tag{3.15}$$

Choosing L to be traceless, possibly after transformation, we haveTr $L = 0$ which gives $L_{bb} = -L_{aa}$. The eigenvalues will be $\pm\lambda$, from which follows that $\det L = -\lambda^2$; inserting the expression for L gives

$$L_{aa}(-L_{aa}) - L_{ab}L_{ba} = -\lambda^2 \implies L_{aa}^2 + L_{ab}L_{ba} = \lambda^2. \tag{3.16}$$

Furthermore, we have

$$\begin{aligned} L|a\rangle = \lambda|a\rangle \implies & L_{aa}|a\rangle + L_{ba}|b\rangle + L_{ab}\alpha e^{-i\beta}|a\rangle - L_{aa}\alpha e^{-i\beta}|b\rangle = \lambda|a\rangle \implies \\ \implies & L_{aa} + L_{ab}\alpha e^{-i\beta} = \lambda \text{ and} \qquad (3.17) \\ & L_{ba} - L_{aa}\alpha e^{-i\beta} = 0. \qquad (3.18) \end{aligned}$$

$$\begin{aligned} L|b\rangle = \lambda|b\rangle \implies & L_{aa}\alpha e^{i\beta}|a\rangle + L_{ba}\alpha e^{i\beta}|b\rangle + L_{ab}|a\rangle - L_{aa}|b\rangle = -\lambda|b\rangle \implies \\ \implies & L_{aa}\alpha e^{i\beta} + L_{ab} = 0 \text{ and} \qquad (3.19) \\ & L_{ba}\alpha e^{i\beta} - L_{aa} = -\lambda. \qquad (3.20) \end{aligned}$$

Combining 3.17 and 3.20 gives us

$$L_{aa} - L_{ba}\alpha e^{i\beta} = L_{aa} + L_{ab}\alpha e^{-i\beta} \implies L_{ba} = -L_{ab}e^{-2i\beta}. \qquad (3.21)$$

from which we deduce that $L_{aa}^2 - L_{ab}^2 e^{-2i\beta} = \lambda^2$. Squaring the equation 3.19 gives $L_{ab}^2 = L_{aa}^2\alpha^2 e^{2i\beta}$. Combined we get $L_{aa}^2\left(1-\alpha^2\right) = \lambda^2 \implies L_{aa} = \frac{\lambda}{\sqrt{1-\alpha^2}}$. 3.19 and 3.18 respectively give $L_{ab} = -\alpha e^{i\beta}L_{aa}, L_{ba} = \alpha e^{-i\beta}L_{aa}$, from which the desired result 3.14 is obtained. □

For $\alpha \neq 0$, an unbalanced phase jump is obtained, in which case the dynamics are complicated.[4]

3.3 Markovianity, the quantum dynamical semigroup

Consider an open system where the environment lacks memory. The composite system consisting of the system and environment envolves in time according to an operator $U(t_1, t_2)$. This is known as unitary time evolution. We assume the initial state is $\rho(0) = \rho_S(0) \otimes \rho_B$. Tracing out the environment yields a time-dependent system density matrix $\rho_S(t)$. This can also be described in terms of a dynamical map $V(t)$. The relationship between the dynamical map and unitary time evolution according to $U(t_1, t_2)$ is illustrated in Figure 3.3.[2]

$$\begin{array}{ccc} \rho(0) = \rho_S(0) \otimes \rho_B & \xrightarrow{\text{unitary evolution}} & \rho(t) = U(t,0)[\rho_S(0) \otimes \rho_B]U^\dagger(t,0) \\ \Big\downarrow \text{tr}_B & & \Big\downarrow \text{tr}_B \\ \rho_S(0) & \xrightarrow{\text{dynamical map}} & \rho_S(t) = V(t)\rho_S(0) \end{array}$$

Figure 3.3: Figure courtesy of [2].

Definition 3.3.1. The dynamical map is a super-operator $V(t)$ that determines the time evolution of the system density matrix $\rho_S(t)$:[2]

$$\rho_S(t) = V(t)\rho_S(0). \qquad (3.22)$$

Definition 3.3.2. The semigroup property for a dynamical map $V(t)$ means that[2]

$$V(t_1 + t_2) = V(t_1)V(t_2). \qquad (3.23)$$

3.4 The Lindblad master equation as the most general generator of the quantum dynamical semigroup

Markvoian time evolution of an open system is described by the quantum dynamical semigroup. This is the semigroup of dynamical maps $V(t)$ such that the system density matrix at time t may be written as[2]

$$\rho_S(t) = V(t)\rho_S(0). \qquad (3.24)$$

The Lindblad master equation arises mathematically as the most general generator of the quantum dynamical semigroup. A generator for the quantum dynamical semigroup is a super-operator $\mathcal{L}$ for which[2]

$$V(t) = e^{\mathcal{L}t}. \qquad (3.25)$$

which, in other words means

$$\rho_S(t) = e^{\mathcal{L}t}\rho_S(0), \tag{3.26}$$

$$\partial_t \rho_S(t) = \mathcal{L}e^{\mathcal{L}t}\rho_S(0) = \mathcal{L}\rho_S(t). \tag{3.27}$$

Thus, deriving the Lindblad master equation means producing the most general super-operator $\mathcal{L}$. This is for example done in [2]. We start by considering the unitary time evolution operator for the coupled system and environment, which after tracing out the environment degrees of freedom produces an expression for $V(t)$ in terms of how this time evolution operator acts on the reference state for the environment ρ_B:

Proposition 3.4.1. *Consider a system with environment that has the time evolution operator $U(t_1, t_2)$ and initial state $\rho_S(0) \otimes \rho_B$, where the spectral composition of ρ_B is $\rho_B = \sum_\beta e_\beta |\beta\rangle\langle\beta|$. Then the dynamical map for the system density matrix ρ_S may be expressed as*

$$\rho_S(t) = V(t)\rho_S(0) = \sum_{\alpha,\beta} W_{\alpha\beta}(t)\rho_S(0)W_{\alpha\beta}(t)^\dagger. \tag{3.28}$$

where $W_{\alpha\beta}(t) = \sqrt{e_\beta}\langle\alpha|U(t,0)|\beta\rangle$ are operators acting on the system Hilbert space.[2]

Derivation. We have

$$\rho(t) = \rho_S(t) \otimes \rho_B = U(t,0)\rho_S(0) \otimes \rho_B U^\dagger(t,0), \tag{3.29}$$

yielding

$$V(t)\rho_S(0) = \mathrm{Tr}^{(2)}\left[U(t,0)\rho_S(0) \otimes \rho_B U^\dagger(t,0)\right]. \tag{3.30}$$

Using completeness, we have

$$U(t,0) = \left(\sum_\alpha |\alpha\rangle\langle\alpha|\right) U(t,0) \left(\sum_\beta |\beta\rangle\langle\beta|\right) = \sum_{\alpha,\beta} \langle\alpha|U(t,0)|\beta\rangle |\alpha\rangle\langle\beta|, \tag{3.31}$$

insertion into the partial trace yields

$$V(t)\rho_S(0) = \sum_{\alpha,\beta} e_\beta \langle\alpha|U(t,0)|\beta\rangle \rho_S(0) \langle\alpha|U(t,0)|\beta\rangle^\dagger = \sum_{\alpha,\beta} W_{\alpha\beta}(t)\rho_S(0)W_{\alpha\beta}^\dagger(t). \tag{3.32}$$

End of derivation.

But we have limited knowledge about the properties of the $W_{\alpha b}(t)$ operators. To proceed with the derivation of the Lindblad master equation, we express the dynamical map $V(t)$ in terms of basis operators in Fock-Liouville space $\{F_i\}_{i=1}^{N^2}$. Fock-Liouville space is the linear space of operators acting on the system Hilbert space, with the inner product defined by $(F_i, F_j) = Tr\left[F_i^\dagger F_j\right]$. This yields:

Proposition 3.4.2. *The dynamical map for the system density matrix ρ_S of an open quantum system subject to Markovian time evolution may be written as*

$$\rho_S(t) = V(t)\rho_S(0) = \sum_{i,j} c_{ij} F_i \rho_S(0) F_j^\dagger. \tag{3.33}$$

where c_{ij} forms a self-adjoint, positive semi-definite matrix, and F_i are basis operators in Fock-Liouville space; that is, the space of operators on the system Hilbert space, with the inner product defined by $(F_i, F_j) = Tr\left[F_i^\dagger F_j\right]$.[2]

Derivation. According to Proposition 3.4.1, the dynamical map can be expressed as

$$V(t)\rho_S(0) = \sum_{\alpha,\beta} W_{\alpha\beta}(t)\rho_S(0)W_{\alpha\beta}(t)^\dagger. \tag{3.34}$$

Completeness for the $W_{\alpha\beta}(t)$ operators may be written as

$$W_{\alpha\beta}(t) = \sum_{i=1}^{N^2} (F_i, W_{\alpha\beta}(t))\, F_i, \tag{3.35}$$

insertion into the expression for the dynamical map yields

$$V(t)\rho_S(0) = \sum_{\alpha,\beta}\left(\sum_{i=1}^{N^2}(F_i, W_{\alpha\beta}(t))F_i\right)\rho_S(0)\left(\sum_{j=1}^{N^2}(F_j, W_{\alpha\beta}(t))F_j\right)^\dagger =$$
$$= \sum_{\alpha,\beta}\sum_{i,j=1}^{N^2}(F_i, W_{\alpha\beta}(t))(F_j, W_{\alpha\beta}(t))^* F_i\rho_S(0)F_j^\dagger = \sum_{i,j=1}^{N^2} c_{ij}F_i\rho_S(0)F_j^\dagger. \tag{3.36}$$

Where

$$c_{ij} = \sum_{\alpha,\beta}(F_i, W_{\alpha\beta}(t))(F_j, W_{\alpha\beta}(t))^*. \tag{3.37}$$

This matrix is obviously self-adjoint. It is also positive semi-definite, as[2]

$$v(c_{ij})v^\dagger = \sum_{\alpha,\beta}\left|\left(\sum_i v_i^* F_i, W_{\alpha\beta}(t)\right)\right|^2 \geq 0. \tag{3.38}$$

End of derivation.

With this way of expressing the dynamical map, we can finally take the derivative at $t = 0$ (using the definition of a derivate); this yields the generator for the quantum dynamical semigroup.

Proposition 3.4.3. *The Lindblad master equation is the most general generator of the quantum dynamical semigroup.[2]*

Derivation. According to Lemma 3.4.2, we can express the dynamical map as

$$V(t)\rho_S(t) = \sum_{i,j} c_{ij}F_i\rho_S(0)F_j^\dagger. \tag{3.39}$$

We chose basis vectors $\{F_i\}_{i=1}^{N^2}$ such that $F_{N^2} = \frac{1}{\sqrt{N}}I_S$, making the other operators in the basis traceless. We then get the generator[2]

$$\mathcal{L}\rho_S = \lim_{\epsilon\to 0}\frac{1}{\epsilon}[V(\epsilon)\rho_S(0) - \rho_S(0)] = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left(\left[\frac{1}{N}(c_{N^2N^2}(\epsilon)\rho_S(0)) + \right.\right.$$
$$\left.\left. + \frac{1}{\sqrt{N}}\sum_i\left(c_{iN^2}(\epsilon)F_i\rho_S(0) + c_{N^2i}(\epsilon)\rho_S(0)F_i^\dagger\right) + \sum_{i=[1,N^2],j=[1,N^2]} c_{ij}(\epsilon)F_i\rho_S(0)F_j^\dagger\right] - \rho_S(0)\right). \tag{3.40}$$

Introuducing the coefficients[2]

$$a_{N^2N^2}(\epsilon) = \lim_{\epsilon\to 0}\frac{1}{\epsilon}(c_{N^2N^2}(\epsilon) - N), \tag{3.41}$$
$$a_{iN^2} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}c_{iN^2}(\epsilon), \tag{3.42}$$

and[2]

$$a_{ij} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}c_{ij}(\epsilon), \tag{3.43}$$

this can be rewritten as[2]

$$\mathcal{L}\rho_S = a_{N^2N^2}\rho_S(0) + \frac{1}{\sqrt{N}}\sum_i\left(a_{iN^2}F_i\rho_S(0) + a_{iN^2}^*\rho_S(0)F_i^\dagger\right) + \sum_{i,j}a_{ij}F_i\rho_S(0)F_j^\dagger. \tag{3.44}$$

Introduce the operators (they are not self-adjoint!)[2]

$$F = \frac{1}{\sqrt{N}}\sum_{i=1}^{N^2-1}a_{iN^2}F_i, \tag{3.45}$$

$$G = \frac{1}{2N}a_{N^2N^2}I^{(1)} + \frac{1}{2}\left(F + F^\dagger\right), \tag{3.46}$$

and the Hermitian operator $H = \frac{1}{2i}\left(F^\dagger - F\right)$; we then get[2]

$$\mathcal{L}\rho_S = [H, \rho_S(0)] + \{G, \rho_S(0)\} + \sum_{i,j} a_{ij} F_i \rho_S(0) F_j^\dagger. \tag{3.47}$$

If the norm of the system density matrix, we must have[2]

$$\mathrm{Tr}\, \partial_t \rho_S = \mathrm{Tr}\, \mathcal{L}\rho_S = 0, \tag{3.48}$$

which gives[2]

$$\mathrm{Tr}\, 2G + \mathrm{Tr} \sum_{i,j} a_{ij} F_i \rho_S(0) F_j^\dagger = 0 \implies G = -\frac{1}{2} \sum_{i,j} a_{ij} F_i F_j^\dagger. \tag{3.49}$$

The first standard form of the Lindblad master equation is then obtained:[2]

$$\mathcal{L}\rho_S = [H, \rho_S(0)] + \sum_{i,j} a_{ij} \left(F_i \rho_S(0) F_j^\dagger - \frac{1}{2} \left\{ F_i F_j^\dagger, \rho_S(0) \right\} \right). \tag{3.50}$$

End of derivation.

3.5 The Lindblad master equation through microscopic derivations (weak-coupling limit)

It has been earlier how the Lindblad master equation arises mathematically. Now we consider how the Lindblad master equation may arise from a microscopic model of the interactions between the system and environment in form of an interaction Hamiltonian $H_I(t)$. This is interesting from a fundamental perspective as it highlights how various approximations are used when deriving the Lindblad master equation. We study the limit where the environment is weakly coupled to the reservoir. The derivation is most easily performed by starting off with interaction picture time evolution equation, which after time averaging yields the so-called Redfield equation[2]:

Proposition 3.5.1. *The Redfield equation. Time evolution in the interaction picture may, under the Born-Markov approximation and assuming that* $\mathrm{Tr}_B\left[H_I(t), \rho_I(0)\right] = 0$*, be written as[2]*

$$\partial_t \rho_S(t) = -\int_0^\infty \mathrm{Tr}_B \left[H_I(t), \left[H_I(t-s), \rho_S(t) \otimes \rho_B\right]\right] \mathrm{d}s. \tag{3.51}$$

Derivation. We start off with the interaction picture time evolution

$$\partial_t \rho_I(t) = -i\left[H_I(t), \rho_I(t)\right]. \tag{3.52}$$

Integrating from time 0 to t gives[2]

$$\rho_I(t) = \rho_I(0) - i\int_0^t \left[H_I(s), \rho_I(s)\right] \mathrm{d}s. \tag{3.53}$$

Re-insertion into the previous expression yields[2]

$$\begin{aligned} \partial_t \rho_I(t) &= -i\left[H_I(t), \rho_I(0) - i\int_0^t \left[H_I(s), \rho_I(s)\right] ds\right] = -i\left[H_I(t), \rho_I(0)\right] + \\ &+ \left[H_I(t), \int_0^t \left[H_I(s), \rho_I(s)\right] \mathrm{d}s\right] = -i\left[H_I(t), \rho_I(0)\right] + \int_0^t \left[H_I(t), \left[H_I(s), \rho_I(s)\right]\right] \mathrm{d}s. \end{aligned} \tag{3.54}$$

Due to the linearity and time-independence of the trace operator, we have $\mathrm{Tr}_B \partial_t \rho_I(t) = \partial_t \mathrm{Tr}_B \rho_I(t)$. Taking the partial trace of the time evolution thus yields[2]

$$\partial_t \rho_S(t) = -\mathrm{Tr}_B \int_0^t \left[H_I(t), \left[H_I(s), \rho_I(s)\right]\right] \mathrm{d}s. \tag{3.55}$$

Now we apply the Born approximation and assume the coupling between the system and the reservoir to be weak. The system will exert little influence on the reservoir, giving an uncorrelated product state

$\rho(t) = \rho_S(t) \otimes \rho_B$ for the composite system. We then apply the Markov approximation, which consists of first replacing $\rho_S(s)$ by $\rho_S(t)$, after having substituted $s = t - s$[2]:

$$\begin{aligned}\partial_t \rho_S(t) &= -\int_0^t \mathrm{Tr}_B \left[H_I(t), \left[H_I(s), \rho_S(t) \otimes \rho_B\right]\right] \mathrm{d}s = \\ &= [s = t - s] = -\int_0^t \mathrm{Tr}_B \left[H_I(t), \left[H_I(s), \rho_S(t) \otimes \rho_B\right]\right] \mathrm{d}s. \end{aligned} \tag{3.56}$$

Letting $t \to \infty$, we get

$$\partial_t \rho_S(t) = -\int_0^\infty \mathrm{Tr}_B \left[H_I(t), \left[H_I(t-s), \rho_S(t) \otimes \rho_B\right]\right] \mathrm{d}s. \tag{3.57}$$

End of derivation.

The Markov approximation is justified when the relaxation time of the system - that is, the time scale τ_R over which ρ_S varies appreachably is much larger than the environment time scale τ_B over which the reservoir correlation functions decay.[bp] We now apply the secular approximation to equation 3.51. The secular approximation means time averaging over rapidly oscillating terms in the interaction Hamiltonian, and is valid when the typical inverse frequence difference $\tau_S = |\omega - \omega'|^{-1}$ is much smaller than the relaxation time τ_R[2]. Decompose the Schrödinger picture interaction Hamiltonian acoording to (where A_α and B_α are self-adjoint operators acting on the system and environment, respectively):[2]

$$H_I = \sum_\alpha A_\alpha \otimes B_\alpha. \tag{3.58}$$

The system Hamiltonian H_S is assumed to have a discrete set of energy non-degenerate eigenvalues ϵ, with[2]

$$A_\alpha(\omega) = \sum_{\epsilon - \epsilon' = \omega} \Pi_\epsilon A_\alpha \Pi_{\epsilon'}. \tag{3.59}$$

Where the Π_ϵ operators are projection operators onto the corresponding eigenvectors. These operators are a decomposition of the A_α operator into eigenoperators of the system Hamiltonian belonging to the frequencies $\mp\omega$:[2]

$$\begin{aligned}\left[H_S, A_\alpha(\omega)\right] &= \sum_{\epsilon' - \epsilon = \omega} H_S \Pi_\epsilon A_\alpha \Pi_{\epsilon'} - \Pi_\epsilon A_\alpha \Pi_{\epsilon'} H_S = \\ &= \sum_{\epsilon' - \epsilon = \omega} H_S \Pi_\epsilon A_\alpha \Pi_{\epsilon'} - \Pi_\epsilon A_\alpha \Pi_{\epsilon'} H_S = \\ &= \sum_{\epsilon' - \epsilon = \omega} \epsilon \Pi_\epsilon A_\alpha \Pi_{\epsilon'} - \Pi_\epsilon A_\alpha \Pi_{\epsilon'} \epsilon' = \\ &= -\omega \sum_{\epsilon' - \epsilon = \omega} \Pi_\epsilon A_\alpha \Pi_{\epsilon'} - \Pi_\epsilon A_\alpha \Pi_{\epsilon'} = \\ &= -\omega A_\alpha(\omega), \end{aligned} \tag{3.60}$$

$$\left[H_S, A_\alpha^\dagger(\omega)\right] = \omega A_\alpha^\dagger(\omega). \tag{3.61}$$

$$\begin{aligned}\sum_\omega A_\alpha(\omega) &= \sum_\omega \sum_{\epsilon' - \epsilon = \omega} \Pi_\epsilon A_\alpha \Pi_{\epsilon'} = \sum_\omega \sum_{\epsilon, \epsilon'} (\epsilon - \epsilon' = \omega) \Pi_\epsilon A_\alpha \Pi_{\epsilon'} = \\ &= \sum_{\epsilon, \epsilon'} \Pi_\epsilon A_\alpha \Pi_{\epsilon'} = \sum_\epsilon \Pi_\epsilon A_\alpha \sum_{\epsilon'} \Pi_{\epsilon'} = I A_a I = A_\alpha. \end{aligned} \tag{3.62}$$

In the interaction picture, we obtain the operators (the Schrödinger picture operators are $A_\alpha(\omega)$ and B_α)[2]

$$\partial_t A_\alpha(\omega, t) = [iH_S, A_\alpha(\omega, t)] = -i\omega A_\alpha(\omega, t) \implies A_\alpha(\omega, t) = e^{-i\omega t} A_\alpha(\omega), \tag{3.63}$$

and[2]

$$A_\alpha^\dagger(\omega,t) = e^{i\omega t}A_\alpha^\dagger(\omega), \tag{3.64}$$

as well as[2]

$$B_\alpha(t) = U_B^\dagger B_\alpha U_B = e^{iH_B t}B_\alpha e^{-iH_B t}, \tag{3.65}$$

and[2]

$$B_\alpha^\dagger(t) = U_B^\dagger B_\alpha^\dagger U_B = e^{iH_B t}B_\alpha^\dagger e^{-iH_B t}. \tag{3.66}$$

We get the interaction picture interaction Hamiltonian:[2]

$$H_I(t) = \sum_\alpha A_\alpha(t)\otimes B_\alpha(t) = \sum_{\alpha,\omega} e^{-i\omega t}A_\alpha(\omega)\otimes B_\alpha(t) = \sum_{\alpha,\omega} e^{i\omega t}A_\alpha^\dagger(\omega)\otimes B_\alpha^\dagger(t). \tag{3.67}$$

Introduce the super-operator He according to

$$\mathrm{He}(A) = A + A^\dagger. \tag{3.68}$$

That is, A plus its Hermitian conjugate. Insertion into the Born-Markov approximation yields (see section A.1):

$$\begin{aligned}\partial_t\rho_S(t) = \int_0^\infty \mathrm{d}s\mathrm{Tr}_B\mathrm{He}\Bigg[\sum_{\alpha,\beta}\sum_{\omega,\omega'} e^{i(\omega'-\omega)t}e^{i\omega s}\big(A_\beta(\omega)\rho_S(t)A_\alpha^\dagger(\omega')\otimes B_\beta(t-s)\rho_B B_\alpha^\dagger(t) - \\ -A_\alpha^\dagger(\omega')A_\beta(\omega)\rho_S(t)\otimes B_\alpha^\dagger(t)B_\beta(t-s)\rho_B\big)\Bigg].\end{aligned} \tag{3.69}$$

Introduce the one-sided Fourier transforms of the reservoir correlation functions $\left\langle B_\alpha^\dagger(t)B_\beta(t-s)\right\rangle$ (these functions only depend on the frequency ω and not the time t as the bath ρ_B is assumed to be stationary):

$$\Gamma_{\alpha\beta}(\omega) = \int_0^\infty e^{i\omega s}\left\langle B_\alpha^\dagger(t)B_\beta(t-s)\right\rangle \mathrm{d}s. \tag{3.70}$$

Insertion into 3.69 gives

$$\partial_t\rho_S(t) = \mathrm{He}\left[\sum_{\alpha,\beta}\sum_{\omega,\omega'} e^{i(\omega'-\omega)t}\Gamma_{\alpha\beta}(\omega)\left(A_\beta(\omega)\rho_S(t)A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega')A_\beta(\omega)\rho_S(t)\right)\right]. \tag{3.71}$$

The secular approximation; that is, neglecting rapidly oscillating terms for which $\omega' \neq \omega$, yields[2]

$$\partial_t\rho_S(t) = \mathrm{He}\left[\sum_{\alpha,\beta}\sum_{\omega}\Gamma_{\alpha\beta}(\omega)\left(A_\beta(\omega)\rho_S(t)A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega)A_\beta(\omega)\rho_S(t)\right)\right]. \tag{3.72}$$

We introduce functions $\gamma_{\alpha\beta}$ and $S_{\alpha\beta}$ according to[2]

$$\gamma_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega), \tag{3.73}$$

and

$$S_{\alpha\beta}(\omega) = \frac{1}{2i}\left(\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}^*(\omega)\right). \tag{3.74}$$

The $S_{\alpha\beta}(\omega)$ coefficients thus form a Hermitian matrix. We now wish to show that the $\gamma_{\alpha\beta}$ coefficients form a positive matrix:[2]

$$\begin{aligned}\gamma_{\alpha\beta}(\omega) =& \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega) = \Gamma_{\alpha\beta}(\omega) + \int_0^\infty e^{-i\omega s}\left\langle B_\beta^\dagger(t)B_\alpha(t-s)\right\rangle^* \mathrm{d}s = \\ =& \Gamma_{\alpha\beta}(\omega) + \int_0^\infty e^{-i\omega s}\left\langle B_\alpha(t-s)^\dagger B_\beta(t)\right\rangle \mathrm{d}s = [s=-s] = \\ =& \Gamma_{\alpha\beta}(\omega) - \int_0^{-\infty} e^{i\omega s}\left\langle B_\alpha(t+s)^\dagger B_\beta(t)\right\rangle \mathrm{d}s = \\ =& \int_0^\infty e^{i\omega s}\left\langle B_\alpha^\dagger(s)B_\beta(0)\right\rangle \mathrm{d}s + \int_{-\infty}^0 e^{i\omega s}\left\langle B_\alpha(s)^\dagger B_\beta(0)\right\rangle \mathrm{d}s = \\ =& \int_{-\infty}^\infty e^{i\omega s}\left\langle B_\alpha^\dagger(s)B_\beta(0)\right\rangle \mathrm{d}s > 0.\end{aligned} \tag{3.75}$$

Which was the result we wished to show. Now

$$\begin{aligned}
\partial_t \rho_S(t) = & \sum_{\alpha,\beta} \sum_{\omega} \left(\left(\frac{1}{2} \gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega) \right) \left(A_\beta(\omega) \rho_S(t) A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega) A_\beta(\omega) \rho_S(t) \right) + \right. \\
& \left. + \left(\frac{1}{2} \gamma_{\alpha\beta}(\omega) - i S_{\alpha\beta}(\omega) \right) \left(A_\alpha(\omega) \rho_S(t) A_\beta^\dagger(\omega) - \rho_S(t) A_\alpha(\omega) A_\beta^\dagger(\omega) \right) \right) = \\
= & -i \sum_{\alpha,\beta} \sum_{\omega} \left[S_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_S(t) \right] + \\
& + \sum_{\alpha,\beta} \sum_{\omega} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S(t) A_a^\dagger(\omega) - \frac{1}{2} \left\{ A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_S(t) \right\} \right) = \\
= & -i \left[H_{LS}, \rho_S(t) \right] + \mathcal{D}(\rho_S(t)) .
\end{aligned} \tag{3.76}$$

the first standard form of the Lindblad master equation. It can be shown that the $\gamma_{\alpha\beta}$ coefficients form a positive matrix, from which follows that 3.76 is diagonalizable.[2]

Chapter 4

Qubit coherence protection

4.1 Background

Qubits are quantum mechanical systems with a Hilbert space spanned by the basis vectors $|0\rangle$ and $|1\rangle$. This means that they, contrary to a classical bit, may reside in a superposition of two states. They can both be used for solving quantum mechanical problems, and solving traditional problems more efficiently by utilising superposition and entanglement. Quantum computers, that is, a system consisting of qubits and quantum logic gates, operate on the qubits by unitary transformations. No quantum computer, however, is perfectly isolated from its environment. Interaction with the environment causes dissipation, leading to decoherence and destroying the entanglement between qubits. To prevent dissipation, there are various coherence protection schemes[6]. It has been shown that it is possible to protect the qubits of any quantum computer while simultaneously controlling the time evolution of the qubits, through Hamiltonians that are rapidly switched on and off. Any protection through external driving needs to be performed in a fashion so as not to disturb the computation in progress[5].

In this study of qubit protection, we do not consider any many-qubit system, and use the Lindblad master equation to model dissipation caused by spontaneous emission. The driving is continous rather than pulsed. It is based on a previous study by Zong et al. [6].

4.2 Mathematics for the system

We represent the two-level qubit system with a $2x2$ density matrix:

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}. \tag{4.1}$$

We consider a qubit subject to Lindblad dissipation:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \left(L\rho L^\dagger - \frac{1}{2}L^\dagger L\rho - \frac{1}{2}\rho L^\dagger L \right). \tag{4.2}$$

The Hamiltonian H is the same as for the corresponding closed system, and the Lindblad operator L describes the interaction with the environment. For our qubit, we will use the Hamiltonian

$$H = H_0 + H_d = \frac{1}{2}\hbar\omega\sigma_z + \frac{1}{2}\hbar\omega\bar{A}\cdot\bar{\sigma}. \tag{4.3}$$

Where we have introduced the Pauli spin matrices $\bar{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. The H_0 part is the Hamiltonian for the closed system, while the H_d represents an external resonant driving. We will also consider the case of a non-resonant driving ($\Omega \neq \omega$); $H_d = \frac{1}{2}\hbar A\left(\sigma_x cos\left(\Omega t\right) + \sigma_y sin\left(\Omega t\right)\right)$. The Lindblad operator is given by

$$L = \sqrt{\gamma}\left|0\right\rangle\left\langle 1\right|. \tag{4.4}$$

Where $|1\rangle$ and $|0\rangle$ are unit eigenvectors for the Hamiltonian H_0. This will cause the qubit state to decohere, which means off-diagonal elements of the density matrix become small (the superposition of $|1\rangle$ and $|0\rangle$ is destroyed). We define coherence as the product of the off-diagonal elements of the density matrix, $4\rho_{01}\rho_{10}$.

4.3 Problem formulation

Given a qubit subject to spontaneous emission, how does the transient behavior of the qubit depend on the driving parameters $\bar{A}$ given an initial pure state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$? How does the steady-state coherence depend on $\bar{A}$? How does the transient coherence depend on the driving frequency Ω? (We assume a decay rate of $\gamma = 0.25$, and that the behavior is not affected by A_z.)

4.4 Numerical results

4.4.1 Behavior of the qubit over time

A 2x2 density matrix has a representation as a Bloch vector (n_x, n_y, n_z). This representation may be used to illustrate the time-dependent behavior of the qubit starting from an initial superposition state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$; see Figure 4.1.

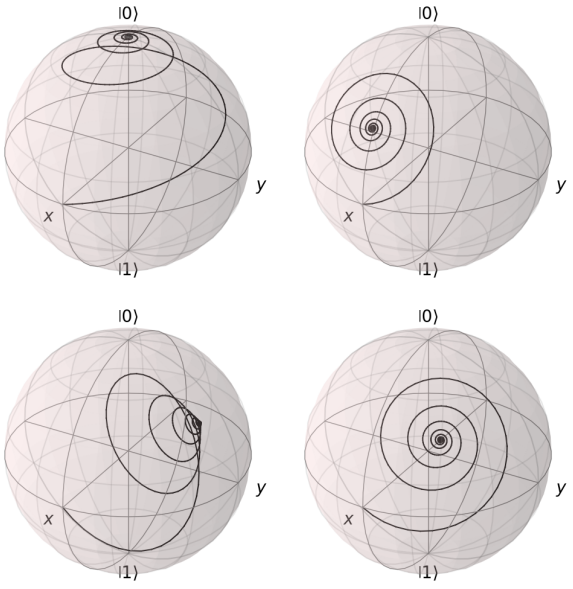


Figure 4.1: Bloch vector components over time; top left to bottom right: no driving, A_x driving, A_y driving, A_x+A_y driving

4.4.2 Coherence by A

Simulation of the qubit is performed until a steady state occurs; this is defined as the coherence varying no more than 10^{-4} over a couple of time steps. The dependence of the steady-state coherence by driving amplitude A_x is shown in Figure 4.2. We see that there is an optimal driving amplitude, and a maximum achievable coherence. Simultaneously varying A_x and A_y shows that the coherence only depends on the amplitude $\left|\bar{A}\right|$; see Figure 4.3.

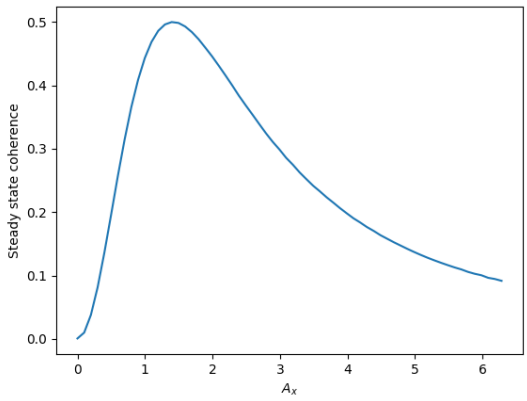


Figure 4.2: Coherence by driving amplitude A_x

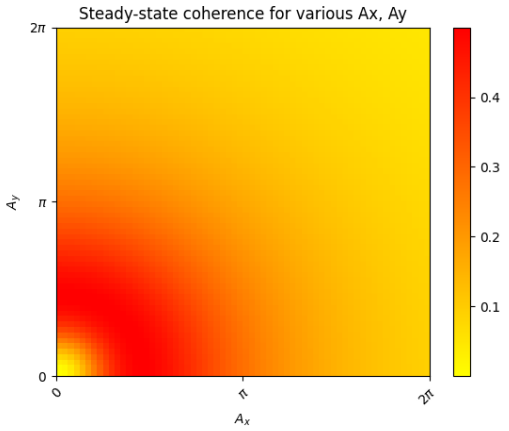


Figure 4.3: Coherence by driving amplitudes A_x,A_y

4.4.3 Transient coherence by Ω

The driving frequency Ω will affect the final coherence, and how much the coherence oscillates before settling for a stationary state. This is shown in Figure 4.4.

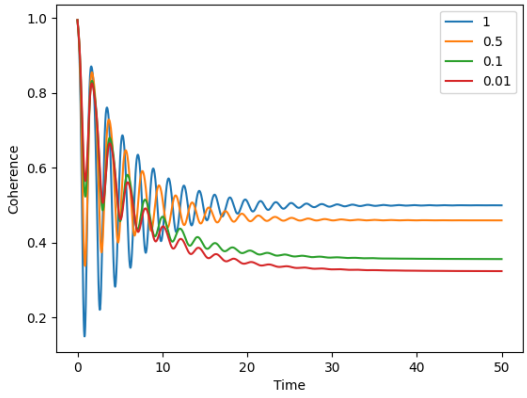


Figure 4.4: Transient coherence for various Ω

4.5 Analysis of results

The obtained results show that the achievable coherence depends on the amplitude $|A|$, with a maximum achievable coherence. The driving frequency Ω should ideally be as close as possible to ω, mismatches limit the achievable coherence.

4.6 Discussion

There are a multiple of limitations with this toy application. First of all, it does not in any way account for the usability of the driven qubit resource. Driving a qubit interferes with using it in a quantum circuit, for which reason a pulsed drive is often used. This requires appropriate timing of the gating operations, which is not accounted for in this model either[5]. There are also many ways in which dissipation to the environment can be caused, and the interaction with the environment need not necessarily be Markvoian.

Appendix

A.1 Details of secular approximation

For Hermitian operators A, B, C, we have:

$$[A,[B,C]] = [A, BC - CB] = ABC - ACB + CBA - BCA = \mathrm{He}\left(BCA - ABC\right). \tag{A.1}$$

Putting $A = H_I(t)$, $B = H_I(t-s), C = \rho_S(t) \otimes \rho_B$, we get

$$[H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]] = \mathrm{He}\left(H_I(t-s)\rho_S(t) \otimes \rho_B H_I(t) - H_I(t) H_I(t-s) \rho_S(t) \otimes \rho_B\right). \tag{A.2}$$

Insertion into the Born-Markov approximation yields

$$\begin{aligned}
\partial_t \rho_S(t) &= -\int_0^\infty \mathrm{d}s \mathrm{Tr}_B \left[H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]\right] = \\
&= -\int_0^\infty \mathrm{d}s \mathrm{Tr}_B \mathrm{He}\left[H_I(t), H_I(t-s)\rho_S(t) \otimes \rho_B - \rho_S(t) \otimes \rho_B H_I(t-s)\right] = \\
&= \int_0^\infty \mathrm{d}s \mathrm{Tr}_B \mathrm{He}\left[H_I(t-s)\rho_S(t) \otimes \rho_B H_I(t) - H_I(t) H_I(t-s) \rho_S(t) \otimes \rho_B\right] = \\
&= \int_0^\infty \mathrm{d}s \mathrm{Tr}_B \mathrm{He}\left[\sum_{\beta,\omega} e^{-i\omega(t-s)} A_\beta(\omega) \otimes B_\beta(t-s)\rho_S(t) \otimes \rho_B \sum_{\alpha,\omega'} e^{i\omega' t} A_\alpha^\dagger(\omega') \otimes B_\alpha^\dagger(t) - \right. \\
&\quad \left. - \sum_{\alpha,\omega'} e^{i\omega' t} A_\alpha^\dagger(\omega') \otimes B_\alpha^\dagger(t) \sum_{\beta,\omega} e^{-i\omega(t-s)} A_\beta(\omega) \otimes B_\beta(t-s)\rho_S(t) \otimes \rho_B\right] = \\
&= \int_0^\infty \mathrm{d}s \mathrm{Tr}_B \mathrm{He}\left[\sum_{\beta,\omega}\sum_{\alpha,\omega'} e^{-i\omega(t-s)} e^{i\omega' t} \left(A_\beta(\omega)\rho_S(t) A_\alpha^\dagger(\omega') \otimes B_\beta(t-s)\rho_B B_\alpha^\dagger(t) - \right.\right. \\
&\quad \left.\left. - A_\alpha^\dagger(\omega') A_\beta(\omega)\rho_S(t) \otimes B_\alpha^\dagger(t) B_\beta(t-s)\rho_B\right)\right] = \\
&= \int_0^\infty \mathrm{d}s \mathrm{Tr}_B \mathrm{He}\left[\sum_{\alpha,\beta}\sum_{\omega,\omega'} e^{i(\omega'-\omega)t} e^{i\omega s} \left(A_\beta(\omega)\rho_S(t) A_\alpha^\dagger(\omega') \otimes B_\beta(t-s)\rho_B B_\alpha^\dagger(t) - \right.\right. \\
&\quad \left.\left. - A_\alpha^\dagger(\omega') A_\beta(\omega)\rho_S(t) \otimes B_\alpha^\dagger(t) B_\beta(t-s)\rho_B\right)\right].
\end{aligned} \tag{A.3}$$

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