

# Chapter 6

## Dynamics of open quantum systems

### 6.1 Introduction

Postulate 2 of quantum mechanics tells us that the evolution of any isolated quantum system is governed by the Schrödinger equation.

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle \quad (6.1)$$

However, in nature most quantum systems are *not* isolated. They are constantly interacting with all the other systems around them, which we call their *environment*. While in principle one could “zoom out” from the system of interest and attempt to solve the Schrödinger equation for all of these systems, in practise this is often unwieldy. There are often simply too many interacting modes and particles for this to be feasible, in fact, the environment of a system may include the whole lab, planet or beyond (!), if all interactions between systems are taken into account.

Systems interacting with an environment are called *open quantum systems*. We would like a means to describe the evolution of the systems we are interested in without having to solve the Schrödinger equation for the whole environment. While this is not always possible, we will see in this chapter that, in some important physical situations, one can derive equations to describe the evolution of open quantum systems.

System and environment are interacting, and hence, will tend to become entangled. This means that the global state no longer factorises and we cannot assign a state vector to the system or environment individually. For this reason we need to use the density matrix formalism (recall that the reduced state of a system in

an entangled state is a mixed state, which requires a density matrix for a compact description.) Therefore, first we shall review the density matrix formalism.

Please note that this material is not taught as standard in undergraduate-level textbooks, and specialised texts on open quantum systems are usually far too specialised and detailed for this course. One of the few undergraduate textbooks which does cover open quantum systems at a similar level to here is Quantum physics By Michel Le Bellac (Cambridge).

## 6.2 Density Matrices revised

A density matrix (operator) is a Hermitian operator which represents the state of a system. It widens the state vector formalism to a more general setting which can also compactly represent states which have been prepared probabilistically (using classical randomness) or are reduced states of a larger entangled state.

The density matrix for a pure state  $|\psi\rangle$  is simply the projector  $|\psi\rangle\langle\psi|$  and for an ensemble of states  $|\psi_j\rangle$ , each prepared with probability  $p_j$  is

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| \quad (6.2)$$

The expectation value for any operator  $\hat{O}$  is given by the expression

$$\langle\hat{O}\rangle = \text{Tr}[\rho\hat{O}]. \quad (6.3)$$

In general, a physical density operator must satisfy the following requirements

- Unit Trace:  $\text{Tr}[\rho] = 1$ .
- Hermiticity:  $\rho = \rho^\dagger$ .
- Positive semi-definiteness:  $\rho$  has no negative eigenvalues.

A general density operator can be written in terms of orthonormal basis  $|\phi_j\rangle$

$$\rho = \sum_{j,k} \rho_{j,k} |\phi_j\rangle\langle\phi_k| \quad (6.4)$$

where  $\rho_{j,k} = \langle\phi_j|\rho|\phi_k\rangle$ .

If we are working with a joint system composed of system A with basis  $|\alpha_j\rangle$  and system B with basis  $|\beta_j\rangle$ , we may write a general density matrix for the joint system with respect to tensor product basis  $|\alpha_j\rangle|\beta_k\rangle$

$$\rho = \sum_{j,k,l,m} \rho_{j,k,l,m} |\alpha_j\rangle |\beta_k\rangle \langle \alpha_l| \langle \beta_m| \quad (6.5)$$

where  $\rho_{j,k,l,m} = \langle \alpha_j | \langle \beta_k | \rho | \alpha_l \rangle | \beta_m \rangle$ .

Given a joint state for systems  $A$  and  $B$ , a *reduced state* of a system is a density matrix which specifies all the local properties of system  $A$  or  $B$  alone. It may be obtained using the partial trace operation

$$\rho_A = \text{Tr}_B \rho = \sum_l \rho_{j,l,k,l} |\alpha_j\rangle \langle \alpha_k| \quad (6.6)$$

or similarly

$$\rho_B = \text{Tr}_A \rho = \sum_l \rho_{l,j,l,k} |\beta_j\rangle \langle \beta_k|. \quad (6.7)$$

## Unitary evolution of density matrices

In previous chapters we have seen that in a closed system, a pure state, described as state vector  $|\psi(t)\rangle$  evolves under the Schrödinger equation via a unitary evolution operator  $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ , where  $U(t) = \exp[-i\hat{H}t/\hbar]$  and  $\hat{H}$  is the Hamiltonian of the system.

Consider a closed system prepared in a *mixed state* at time  $t = 0$ . This state can be described by density matrix

$$\rho(0) = \sum_j p_j |\psi_j\rangle \langle \psi_j| \quad (6.8)$$

If the system evolves under Hamiltonian  $\hat{H}$ , then each of the state vectors  $|\psi_j\rangle$  will evolve to  $U(t)|\psi_j\rangle$  and the full mixed state  $\rho$  will evolve as follows:

$$\begin{aligned} \rho(t) &= \sum_j p_j U(t) |\psi_j\rangle \langle \psi_j| U^\dagger(t) \\ &= U(t) \rho(0) U^\dagger(t). \end{aligned} \quad (6.9)$$

We see that the initial state  $\rho(0)$  is multiplied from the left by  $U(t)$  and from the right by  $U^\dagger(t)$ . We can derive a version of the Schrödinger equation for mixed

states using similar methods to those in the previous chapters

$$\begin{aligned}
\frac{\partial}{\partial t}\rho(t) &= \frac{\partial}{\partial t} (U(t)\rho(0)U^\dagger(t)) \\
&= \dot{U}(t)\rho(0)U^\dagger(t) + U(t)\rho(0)\dot{U}^\dagger(t) \\
&= -\frac{i}{\hbar}\hat{H}U(t)\rho(0)U^\dagger(t) + \frac{i}{\hbar}U(t)\rho(0)U^\dagger(t)\hat{H} \\
&= -\frac{i}{\hbar}[\hat{H}, \rho(t)]
\end{aligned} \tag{6.10}$$

where  $\dot{U}(t) = \partial U(t)/\partial t = -(i\hat{H}/\hbar)U(t)$ . This compact equation is a density matrix formulation of the Schrödinger equation, and is sometimes called the von Neumann equation.

### Purity: Pure states versus mixed states

Recall that a pure state is any state which can be expressed as a single projector, e.g. in the form:

$$\rho = |\psi\rangle\langle\psi| \tag{6.11}$$

Pure states are the states which can be equally described in the state vector picture by state vector  $|\psi\rangle$ .

A mixed state is one which cannot be expressed as a single projector, but must necessarily be written as a sum of projectors

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| \tag{6.12}$$

where  $\sum_j p_j = 1$ .

Purity is a useful measure of “how pure” a state is. It is equal to the simple expression  $\text{Tr}[\rho^2]$ . For any pure state  $\text{Tr}[\rho^2] = \text{Tr}[|\psi\rangle\langle\psi|] = 1$ , whereas for all mixed states  $\text{Tr}[\rho^2] < 1$ . Unitary evolution does not change the purity of a state. This is easy to show using the cyclic properties of trace:

$$\text{Tr}[\rho(t)^2] = \text{Tr}[U(t)\rho(0)U(t)^\dagger U(t)\rho(0)U(t)^\dagger] = \text{Tr}[U(t)\rho(0)^2 U(t)^\dagger] = \text{Tr}[\rho(0)^2] \tag{6.13}$$

This means that any closed system which starts in a pure (or mixed) state will remain as a pure (mixed) state for the whole of its evolution.

## 6.3 Super-operators and non-unitary evolution

Since unitary operators preserve purity, then it is impossible to create a mixed state from a pure state via unitary evolution. This means that there must be additional types of quantum evolution, which can change the purity of the state, and it is these which we shall study in this chapter.

As we have already seen, mixed states arise in two contexts. Firstly, when classical randomness is employed in the creation of a state. Secondly, when a system becomes entangled with another system, and we consider its reduced state.

We shall first consider the former setting and construct a thought experiment. We will start with a system in pure state  $\rho = |\psi\rangle\langle\psi|$  and we wish to construct a mixed state. Let us imagine that we know how to implement a set of unitary transformations  $U_j$  for  $j = 1, 2, \dots, n$  on the system (by implementing certain Hamiltonians for a certain time). Each of these will transform the state of the system to  $U_j\rho U_j^\dagger$ .

Now let us introduce classical randomness. Imagine we choose the unitary transformation which will be applied by using a random number generator, selecting unitary  $U_j$  with probability  $p_j$ . We know how to construct a density matrix for the state  $\rho'$  which will be created

$$\rho' = \sum_j p_j U_j \rho U_j^\dagger \quad (6.14)$$

Although constructed using unitary evolution operators, the overall evolution is not unitary, due to the classical randomness. This evolution can transform a state from a pure state to a mixed state. To see an example of this, imagine we start in pure spin-half state  $|\uparrow\rangle$ , and apply unitaries  $\mathbb{1}$  and  $\sigma_X$  with equal probability. The state which results is the mixed state  $(1/2)(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)$ .

### Superoperators

In the state vector picture, operators played a very important role. An operator  $\hat{O}$  was defined as a mathematical object which transformed one vector to another

$$|\psi'\rangle = \hat{O}|\psi\rangle. \quad (6.15)$$

We are now studying the transformation of operators (the density operator) themselves. For this we need to define a new mathematical object, called a *superoperator*.

A superoperator  $S[\cdot]$  is a mathematical object which transforms one operator to another.

$$\rho' = S[\rho] \quad (6.16)$$

E.g., in the previous example

$$\rho' = S[\rho] = \sum_j p_j U_j \rho U_j^\dagger \quad (6.17)$$

We notice that to write down the transformation, we are summing over operators  $U_j$  multiplied from the left and (as Hermitian conjugates) from the right. In fact, all superoperators which occur in quantum mechanics may be written in the form:

$$S[\rho] = \sum_j K_j \rho K_j^\dagger \quad (6.18)$$

where  $K_j$  are linear operators which satisfy,

$$\sum_j K_j^\dagger K_j = \mathbb{1}. \quad (6.19)$$

This is called the “operator-sum” representation of the super-operator, or, more commonly, its Kraus representation. The operators  $K_j$  are called Kraus operators. In the above example, the Kraus operators are  $K_j = \sqrt{p_j} U_j$ . We can verify that  $\sum_j K_j^\dagger K_j = \sum_j p_j U_j^\dagger U_j = \sum_j p_j \mathbb{1} = \mathbb{1}$ .

It is important to note that the operators  $K_j$  do not have to be unitary. Indeed, even in the above example they are not unitary, only proportional to unitary.

Any super-operator  $S[\rho]$  which can be expressed as a Kraus decomposition has the following properties.

- If  $\rho$  is Hermitian, has trace 1 and no negative eigenvalues (i.e. a physical density operator) then  $\rho' = S[\rho]$  is Hermitian, trace 1 and has no negative eigenvalues.

The proofs of the first two of these properties are straight-forward, and we shall list them here. To prove the Hermiticity of  $S[\rho]$ , we use the fact that if  $\rho' = S[\rho]$ ,

$$(\rho')^\dagger = \left( \sum_j K_j \rho K_j^\dagger \right)^\dagger \quad (6.20)$$

We then use the rule for taking Hermitian conjugates of products  $(ABC)^\dagger = C^\dagger B^\dagger A^\dagger$ , therefore

$$(\rho')^\dagger = \sum_j K_j \rho K_j^\dagger = \rho' \quad (6.21)$$

and therefore  $\rho'$  is Hermitian.

To prove that the trace of  $\rho'$  is 1, we use the linearity and cyclic property of Trace

$$\begin{aligned} \text{Tr}[\rho'] &= \text{Tr}\left[\sum_j K_j \rho K_j^\dagger\right] \\ &= \sum_j \text{Tr}[K_j \rho K_j^\dagger] \\ &= \sum_j \text{Tr}[K_j^\dagger K_j \rho] \\ &= \text{Tr}\left[\sum_j K_j^\dagger K_j \rho\right] \\ &= \text{Tr}[\rho] \end{aligned} \quad (6.22)$$

Kraus form superoperators transform physical density matrices to physical density matrices, and for this reason they represent all physical evolutions of density matrices studied in quantum mechanics. In addition to the above three properties, there is in fact one further, more subtle, property which physical transformations in quantum mechanics need to fulfil. This is called complete positivity.

### Off-syllabus: Complete positivity

For a transformation to be physical, it must transform the density matrix to a physical state even if it only acts on a sub-system. Consider two sub-systems  $A$  and  $B$ . Surprisingly there exist superoperators where  $S[\rho_A]$  on reduced state  $\rho_A$  never has a negative eigenvalue, but the superoperator acting on the full state  $S[\rho_{AB}]$  can have negative eigenvalues<sup>1</sup>. A superoperator where  $S[\rho_A]$  and  $S[\rho_{AB}]$  can never have negative eigenvalues, where system  $B$  can be of any dimension, is called *completely positive*.

<sup>1</sup>An example of this is the transpose operation, which switches columns and rows in the density matrix. It is possible to show that the transpose operation is positive semi-definite on a full system, but can lead to negative eigenvalues if it acts on a sub-system alone.

It has been shown that any superoperator  $S[\cdot]$  which preserves Hermiticity, Trace and is completely positive can be written in Kraus decomposition form, which is why all transformations which arise in quantum evolution can be written in this form.

## 6.4 Open quantum systems

In this section, we return to the main focus of this chapter, open quantum systems, that is, systems interacting with a large environment, which represents all other objects and fields which may have an influence on the system we are studying, and the state of which we do not want to include in our calculations. Taken together, the system plus the environment constitute a closed system, (this assumes that the environment includes *everything* which may affect the system we are studying). Closed systems evolve unitarily under the Schrödinger equation. In principle we could study the evolution of the system in question by solving this equation, and then computing the reduced state of the system. However, the environment will usually be so large that this is unpractical. An alternative approach, and the approach taken in many studies of open quantum systems, is to attempt to derive an evolution equation for the reduced state of the system  $\rho$  alone.

In other words, we would like to find an equation of the form

$$\dot{\rho}(t) = \frac{\partial \rho(t)}{\partial t} = S[\rho(t)] \quad (6.23)$$

for some superoperator  $S$ , in analogy to the Schrödinger equation, which has the form

$$\frac{\partial |\psi(t)\rangle}{\partial t} = \hat{O} |\psi(t)\rangle \quad (6.24)$$

where operator  $\hat{O} = -i\hat{H}/\hbar$ .

Via the definition of the derivative,  $\dot{\rho}(t)$  can be written

$$\dot{\rho}(t) = \lim_{\delta t \rightarrow 0} \frac{\rho(t + \delta t) - \rho(t)}{\delta t} \quad (6.25)$$

which we can rewrite as the  $\delta t \rightarrow 0$  limit of

$$\rho(t + \delta t) = \rho(t) + \dot{\rho}(t)\delta t \quad (6.26)$$

We see that, to achieve an evolution equation of the form of equation (6.23)  $\rho(t + \delta t)$  must only depend on the state of the system immediately before, i.e.



$\rho(t)$ . In other words, the evolution of our system cannot depend on a) the state of the environment or b) The state  $\rho(t')$  for some earlier time  $t' < t$ . Evolution of this type is called *Markovian*. Roughly speaking, Markovian evolution means that the way the system will immediately change depends only on its state now. Because of this, in general, Markovian systems are easier to study and analyse than non-Markovian systems.

### Examples of Markovian and non-Markovian evolution

Markovian evolution is also important in classical probability theory. Many types of classical evolution can be classified as Markovian or non-Markovian.

- **The weather** is a good example of a system which is *not* Markovian. The probability that it rains today is influenced by the weather yesterday, last week and last year.
- The board-game **Snakes and Ladders** *does* exhibit Markovian behaviour. As you play the game, the probability that you land on a ladder or a snake depends *only* on your current position, not on the history of the game previously.

Another important aspect of Markovian evolution in interacting systems, is that the evolution of the system we are studying, depends only on *its* reduced state at time  $t$ , not on the state of the other system. This can be understood in terms of the flow of information. Information must flow from the system we study into the environment, but not vice versa.

The assumptions of Markovianity are strict and it is therefore not surprising that most forms of evolution for interacting quantum systems are *not* Markovian. However, for many of the most important open systems which we would like to study, the evolution *is* Markovian (to a very high degree of approximation). For example, in spontaneous emission from atoms, photons are emitted from an atom, due to the interaction with the electromagnetic field surrounding it, but these photons never (or at least are very very unlikely to) return to interact again with the atom. Here, the flow of influence or “information” is one way, and the evolution is Markovian.

When the evolution of an open quantum system is Markovian it is possible to write down an evolution equation in the form of equation (6.23). This type of equation is called a *master equation*. In the next section, we will see that

Markovian master equations can always be written in a certain form, and that we can use phenomenological approaches to write down Master equations based on observations of the physics of a system, as an alternative to lengthy derivations from first principles.

## 6.5 The Markovian master equation

For an open quantum system interacting with its environment in a Markovian manner, we would like to derive an evolution equation of the form,

$$\dot{\rho}(t) = \frac{\partial \rho(t)}{\partial t} = S[\rho(t)] \quad (6.27)$$

To do so, there are a number of ways we could proceed. One would be to write down a Hamiltonian for the full system and environment, and manipulate this expression, by performing a partial trace over the environment, to derive a master equation. This approach is the most rigorous, and is the approach taken in most text-books on open quantum systems. However, derivations can be very complex, and the methods used can be very specific to the form of the Hamiltonian in question.

Here, we shall take an alternative approach<sup>2</sup>. We shall derive a general form in which *all* Markovian master equations can be expressed. We will then see that it is possible to understand this equation phenomenologically. In other words, we can associate the operators in the equation with particular observed events (such as the emission of a photon in spontaneous emission), allowing us to construct master equations via good guess work, and clarify our understanding of rigorously derived Master equations.

We shall start with the equation

$$\rho(t + \delta t) = \rho(t) + \delta t \dot{\rho}(t) \quad (6.28)$$

which is exact in the limit  $\delta t$  goes to zero. We will use this expression to derive an expression for  $\dot{\rho}(t)$ , taking the limit at the end of our calculation. We will start by deriving an approximate expression for  $\dot{\rho}(t)$  which is accurate to the first order in  $\delta t$ . The reason for this is that at the end of the calculation we are going to take the limit  $\delta t \rightarrow 0$ . In this limit, all terms in that approximation proportional to

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<sup>2</sup>Due to John Preskill at Caltech.

$(\delta t)^2$ ,  $(\delta t)^3$  and higher will vanish much faster than terms proportional to  $\delta t$ , and we can neglect them.

We are going to derive a general form for  $\dot{\rho}(t)$  based on just two assumptions. The first assumption is that the evolution is Markovian, and thus has an equation of the form of equation (6.27), and secondly that there is a physical superoperator which transforms  $\rho(t)$  to  $\rho(t + \delta t)$  which can therefore be expressed as a Kraus decomposition. From these two assumptions we will show that the master equation has to take a particular form, called the Lindblad form.

To simplify notation, we will consider  $\rho(0)$  and  $\rho(\delta t)$  instead of  $\rho(t)$  and  $\rho(t + \delta t)$ , but the argument below also applies for the general case. The assumption that the transformation from  $\rho(0)$  to  $\rho(\delta t)$  has a Kraus decomposition means we can write

$$\rho(\delta t) = S[\rho(0)] = \sum_j K_j(\delta t) \rho(0) K_j^\dagger(\delta t) \quad (6.29)$$

where the Kraus operators  $K_j(\delta t)$  are functions of  $\delta t$ . Equation (6.29) must be the same as equation (6.28), rewritten here for  $\rho(0)$  and  $\rho(\delta t)$ ,

$$\rho(\delta t) = \rho(0) + \delta t \dot{\rho}(0) \quad (6.30)$$

Comparing these two equations we see that for them to be equal, up to first order in  $\delta t$ , the Kraus operators must have the following forms. There must be one Kraus operator (let's label this  $K_0$ ) which is given by

$$K_0 = \mathbb{1} + \delta t A \quad (6.31)$$

where  $A$  is a linear operator, and the remaining Kraus operators (which we label  $K_j$ ) must have the form

$$K_j = \sqrt{\delta t} L_j \quad (6.32)$$

where  $L_j$  are linear operators. To verify that these Kraus operators do give us the form of equation (6.30), we substitute them into equation (6.29),

$$\begin{aligned} \rho(\delta t) &= K_0 \rho(0) K_0^\dagger + \sum_{j=1}^{\infty} K_j(\delta t) \rho(0) K_j^\dagger(\delta t) \\ &= (\mathbb{1} + \delta t A) \rho(0) (\mathbb{1} + \delta t A^\dagger) + \delta t \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger \\ &= \rho(0) + \delta t A \rho(0) + \delta t \rho(0) A^\dagger + O((\delta t)^2) + \delta t \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger \end{aligned} \quad (6.33)$$

where we shall neglect the terms of order  $(\delta t)^2$  to write:

$$\rho(\delta t) = \rho(0) + \delta t \left( A\rho(0) + \rho(0)A^\dagger + \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger \right) \quad (6.34)$$

comparing this equation with equation (6.30) we can simply read off an expression for  $\dot{\rho}(0)$ , which, since we assume that the evolution is not time-varying, will be equal to  $\dot{\rho}(t)$ ,

$$\dot{\rho}(0) = A\rho(0) + \rho(0)A^\dagger + \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger. \quad (6.35)$$

If the evolution is constant in time, this derivation does not depend on the value of  $t$  and the following equation also holds,

$$\dot{\rho}(t) = A\rho(t) + \rho(t)A^\dagger + \sum_{j=1}^{\infty} L_j \rho(t) L_j^\dagger. \quad (6.36)$$

Any linear operator  $A$  can be decomposed as  $A = B + iC$  where  $B$  and  $C$  are Hermitian operators. This is equivalent to decomposing a complex number  $z = x + iy$ . You can verify that this can be done for any linear operator  $A$  as an exercise (Hint: It is easiest to prove it for any matrix, which is an equivalent statement).

In our derivation, it will be convenient to express operator  $A$  as follows

$$A = -\frac{i}{\hbar}H + M \quad (6.37)$$

where  $H$  and  $M$  are Hermitian. Hence

$$K_0 = \mathbb{1} + \delta t \left( -\frac{i}{\hbar}H + M \right) \quad (6.38)$$

Recall that Kraus operators satisfy a condition  $\sum_j K_j^\dagger K_j = \mathbb{1}$ . We can use this to

identify the value of  $M$ .

$$\begin{aligned}
 \mathbb{1} &= \sum_j K_j^\dagger K_j \\
 &= \left( \mathbb{1} + \delta t \left( +\frac{i}{\hbar} H + M \right) \right) \left( \mathbb{1} + \delta t \left( -\frac{i}{\hbar} H + M \right) \right) + \delta t \sum_{j=1}^{\infty} L_j^\dagger L_j \\
 &= \mathbb{1} + \delta t \left( -\frac{i}{\hbar} H + M \right) + \delta t \left( +\frac{i}{\hbar} H + M \right) + O((\delta t)^2) + \delta t \sum_{j=1}^{\infty} L_j^\dagger L_j
 \end{aligned} \tag{6.39}$$

Neglecting the term of order  $(\delta t)^2$ , and cancelling terms, this implies that

$$\delta t \, 2M = -\delta t \sum_{j=1}^{\infty} L_j^\dagger L_j \tag{6.40}$$

and thus

$$M = -\frac{1}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j \tag{6.41}$$

Thus we can write

$$\dot{\rho}(t) = \left( -\frac{iH}{\hbar} - \frac{1}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j \right) \rho(t) + \rho(t) \left( +\frac{iH}{\hbar} - \frac{1}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j \right) + \sum_{j=1}^{\infty} L_j \rho(t) L_j^\dagger. \tag{6.42}$$

This equation looks rather fearsome, but we can write it in a simpler way by defining an operator called the *effective Hamiltonian*

$$H_{\text{eff}} = H - i\frac{\hbar}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j \tag{6.43}$$

This is not a proper Hamiltonian, since it is not a Hermitian operator, but it plays a similar role to the Hamiltonian in the master equation, as we shall see below.

Written in terms of the effective Hamiltonian, our master equation takes the simpler form

$$\dot{\rho}(t) = -\frac{i}{\hbar} \left( H_{\text{eff}} \rho(t) - \rho(t) H_{\text{eff}}^\dagger \right) + \sum_{j=1}^{\infty} L_j \rho(t) L_j^\dagger. \tag{6.44}$$

This is called the Lindblad equation, or the Lindblad form of the master equation. We derived it only assuming Markovian evolution and that all evolution must be described by a Kraus decomposition superoperator. Therefore the state of all Markovian open systems will evolve according to an equation of this form.

The treatment so far has been solely a mathematical derivation. Now we introduce the physics. We need to identify the physical meaning of the operators  $H$  and  $L_j$ . First let's look at what happens if we set all the  $L_j$  operators to zero. In that case,  $H_{\text{eff}}$  is simply equal to  $H$ , and the evolution equation reduces to

$$\dot{\rho}(t) = -\frac{i}{\hbar} (H\rho(t) - \rho(t)H) = -\frac{i}{\hbar} [H, \rho(t)] \quad (6.45)$$

This equation is identical to equation (6.10) the Von Neumann equation which we derived above, which is the evolution equation (equivalent to the Schrödinger equation) for closed systems in the density matrix formalism, and we can identify  $H$  as the Hamiltonian describing the dynamics of the system we are studying alone. This implies that the  $L_j$  operators are responsible for the irreversible dynamics due to a coupling with the environment.

Indeed, we find that this is the case, the operator  $H$  represents the Hamiltonian of the system we are studying, if interactions with the environment are not taken into account, and the  $L_j$  operators, called *jump operators* represent processes associated with the interaction with the environment. These are best illustrated by an example. The example we will study here is spontaneous emission.

### Example: Spontaneous Emission

Consider a two-level atom, its ground state  $|g\rangle$  at energy 0 and its excited state  $|e\rangle$  with energy  $\hbar\omega$ . The Hamiltonian for the atom is  $H = \hbar\omega|e\rangle\langle e|$ . Spontaneous emission occurs due to the interaction between the atom and all the modes of the electromagnetic field surrounding it. These interact via a Jaynes-Cummings Hamiltonian of the form derived (for a single mode) in chapter 4. We saw there that an atom may interact with an empty mode by decaying from excited to ground state via the emission of a photon. Unlike in the cavity mode case, where the photon was then reabsorbed, photons emitted into free-space are not likely to be reabsorbed by the atom, and the system's evolution is therefore Markovian. By solving the Schrödinger equation under a number of approximations, and then tracing out the state of the electromagnetic field modes, one may derive a Lindblad form master equation. The derivation is known as Wigner-Weisskopf theory and may be found in textbooks on quantum optics.

In this master equation we take the Hamiltonian of the system  $H = \hbar\omega|e\rangle\langle e|$  and a single jump operator  $L = \gamma|g\rangle\langle e|$ . The jump operator embodies the spontaneous decay of the atom. You can see that the form of the jump operator captures very literally, the operator transforms state  $|e\rangle$  to the ground state  $|g\rangle$ , just as occurs in spontaneous emission. As we shall see below, the constant  $\gamma$  is related to the rate at which spontaneous emission occurs.

Inserting these operators into equation (6.44) we obtain the master equation derived in Wigner-Weisskopf theory. First we derive the effective Hamiltonian for this evolution

$$\begin{aligned} H_{\text{eff}} &= \hbar\omega|e\rangle\langle e| - \frac{i\hbar}{2}|\gamma|^2|e\rangle\langle g|g\rangle\langle e| \\ &= \hbar\omega|e\rangle\langle e| - \frac{i\hbar}{2}|\gamma|^2|e\rangle\langle e| \\ &= \left(\hbar\omega - \frac{i\hbar}{2}|\gamma|^2\right)|e\rangle\langle e| \end{aligned} \quad (6.46)$$

The master equation for the problem is then

$$\dot{\rho}(t) = -\frac{i}{\hbar} \left( H_{\text{eff}}\rho(t) - \rho(t)H_{\text{eff}}^\dagger \right) + L\rho(t)L^\dagger. \quad (6.47)$$

Let us assume that the initial state of the atom is the excited state  $\rho(0) = |e\rangle\langle e|$ . To simplify the calculation, we will consider a time-evolving state of the form

$$\rho(t) = \rho_{ee}(t)|e\rangle\langle e| + \rho_{gg}(t)|g\rangle\langle g| \quad (6.48)$$

For a full treatment we should also have included terms  $\rho_{eg}(t)|e\rangle\langle g|$  and  $\rho_{ge}(t)|g\rangle\langle e|$ , but, we find that  $\rho(0) = |e\rangle\langle e|$ , then  $\rho_{eg}(t) = \rho_{ge}(t) = 0$  for all time. We neglect these terms here to simplify the calculation.

We now substitute equation (6.48) into the master equation. To solve it, let us first consider how  $L$  and  $H_{\text{eff}}$  act on states  $|e\rangle$  and  $|g\rangle$ ,

$$\begin{aligned} H_{\text{eff}}|e\rangle &= \hbar(\omega - i|\gamma|^2/2)|e\rangle & H_{\text{eff}}|g\rangle &= 0 \\ L|e\rangle &= \gamma|g\rangle & L|g\rangle &= 0 \end{aligned} \quad (6.49)$$

And thus, using equation (6.48)

$$\begin{aligned} H_{\text{eff}}\rho(t) &= \hbar(\omega - i|\gamma|^2/2)\rho_{ee}(t)|e\rangle\langle e| \\ \rho(t)H_{\text{eff}}^\dagger &= \hbar(\omega + i|\gamma|^2/2)\rho_{ee}(t)|e\rangle\langle e| \\ L\rho(t)L^\dagger &= |\gamma|^2\rho_{ee}(t)|g\rangle\langle g| \end{aligned} \quad (6.50)$$

Substituting these expressions into equation (6.47) we find

$$\begin{aligned}
 \dot{\rho}(t) &= \dot{\rho}_{ee}(t)|e\rangle\langle e| + \dot{\rho}_{gg}(t)|g\rangle\langle g| \\
 &= -\frac{i}{\hbar} (\hbar(\omega - i|\gamma|^2/2) - \hbar(\omega + i|\gamma|^2/2)) \rho_{ee}(t)|e\rangle\langle e| + |\gamma|^2 \rho_{ee}(t)|g\rangle\langle g| \\
 &= -|\gamma|^2 \rho_{ee}(t)|e\rangle\langle e| + |\gamma|^2 \rho_{ee}(t)|g\rangle\langle g|
 \end{aligned} \tag{6.51}$$

If we multiply  $\langle e|$  from the left and  $|e\rangle$  from the right we obtain:

$$\dot{\rho}_{ee}(t) = -|\gamma|^2 \rho_{ee}(t). \tag{6.52}$$

If we multiply  $\langle g|$  from the left and  $|g\rangle$  from the right we obtain:

$$\dot{\rho}_{gg}(t) = |\gamma|^2 \rho_{ee}(t). \tag{6.53}$$

Equation (6.52) is a simple first order differential equation, which we integrate to find:

$$\rho_{ee}(t) = \exp[-|\gamma|^2 t] \rho_{ee}(0). \tag{6.54}$$

and

$$\rho_{gg}(t) = 1 - \exp[-|\gamma|^2 t] \rho_{ee}(0). \tag{6.55}$$

This equation tells us that the probability of measuring that the state of the atom in the excited state  $|e\rangle$  will decay exponentially in time with rate  $|\gamma|^2$ . This is precisely the behaviour we observe in spontaneous emission.

## Phenomenological master equations

The master equation for spontaneous emission was very simple, and amounted to just specifying the system Hamiltonian  $H$  and the jump operator  $L = \gamma|g\rangle\langle e|$ . This operator is called a jump operator because it embodies the “jump” from excited to ground state which occurs when a photon is emitted. The jump operator represents this process quite literally, transforming state  $|e\rangle$  into  $|g\rangle$ .

We could have constructed the master equation by

1. Identifying the system Hamiltonian  $H$
2. Identifying the jump operator  $L$  corresponding to the irreversible dynamics due to interaction with the environment.



We can build up a tool-box of jump operators corresponding to different types of system-environment interaction, and construct master equations to suit a particular problem. Two examples of this are given in problem sheet 5.

Phenomenological approaches are not rigorous derivations, essentially they are a form of intelligent guesswork, but they are often a powerful method for quickly constructing models of open systems which often can be shown to match the evolution predicted by rigorous calculation or observed in experiment. In particular, the phenomenological approach does not predict the value of rates such as  $|\gamma|^2$ , which would be provided by a full calculation.

### Example jump operators

- **Random magnetic field:** If a spin encounters a randomly varying magnetic field it will shift the energies of the spin energy levels. This leads to random phase shifts. The classical randomness which this contributes to the evolution causes the quantum state of the spin to become mixed. A jump operator which implements this dephasing behaviour is  $L = \gamma(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|) = \gamma\sigma_z$ , where  $|\gamma|^2$  is a rate in the evolution equations.
- **Damped quantum oscillator** (leaking cavity): In a physical optical cavity, photons are not captured indefinitely. Over time, they leak from the cavity and are lost. This process is mathematically equivalent to a damped Harmonic oscillator and is described by jump operator  $L = \gamma\hat{a}$ . This jump operator has a literal interpretation, it is proportional to the lowering operator, which annihilates photons.

Phenomenological master equations play an important role in a number of current research areas, since they are a key tool for modelling quantum systems interacting with the world around them. For example, they are used to model noise and errors in quantum computation, in modelling quantum effects in nano-scale devices such as quantum dots and in studying the transport of energy in molecules associated with photo-synthesis in biological systems.