

3

Open quantum systems

3.1 Introduction

As discussed in Chapter 1, to understand the general evolution, conditioned and unconditioned, of a quantum system, it is necessary to consider coupling it to a second quantum system. In the case in which the second system is much larger than the first, it is often referred to as a *bath*, *reservoir* or *environment*, and the first system is called an *open system*. The study of open quantum systems is important to quantum measurement for two reasons.

First, all real systems are open to some extent, and the larger a system is, the more important its coupling to its environment will be. For a macroscopic system, such coupling leads to very rapid *decoherence*. Roughly, this term means the irreversible loss of quantum coherence, that is the conversion of a quantum superposition into a classical mixture. This process is central to understanding the emergence of classical behaviour and ameliorating, if not solving, the so-called *quantum measurement problem*.

The second reason why open quantum systems are important is in the context of generalized quantum measurement theory as introduced in Chapter 1. Recall from there that, by coupling a quantum system to an ‘apparatus’ (a second quantum system) and then measuring the apparatus, a generalized measurement on the system is realized. For an open quantum system, the coupling to the environment is typically continuous (present at all times). In some cases it is possible to *monitor* (i.e. continuously measure) the environment so as to realize a continuous generalized measurement on the system.

In this chapter we are concerned with introducing open quantum systems, and with discussing the first point, decoherence. We introduced the decoherence of a macroscopic apparatus in Section 1.2.3, in the context of the von Neumann chain and Heisenberg’s cut. To reiterate that discussion, direct projective measurements on a quantum system do not adequately describe realistic measurements. Rather, one must consider making measurements on an apparatus that has been coupled to the system. But how does one make a direct observation on the apparatus? Should one introduce yet another system to model the readout of the meter coupled to the actual system of study, and so on with meters upon meters *ad infinitum*? This is the von Neumann chain [vN32]. To obtain a finite theory, the experimental result must be considered to have been recorded definitely at some point: Heisenberg’s cut [Hei30].

The quantum measurement problem is that there is no physical basis for inserting a cut at any particular point. However, there is a physical basis for determining the point in the chain *after which* the cut may be placed without affecting any theoretical predictions. This point is the point at which, for all practical purposes, the meter can be treated as a classical, rather than a quantum, object. That such a point exists is due to decoherence brought about by the environment of the apparatus.

Consider, for example, the single-photon measurement discussed in Section 1.5. The system of study was the electromagnetic field of a single-mode microwave cavity. The meter was an atomic system, suitably prepared. This meter clearly still behaves as a quantum system; however, as other experiments by the same group have shown [RBH01], the atomic ‘meter’ is in turn measured by ionization detectors. These detectors are, of course, rather complicated physical systems involving electrical fields, solid-state components and sophisticated electronics. Should we include these as quantum systems in our description? No, for two reasons.

First, it is too hard. Quantum systems with many degrees of freedom are generally intractable. This is due to the exponential increase in the dimension of the Hilbert space with the number of components for multi-partite systems, as discussed in Section A.2. Except for cases in which the Hamiltonian has an exceptionally simple structure, numerical solutions are necessary for the quantum many-body problem.

Exercise 3.1 *For the special case of a Hamiltonian that is invariant under particle permutations show that the dimension of the total Hilbert space increases only linearly in the number of particles.*

However, even on today’s supercomputers, numerical solutions are intractable for 100 particles or more. Detectors typically have far more particles than this, and, more importantly, they typically interact strongly with other systems in their environment.

Second, it is unnecessary. Detectors are not arbitrary many-body systems. They are designed for a particular purpose: to be a detector. This means that, despite its being coupled to a large environment, there are certain properties of the detector that, if initially well defined, remain well defined over time. These classical-like properties are those that are *robust* in the face of decoherence, as we will discuss in Section 3.7. Moreover, in an ideal detector, one of these properties is precisely the one which becomes correlated with the quantum system and apparatus, and so constitutes the *measurement result*. As we will discuss in Section 4.8, sometimes it may be necessary to treat the detector dynamics in greater detail in order to understand precisely what information the experimenter has obtained about the system of study from the measurement result. However, in this case it is still unnecessary to treat the detector as a quantum system; a classical model is sufficient.

The remainder of this chapter is organized as follows. In Section 3.2 we introduce the simplest approach to modelling the evolution of open quantum systems: the *master equation* derived in the Born–Markov approximations. In Section 3.3 we apply this to the simplest (and historically first) example: radiative damping of a two-level atom. In the same section we also describe damping of an optical cavity; this treatment is very similar, insofar as both involve a rotating-wave approximation. In Section 3.4 we consider systems in which the

rotating-wave approximation cannot be made: the spin–boson model and Brownian motion. In all of these examples so far, the reservoir consists of harmonic oscillators, modes of a bosonic field (such as the electromagnetic field). In Section 3.5 we treat a rather different sort of reservoir, consisting of a fermionic (electron) field, coupled to a single-electron system.

In Section 3.6 we turn to more formal results: the mathematical conditions that a Markovian theory of open quantum systems should satisfy. Armed with these examples and this theory, we tackle the issue of decoherence and its relation to the quantum measurement problem in Section 3.7, using the example of Brownian motion. Section 3.8 develops this idea in the direction of continuous measurement (which will be considered in later chapters), using the examples of the spin–boson model, and the damped and driven atom. The ground-breaking decoherence experiment from the group of Haroche is analysed in Section 3.9 using the previously introduced damped-cavity model. In Section 3.10 we discuss two more open systems of considerable experimental interest: a quantum electromechanical oscillator and a superconducting qubit. Finally (apart from the further reading), we present in Section 3.11 a Heisenberg-picture description of the dynamics of open quantum systems, and relate it to the descriptions in earlier sections.

3.2 The Born–Markov master equation

In this section we derive a general expression for the evolution of an open quantum system in the Born and Markov approximations. This will then be applied to particular cases in subsequent sections. The essential idea is that the system couples weakly to a very large environment. The weakness of the coupling ensures that the environment is not much affected by the system: this is the Born approximation. The largeness of the environment (strictly, the closeness of its energy levels) ensures that from one moment to the next the system effectively interacts with a different part of the environment: this is the Markov approximation.

Although the environment is relatively unaffected by the system, the system is profoundly affected by the environment. Specifically, it typically becomes entangled with the environment. For this reason, it cannot be described by a pure state, even if it is initially in a pure state. Rather, as shown in Section A.2.2, it must be described by a mixed state ρ . The aim of the Born–Markov approximation is to derive a differential equation for ρ . That is, rather than having to use a quantum state for the system and environment, we can find the approximate evolution of the system by solving an equation for the system state alone. For historical reasons, this is called a *master equation*.

The dynamics of the state ρ_{tot} for the system plus environment is given in the Schrödinger picture by

$$\dot{\rho}_{\text{tot}}(t) = -i[\hat{H}_S + \hat{H}_E + \hat{V}, \rho_{\text{tot}}(t)]. \quad (3.1)$$

Here \hat{H}_S is the Hamiltonian for the system (that is, it acts as the identity on the environment Hilbert space), \hat{H}_E is that for the environment, and \hat{V} includes the coupling between the two. Following the formalism in Section A.1.3, it is convenient to move into an interaction

frame with free Hamiltonian $\hat{H}_0 = \hat{H}_S + \hat{H}_E$. That is, instead of $\hat{H}_{\text{tot}} = \hat{H}_0 + \hat{V}$, we use

$$\hat{V}_{\text{IF}}(t) = e^{i\hat{H}_0 t} \hat{V} e^{-i\hat{H}_0 t}. \quad (3.2)$$

In this *frame*, the Schrödinger-picture equation is

$$\dot{\rho}_{\text{tot;IF}}(t) = -i[\hat{V}_{\text{IF}}(t), \rho_{\text{tot;IF}}(t)], \quad (3.3)$$

where the original solution to Eq. (3.1) is found as

$$\rho_{\text{tot}}(t) = e^{-i\hat{H}_0 t} \rho_{\text{tot;IF}} e^{i\hat{H}_0 t}. \quad (3.4)$$

The equations below are all in the interaction frame, but for ease of notation we drop the IF subscripts. That is, \hat{V} will now denote $\hat{V}_{\text{IF}}(t)$, etc.

Since the interaction is assumed to be weak, the differential equation Eq. (3.3) may be solved as a perturbative expansion. We solve Eq. (3.3) implicitly to get

$$\rho_{\text{tot}}(t) = \rho_{\text{tot}}(0) - i \int_0^t dt_1 [\hat{V}(t_1), \rho_{\text{tot}}(t_1)]. \quad (3.5)$$

We then substitute this solution back into Eq. (3.3) to yield

$$\dot{\rho}_{\text{tot}}(t) = -i[\hat{V}(t), \rho_{\text{tot}}(0)] - \int_0^t dt_1 [\hat{V}(t), [\hat{V}(t_1), \rho_{\text{tot}}(t_1)]]. \quad (3.6)$$

Since we are interested here only in the evolution of the system, we trace over the environment to get an equation for $\rho \equiv \rho_S = \text{Tr}_E[\rho_{\text{tot}}]$ as follows:

$$\begin{aligned} \dot{\rho}(t) = & -i \text{Tr}_E([\hat{V}(t), \rho_{\text{tot}}(0)]) \\ & - \int_0^{t_1} dt_1 \text{Tr}_E([\hat{V}(t), [\hat{V}(t_1), \rho_{\text{tot}}(t_1)]]). \end{aligned} \quad (3.7)$$

This is still an exact equation but is also still implicit because of the presence of $\rho_{\text{tot}}(t_1)$ inside the integral. However, it can be made explicit by making some approximations, as we will see. It might be asked why we carry the expansion to second order in V , rather than use the first-order equation (3.3), or some higher-order equation. The answer is simply that second order is the lowest order which generally gives a non-vanishing contribution to the final master equation.

We now assume that at $t = 0$ there are no correlations between the system and its environment:

$$\rho_{\text{tot}}(0) = \rho(0) \otimes \rho_E(0). \quad (3.8)$$

This assumption may be physically unreasonable for some interactions between the system and its environment [HR85]. However, for weakly interacting systems it is a reasonable approximation. We also split \hat{V} (which, it must be remembered, denotes the Hamiltonian in the interaction frame) into two parts:

$$\hat{V}(t) = \hat{V}_S(t) + \hat{V}_{SE}(t), \quad (3.9)$$

where $\hat{V}_S(t)$ acts nontrivially only on the system Hilbert space, and where $\text{Tr}[\hat{V}_{SE}(t)\rho_{\text{tot}}(0)] = 0$.

Exercise 3.2 Show that this can be done, irrespective of the initial system state $\rho(0)$, by making a judicious choice of \hat{H}_0 .

We now make a very important assumption, namely that the system only weakly affects the bath so that in the last term of Eq. (3.7) it is permissible to replace $\rho_{\text{tot}}(t_1)$ by $\rho(t_1) \otimes \rho_E(0)$. This is known as the *Born approximation*, or the weak-coupling approximation. Under this assumption, the evolution becomes

$$\dot{\rho}(t) = -i[\hat{V}_S(t), \rho(t)] - \int_0^t dt_1 \text{Tr}_E([\hat{V}_{SE}(t), [\hat{V}_{SE}(t_1), \rho(t_1) \otimes \rho_E(0)]]) \quad (3.10)$$

Note that this assumption is not saying that $\rho_{\text{tot}}(t_1)$ is well approximated by $\rho(t_1) \otimes \rho_E(0)$ for all purposes, and indeed this is not the case; the coupling between the system and the environment in general entangles them. This is why the system becomes mixed, and why measuring the environment can reveal information about the system, as will be considered in later chapters, but this factorization assumption is a good one for the purposes of deriving the evolution of the system alone.

The equation (3.10) is an integro-differential equation for the system state matrix ρ . Because it is nonlocal in time (it contains a convolution), it is still rather difficult to solve. We seek instead a local-in-time differential equation, sometimes called a time-convolutionless master equation, that is, an equation in which the rate of change of $\rho(t)$ depends only upon $\rho(t)$ and t . This can be justified if the integrand in Eq. (3.10) is small except in the region $t_1 \approx t$. Since the modulus of $\rho(t_1)$ does not depend upon t_1 , this property must arise from the physics of the bath. As we will show in the next section, it typically arises when the system couples roughly equally to many energy levels of the bath (eigenstates of \hat{H}_E) that are close together in energy. Under this approximation it is permissible to replace $\rho(t_1)$ in the integrand by $\rho(t)$, yielding

$$\dot{\rho}(t) = -i[\hat{V}_S(t), \rho(t)] - \int_0^t dt_1 \text{Tr}_E([\hat{V}(t), [\hat{V}(t_1), \rho(t) \otimes \rho_E(0)]]) \quad (3.11)$$

This is sometimes called the Redfield equation [Red57].

Even though the approximation of replacing $\rho(t_1)$ by $\rho(t)$ is sometimes referred to as a Markov approximation [Car99, GZ04], the resulting master equation (3.11) is not strictly Markovian. That is because it has time-dependent coefficients, as will be discussed in Section 3.4. In fact, it can be argued [BP02] that this additional approximation is not really an additional approximation at all: the original Born master equation Eq. (3.10) would not be expected to be more accurate than the Redfield equation Eq. (3.11).

To obtain a true Markovian master equation, an autonomous differential equation for $\rho(t)$, it is necessary to make a more substantial Markov approximation. This consists of again appealing to the sharpness of the integrand at $t_1 \approx t$, this time to replace the lower limit of the integral in Eq. (3.11) by $-\infty$. In that way we get finally the Born–Markov master equation for the system in the interaction frame:

$$\dot{\rho}(t) = -i[\hat{V}_S(t), \rho(t)] - \int_{-\infty}^t dt_1 \text{Tr}_E([\hat{V}(t), [\hat{V}(t_1), \rho(t) \otimes \rho_E(0)]]) \quad (3.12)$$

We will see in examples below how, for physically reasonable properties of the bath, this gives a master equation with time-independent coefficients, as required. In particular, we require \hat{H}_E to have a continuum spectrum in the relevant energy range, and we require

$\rho_E(0)$ to commute with \hat{H}_E . In practice, the latter condition is often relaxed in order to yield an equation in which $V_S(t)$ may be time-dependent, but the second term in Eq. (3.12) is still required to be time-independent.

3.3 The radiative-damping master equation

In this section we repeat the derivation of the Born–Markov master equation for a specific case: radiative damping of quantum optical systems (a two-level atom and a cavity mode). This provides more insight into the Born and Markov approximations made above.

3.3.1 Spontaneous emission

Historically, the irreversible dynamics of spontaneous emission were introduced by Bohr [Boh13] and, more quantitatively, by Einstein [Ein17], before quantum theory had been developed fully. It was Wigner and Weisskopf [WW30] who showed in 1930 how the radiative decay of an atom from the excited to the ground state could be explained within quantum theory. This was possible only after Dirac’s quantization of the electromagnetic field, since it is the infinite (or at least arbitrarily large) number of electromagnetic field modes which forms the environment or bath into which the atom radiates. The theory of spontaneous emission is described in numerous recent texts [GZ04, Mil93], so our treatment will just highlight key features.

As discussed in Section A.4, the free Hamiltonian for a mode of the electromagnetic field is that of a harmonic oscillator. The total Hamiltonian for the bath is thus

$$\hat{H}_E = \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k, \quad (3.13)$$

where the integer k codes all of the information specifying the mode: its frequency, direction, transverse structure and polarization. The mode structure incorporates the effect of bulk materials with a linear refractive index (such as mirrors) and the like, so this is all described by the Hamiltonian \hat{H}_E . The annihilation and creation operators for each mode are independent and they obey the *bosonic* commutation relations

$$[\hat{b}_k, \hat{b}_l^\dagger] = \delta_{kl}. \quad (3.14)$$

We will assume that only two energy levels of the atom are relevant to the problem, so the free Hamiltonian for the atom is

$$\hat{H}_a = \frac{\omega_a}{2} \hat{\sigma}_z. \quad (3.15)$$

Here ω_a is the energy (or frequency) difference between the ground $|g\rangle$ and excited $|e\rangle$ states, and $\hat{\sigma}_z = |e\rangle\langle e| - |g\rangle\langle g|$ is the inversion operator for the atom. (See Box 3.1.) The coupling of the electromagnetic field to an atom can be described by the so-called dipole-coupling Hamiltonian

$$\hat{V} = \sum_k (g_k \hat{b}_k + g_k \hat{b}_k^\dagger)(\hat{\sigma}_+ + \hat{\sigma}_-). \quad (3.16)$$

Box 3.1 The Bloch representation

Consider a two-level system with basis states $|0\rangle$ and $|1\rangle$. The three *Pauli* operators for the system are defined as

$$\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0|, \quad (3.17)$$

$$\hat{\sigma}_y = i|0\rangle\langle 1| - i|1\rangle\langle 0|, \quad (3.18)$$

$$\hat{\sigma}_z = |1\rangle\langle 1| - |0\rangle\langle 0|. \quad (3.19)$$

These obey the following product relations:

$$\hat{\sigma}_j \hat{\sigma}_k = \delta_{jk} \hat{1} + i\epsilon_{jkl} \hat{\sigma}_l. \quad (3.20)$$

Here the subscripts stand for x , y or z , while $\hat{1}$ is the 2×2 unit matrix, i is the unit imaginary and ϵ_{jkl} is the completely antisymmetric tensor (that is, transposing any two subscripts changes its sign) satisfying $\epsilon_{xyz} = 1$. From this commutation relations like $[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z$ and anticommutation relations like $\hat{\sigma}_x \hat{\sigma}_y + \hat{\sigma}_y \hat{\sigma}_x = 0$ are easily derived.

The state matrix for a two-level system can be written using these operators as

$$\rho(t) = \frac{1}{2}[\hat{1} + x(t)\hat{\sigma}_x + y(t)\hat{\sigma}_y + z(t)\hat{\sigma}_z], \quad (3.21)$$

where x , y , z are the averages of the Pauli operators. That is, $x = \text{Tr}[\hat{\sigma}_x \rho]$ *et cetera*. Recall that $\text{Tr}[\rho^2] \leq 1$, with equality for and only for pure states. This translates to

$$x^2 + y^2 + z^2 \leq 1, \quad (3.22)$$

again with equality iff the system is pure. Thus, the system state can be represented by a 3-vector inside (on) the unit sphere for a mixed (pure) state. The vector is called the *Bloch vector* and the sphere the *Bloch sphere*.

For a two-level atom, it is conventional to identify $|1\rangle$ and $|0\rangle$ with the ground $|g\rangle$ and excited $|e\rangle$ states. Then z is called the atomic inversion, because it is positive iff the atom is inverted, that is, has a higher probability of being in the excited state than in the ground state. The other components, y and x , are called the atomic coherences, or components of the atomic dipole.

Another two-level system is a spin-half particle. Here ‘spin-half’ means that the maximum angular momentum contained in the intrinsic spin of the particle is $\hbar/2$. The operator for the spin angular momentum (a 3-vector) is $(\hbar/2) \times (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$. That is, in this case the Bloch vector (x, y, z) has a meaning in ordinary three-dimensional space, as the mean spin angular momentum, divided by $\hbar/2$.

Nowadays it is common to study a two-level quantum system without any particular physical representation in mind. In this context, it is appropriate to use the term *qubit* – a quantum bit.

Here $\hat{\sigma}_+ = (\hat{\sigma}_-)^{\dagger} = |e\rangle\langle g|$ is the raising operator for the atom. The coefficient g_k (which can be assumed real without loss of generality) is proportional to the dipole matrix element for the transition (which we will assume is non-zero) and depends on the structure of mode k . In particular, it varies as $V_k^{-1/2}$, where V_k is the physical volume of mode k .

It turns out that the rate γ of radiative decay for an atom in free space is of order 10^8 s^{-1} or smaller. This is much smaller than the typical frequency ω_a for an optical transition, which is of order 10^{15} s^{-1} or greater. Since γ is due to the interaction Hamiltonian \hat{V} , it seems reasonable to treat \hat{V} as being small compared with $\hat{H}_0 = \hat{H}_a + \hat{H}_E$. Thus we are justified in following the method of Section 3.2. We begin by calculating \hat{V} in the interaction frame:

$$\hat{V}_{\text{IF}}(t) = \sum_k (g_k \hat{b}_k e^{-i\omega_k t} + g_k \hat{b}_k^{\dagger} e^{i\omega_k t}) (\hat{\sigma}_+ e^{+i\omega_a t} + \hat{\sigma}_- e^{-i\omega_a t}). \quad (3.23)$$

Exercise 3.3 Show this, using the same technique as in Exercise 1.30.

The first approximation we make is to remove the terms in $\hat{V}_{\text{IF}}(t)$ that rotate (in the complex plane) at frequency $\omega_a + \omega_k$ for all k , yielding

$$\hat{V}_{\text{IF}}(t) = \sum_k (g_k \hat{b}_k \hat{\sigma}_+ e^{-i(\omega_k - \omega_a)t} + g_k \hat{b}_k^{\dagger} \hat{\sigma}_- e^{i(\omega_k - \omega_a)t}). \quad (3.24)$$

As discussed in Section 1.5, this is known as the rotating-wave approximation (RWA). It is justified on the grounds that these terms rotate so fast ($\sim 10^{15} \text{ s}^{-1}$) that they will average to zero over the time-scale of radiative decay ($\sim 10^{-8} \text{ s}$) and hence not contribute to this process.¹ This approximation leads to significant simplifications.

Now substitute Eq. (3.24) into the exact equation (3.7) for the system state $\rho(t)$ in Section 3.2. To proceed we need to specify the initial state of the field, which we take to be the vacuum state (see Appendix A). The first term in Eq. (3.7) is then exactly zero.

Exercise 3.4 Show this, and show that it holds also for a field state in a thermal state $\rho_E \propto \exp[-\hat{H}_E/(k_B T)]$.

Hint: Expand ρ_E in the number basis.

For this choice of ρ_E , we have $\hat{V}_S = 0$; later, we will relax this assumption.

For convenience, we now drop the IF subscripts, while still working in the interaction frame. Under the Born approximation, the equation for $\rho(t)$ becomes

$$\dot{\rho} = - \int_0^t dt_1 \{ \Gamma(t - t_1) [\hat{\sigma}_+ \hat{\sigma}_- \rho(t_1) - \hat{\sigma}_- \rho(t_1) \hat{\sigma}_+] + \text{H.c.} \}, \quad (3.25)$$

where H.c. stands for the Hermitian conjugate term, and

$$\Gamma(\tau) = \sum_k g_k^2 e^{-i(\omega_k - \omega_a)\tau}. \quad (3.26)$$

¹ Terms like these are, however, important for a proper calculation of the Lamb frequency shift $\Delta\omega_a$, but that is beyond the scope of this treatment.

Exercise 3.5 Show this, using the properties of the vacuum state and the field operators.

Next, we wish to make the *Markov* approximation. This can be justified by considering the reservoir correlation function (3.26). For an atom in free space, there is an infinite number of modes, each of which is infinite in volume, so the modulus squared of the coupling coefficients is infinitesimal. Thus we can justify replacing the sum in Eq. (3.26) by an integral,

$$\Gamma(\tau) = \int_0^\infty d\omega \rho(\omega) g(\omega)^2 e^{i(\omega_a - \omega)\tau}. \quad (3.27)$$

Here $\rho(\omega)$ is the density of field modes as a function of frequency. This is infinite but the product $\rho(\omega)g(\omega)^2$ is finite. Moreover, $\rho(\omega)g(\omega)^2$ is a smoothly varying function of frequency for ω in the vicinity of ω_a . This means that the reservoir correlation function, $\Gamma(\tau)$, is sharply peaked at $\tau = 0$.

Exercise 3.6 Convince yourself of this by considering a toy model in which $\rho(\omega)g(\omega)^2$ is independent of ω in the range $(0, 2\omega_a)$ and zero elsewhere.

Thus we can apply the Markov approximation to obtain the master equation

$$\dot{\rho} = -i\frac{\Delta\omega_a}{2}[\hat{\sigma}_z, \rho] + \gamma\mathcal{D}[\hat{\sigma}_-]\rho. \quad (3.28)$$

Here the superoperator $\mathcal{D}[\hat{A}]$ is defined for an arbitrary operator \hat{A} by

$$\mathcal{D}[\hat{A}]\rho \equiv \hat{A}\rho\hat{A}^\dagger - \frac{1}{2}(\hat{A}^\dagger\hat{A}\rho + \rho\hat{A}^\dagger\hat{A}). \quad (3.29)$$

The real parameters $\Delta\omega_a$ (the frequency shift) and γ (the radiative decay rate) are defined as

$$\Delta\omega_a - i\frac{\gamma}{2} = -i\int_0^\infty \Gamma(\tau)d\tau. \quad (3.30)$$

Exercise 3.7 Derive Eq. (3.28)

In practice the frequency shift (called the Lamb shift) due to the atom coupling to the electromagnetic vacuum is small, but can be calculated properly only by using renormalization theory and relativistic quantum mechanics.

The solution of Eq. (3.28) at any time $t > 0$ depends only on the initial state at time $t = 0$; there is no memory effect. The evolution is non-unitary because of the \mathcal{D} term, which represents radiative decay. This can be seen by considering the Bloch representation of the atomic state, as discussed in Box 3.1.

Exercise 3.8 Familiarize yourself with the Bloch sphere by finding the points on it corresponding to the eigenstates of the Pauli matrices, and the point corresponding to the maximally mixed state.

For example, the equation of motion for the inversion can be calculated as $\dot{z} = \text{Tr}[\hat{\sigma}_z\dot{\rho}]$, and re-expressing the right-hand side in terms of x , y and z . In this case we find simply

$\dot{z} = -\gamma(z + 1)$, so the inversion decays towards the ground state ($z = -1$) exponentially at rate γ . Thus we can equate γ to the A coefficient of Einstein's theory [Ein17], and $1/\gamma$ to the atomic lifetime. The energy lost by the atom is radiated into the field, hence the term radiative decay. The final state here is pure, but, if it starts in the excited state, then the atom will become mixed before it becomes pure again. This mixing is due to entanglement between the atom and the field: the total state is a superposition of excited atom and vacuum-state field, and ground-state atom and field containing one photon of frequency ω_0 . This process is called spontaneous emission because it occurs even if there are initially no photons in the field.

Exercise 3.9 Show that, if the atom is prepared in the excited state at time $t = 0$, the Bloch vector at time t is $(0, 0, 2e^{-\gamma t} - 1)$. At what time is the entanglement between the atom and the radiated field maximal?

Strictly, the frequency of the emitted photon has a probability distribution centred on ω_0 with a full width-at-half-maximum height of γ . Thus a finite lifetime of the atomic state leads to an uncertainty in the energy of the emitted photon, which can be interpreted as an uncertainty in the energy separation of the atomic transition. The reciprocal relation between the lifetime $1/\gamma$ and the energy uncertainty γ is sometimes referred to as an example of the time–energy uncertainty relation. It should be noted that its meaning is quite different from that of the Heisenberg uncertainty relations mentioned in Section 1.2.1, since time is not a system property represented by an operator; it is merely an external parameter. Nevertheless, this relation is of great value heuristically, as we will see.

We note two important generalizations. Firstly, the atom may be driven coherently by a classical field. As long as the system Hamiltonian which describes this driving is weak compared with \hat{H}_a , it will have negligible effect on the derivation of the master equation in the interaction frame, and can simply be added at the end. Alternatively, this situation can be modelled quantum mechanically by taking the bath to be initially in a coherent state, which will make $\hat{V}_S(t)$ non-zero, and indeed time-dependent in general (this is discussed in Section 3.11.2 below). In any case, the effect of driving is simply to add another Hamiltonian evolution term to the final master equation (3.12) in the interaction frame. If the frequency of oscillation of the driving field is $\omega_0 \approx \omega_a$, then it is most convenient to work in an interaction frame using $\hat{H}_a = \omega_0 \hat{\sigma}_z/2$, rather than $\hat{H}_a = \omega_a \hat{\sigma}_z/2$. This is because, on moving to the interaction frame, it makes the total effective Hamiltonian for the atom time-independent:

$$\hat{H}_{\text{drive}} = \frac{\Omega}{2} \hat{\sigma}_x + \frac{\Delta}{2} \hat{\sigma}_z. \quad (3.31)$$

Here $\Delta = \omega_a + \Delta\omega_a - \omega_0$ is the effective detuning of the atom, while Ω , the *Rabi frequency*, is proportional to the amplitude of the driving field and the atomic dipole moment. Here the phase of the driving field acts as a reference to define the in-phase (x) and in-quadrature (y) parts of the atomic dipole relative to the imposed force. The master equation for a resonantly driven, damped atom is known as the resonance fluorescence master equation.

Exercise 3.10 (a) Show that the Bloch equations for resonance fluorescence are

$$\dot{x} = -\Delta y - \frac{\gamma}{2}x, \quad (3.32)$$

$$\dot{y} = -\Omega z + \Delta x - \frac{\gamma}{2}y, \quad (3.33)$$

$$\dot{z} = +\Omega y - \gamma(z + 1), \quad (3.34)$$

and that the stationary solution is

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{ss}} = \begin{pmatrix} -4\Delta\Omega \\ 2\Omega\gamma \\ -\gamma^2 - 4\Delta^2 \end{pmatrix} (\gamma^2 + 2\Omega^2 + 4\Delta^2)^{-1}. \quad (3.35)$$

(b) Compare $\theta = \arctan(y_{\text{ss}}/x_{\text{ss}})$ and $A = \sqrt{x_{\text{ss}}^2 + y_{\text{ss}}^2}$ with the phase and amplitude of the long-time response of a classical, lightly damped, harmonic oscillator to an applied periodic force with magnitude proportional to Ω and detuning Δ . In what regime does the two-level atom behave like the harmonic oscillator?

Hint: First, define interaction-frame phase and amplitude variables for the classical oscillator; that is, variables that would be constant in the absence of driving and damping.

The second generalization is that the field need not be in a vacuum state, but rather (for example) may be in a thermal state (i.e. with a Planck distribution of photon numbers [GZ04]). This gives rise to *stimulated* emission and absorption of photons. In that case, the total master equation in the Markov approximation becomes

$$\dot{\rho} = -i \left[\frac{\Omega}{2} \hat{\sigma}_x + \frac{\Delta}{2} \hat{\sigma}_z, \rho \right] + \gamma(\bar{n} + 1) \mathcal{D}[\hat{\sigma}_-] \rho + \gamma \bar{n} \mathcal{D}[\hat{\sigma}_+] \rho, \quad (3.36)$$

where $\bar{n} = \{\exp[\hbar\omega_a/(k_B T)] - 1\}^{-1}$ is the thermal mean photon number evaluated at the atomic frequency (we have here restored \hbar). This describes the (spontaneous and stimulated) emission of photons at a rate proportional to $\gamma(\bar{n} + 1)$, and (stimulated) absorption of photons at a rate proportional to $\gamma\bar{n}$.

3.3.2 Cavity emission

Another system that undergoes radiative damping is a mode of the electromagnetic field in an optical cavity. In quantum optics the term ‘cavity’ is used for any structure (typically made of dielectric materials) that will store electromagnetic energy at discrete frequencies. The simplest sort of cavity is a pair of convex mirrors facing each other, but no mirrors are perfectly reflecting, and the stored energy will decay because of transmission through the mirrors.

Strictly speaking, a mode of the electromagnetic field should be a stationary solution of Maxwell’s equations [CRG89] and so should not suffer a decaying amplitude. However, it is often convenient to treat *pseudomodes*, such as those that are localized within a

cavity, as if they were modes, and to treat the amplitude decay as radiative damping due to coupling to the (pseudo-)modes that are localized outside the cavity [GZ04]. This is a good approximation, provided that the coupling is weak; that is, that the transmission at the mirrors is small.

The simplest case to consider is a single mode (of frequency ω_c) of a one-dimensional cavity with one slightly lossy mirror and one perfect mirror. We use \hat{a} for the annihilation operator for the cavity mode of interest and \hat{b}_k for those of the bath as before. The total Hamiltonian for system plus environment, in the RWA, is [WM94a]

$$\hat{H} = \omega_c \hat{a}^\dagger \hat{a} + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_k g_k (\hat{a}^\dagger \hat{b}_k + \hat{a} \hat{b}_k^\dagger). \quad (3.37)$$

The first term represents the free energy of the cavity mode of interest, the second is for the free energy of the many-mode field outside the cavity, and the last term represents the dominant terms in the coupling of the two for optical frequencies.

For weak coupling the Born–Markov approximations are justified just as for spontaneous emission. Following the same procedure leads to a very similar master equation for the cavity field, in the interaction frame:

$$\dot{\rho} = \gamma(\bar{n} + 1)\mathcal{D}[\hat{a}]\rho + \gamma\bar{n}\mathcal{D}[\hat{a}^\dagger]\rho. \quad (3.38)$$

Here \bar{n} is the mean thermal photon number of the external field evaluated at the cavity frequency ω_c . We have ignored any environment-induced frequency shift, since this simply redefines the cavity resonance ω_c .

The first irreversible term in Eq. (3.38) represents emission of photons from the cavity. The second irreversible term represents an incoherent excitation of the cavity due to thermal photons in the external field.

Exercise 3.11 Show that the rate of change of the average photon number in the cavity is given by

$$\frac{d\langle \hat{a}^\dagger \hat{a} \rangle}{dt} = -\gamma \langle \hat{a}^\dagger \hat{a} \rangle + \gamma \bar{n}. \quad (3.39)$$

Note that here (and often from here on) we are relaxing our convention on angle brackets established in Section 1.2.1. That is, we may indicate the average of a property for a quantum system by angle brackets around the corresponding operator.

From Eq. (3.39) it is apparent that γ is the decay rate for the energy in the cavity. Assuming that $\rho(\omega)g(\omega)^2$ is slowly varying with frequency, we can evaluate this decay rate to be

$$\gamma \simeq 2\pi\rho(\omega_c)g(\omega_c)^2. \quad (3.40)$$

Exercise 3.12 Show this explicitly using the example of Exercise 3.6.

Note: This result can be obtained more simply by replacing $\int_{-\infty}^0 d\tau e^{-i\omega\tau}$ by $\pi\delta(\omega)$, which is permissible when it appears in an ω -integral with a flat integrand.

In more physical terms, if the mirror transmits a proportion $T \ll 1$ of the energy in the cavity on each reflection, and the round-trip time for light in the cavity is τ , then $\gamma = T/\tau$.

As in the atomic case, we can include other dynamical processes by simply adding an appropriate Hamiltonian term to the interaction-frame master equation (3.38), as long as the added Hamiltonian is (in some sense) small compared with \hat{H}_0 . In particular, we can include a coherent driving term, to represent the excitation of the cavity mode by an external laser of frequency ω_c , by adding the following driving Hamiltonian [WM94a]:

$$\hat{H}_{\text{drive}} = i\epsilon\hat{a}^\dagger - i\epsilon^*\hat{a}. \quad (3.41)$$

Exercise 3.13 Show that, in the zero-temperature limit, the stationary state for the driven, damped cavity is a coherent state $|\alpha\rangle$ with $\alpha = 2\epsilon/\gamma$.

Hint: Make the substitution $\hat{a} = 2\epsilon/\gamma + \hat{a}_0$, and show that the solution of the master equation is the vacuum state for \hat{a}_0 .

3.4 Irreversibility without the rotating-wave approximation

In the previous examples of radiative decay of an atom and a cavity, the system Hamiltonian \hat{H}_S produced oscillatory motion in the system with characteristic frequencies (ω_a and ω_c , respectively) much larger than the rate of decay. This allowed us to make a RWA in describing the system–environment coupling Hamiltonian as $\sum_k g_k(\hat{s}\hat{b}_k^\dagger + \hat{s}^\dagger\hat{b}_k)$, where \hat{s} is a system lowering operator. That is, the coupling describes the transfer of quanta of excitation of the oscillation between the system and the bath. When there is no such large characteristic frequency, it is not possible to make such an approximation. In this section we discuss two examples of this, the spin–boson model and quantum Brownian motion. We will, however, retain the model for the bath as a collection of harmonic oscillators and the assumption that the interaction between system and environment is weak in order to derive a master equation perturbatively.

3.4.1 The spin–boson model

Consider a two-level system, coupled to a reservoir of harmonic oscillators, such that the total Hamiltonian is

$$\hat{H} = \frac{\Delta}{2}\hat{\sigma}_x + \sum_k \left(\frac{\hat{p}_k^2}{2m_k} + \frac{m_k\omega_k^2\hat{q}_k^2}{2} \right) + \hat{\sigma}_z \sum_k g_k\hat{q}_k, \quad (3.42)$$

where \hat{q}_k are the coordinates of each of the environmental oscillators. This could describe a spin-half particle (see Box 3.1), in the interaction frame with respect to a Hamiltonian proportional to $\hat{\sigma}_z$. Such a Hamiltonian would describe a static magnetic field in the z (‘longitudinal’) direction. Then the first term would describe resonant driving (as in the two-level atom case) by a RF magnetic field in the x – y (‘transverse’) plane, and the last term would describe fluctuations in the longitudinal field. However, there are many other

physical situations for which this Hamiltonian is an approximate description, including quantum tunnelling in a double-well potential [LCD⁺87].

Since the frequency Δ can be small, even zero, we cannot make a RWA in this model. Nevertheless, we can follow the procedure in Section 3.2, where \hat{H}_0 comprises the first two terms in Eq. (3.42). We assume the bath to be in a thermal equilibrium state of temperature $1/(k_B\beta)$ with respect to its Hamiltonian. Then, replacing $\rho(t_1)$ by $\rho(t)$ in Eq. (3.10) yields the master equation with time-dependent coefficients [PZ01]

$$\begin{aligned} \dot{\rho}(t) = & - \int_0^t dt_1 \left(v(t_1) [\hat{\sigma}_z(t), [\hat{\sigma}_z(t-t_1), \rho(t)]] \right. \\ & \left. - i\eta(t_1) [\hat{\sigma}_z(t), \{\hat{\sigma}_z(t-t_1), \rho(t)\}] \right), \end{aligned} \quad (3.43)$$

where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is known as an *anticommutator*, and the kernels are given by

$$v(t_1) = \frac{1}{2} \sum_k g_k^2 \langle \{\hat{q}_k(t), \hat{q}_k(t-t_1)\} \rangle = \int_0^\infty d\omega J(\omega) \cos(\omega t_1) [1 + 2\bar{n}(\omega)], \quad (3.44)$$

$$\eta(t_1) = \frac{i}{2} \sum_k g_k^2 \langle [\hat{q}_k(t), \hat{q}_k(t-t_1)] \rangle = \int_0^\infty d\omega J(\omega) \sin(\omega t_1). \quad (3.45)$$

Here the spectral density function is defined by

$$J(\omega) = \sum_k \frac{g_k^2 \delta(\omega - \omega_k)}{2m_k \omega_k}, \quad (3.46)$$

and $\bar{n}(\omega)$ is the mean occupation number of the environmental oscillator at frequency ω . It is given as usual by the Planck law $1 + 2\bar{n}(\omega) = \coth(\beta\hbar\omega/2)$ (where, in deference to Planck, we have restored his constant). The sinusoidal kernels in Eqs. (3.44) and (3.45) result from the oscillatory time dependence of $\hat{q}_k(t)$ from the bath Hamiltonian.

The time dependence of the operator $\hat{\sigma}_z(t)$, in the interaction frame with respect to \hat{H}_0 , is given by

$$\hat{\sigma}_z(t) = \hat{\sigma}_z \cos(\Delta t) + \hat{\sigma}_y \sin(\Delta t). \quad (3.47)$$

Exercise 3.14 Show this by finding and solving the Heisenberg equations of motion for $\hat{\sigma}_y$ and $\hat{\sigma}_z$, for the Hamiltonian \hat{H}_0 .

Substituting this into Eq.(3.43), and then moving out of the interaction frame, yields the Schrödinger-picture master equation²

$$\dot{\rho} = -i[\hat{H}_{\text{nh}}\rho - \rho\hat{H}_{\text{nh}}^\dagger] - \zeta^*(t)\hat{\sigma}_z\rho\hat{\sigma}_y - \zeta(t)\hat{\sigma}_y\rho\hat{\sigma}_z - D(t)[\hat{\sigma}_z, [\hat{\sigma}_z, \rho]]. \quad (3.48)$$

Here

$$\hat{H}_{\text{nh}} = \left(\frac{\Delta}{2} + \zeta(t) \right) \hat{\sigma}_x \quad (3.49)$$

² With minor corrections to the result in Ref. [PZ01].

is a non-Hermitian operator (the Hermitian part of which can be regarded as the Hamiltonian), while

$$\zeta(t) = \int_0^t dt_1 (v(t_1) - i\eta(t_1)) \sin(\Delta t_1), \quad (3.50)$$

$$D(t) = \int_0^t dt_1 v(t_1) \cos(\Delta t_1). \quad (3.51)$$

The environment thus shifts the free Hamiltonian for the system (via $\text{Re}[\zeta]$) and introduces irreversible terms (via $\text{Im}[\zeta]$ and D). Note that if $\Delta = 0$ only the final term in Eq. (3.48) survives.

To proceed further we need an explicit form of the spectral density function. The simplest case is known as *Ohmic dissipation*, in which the variation with frequency is linear at low frequencies. We take

$$J(\omega) = 2\eta \frac{\omega}{\pi} \frac{\Lambda^2}{\Lambda^2 + \omega^2}, \quad (3.52)$$

where Λ is a cut-off frequency, as required in order to account for the physically necessary fall-off of the coupling at sufficiently high frequencies, and η is a dimensionless parameter characterizing the strength of the coupling between the spin and the environment. After splitting $\zeta(t)$ into real and imaginary parts as $\zeta(t) = f(t) - i\gamma(t)$, we can easily do the integral to find the decay term $\gamma(t)$. It is given by

$$\gamma(t) = \gamma_\infty \left[1 - \left(\cos(\Delta t) + \frac{\Lambda}{\Delta} \sin(\Delta t) \right) e^{-\Lambda t} \right]. \quad (3.53)$$

This begins at zero and decays (at a rate determined by the high-frequency cut-off) to a constant $\gamma_\infty \propto \Lambda^2/(\Lambda^2 + \Delta^2)$. The other terms depend on the temperature of the environment and are not easy to evaluate analytically. The diffusion constant can be shown to approach the asymptotic value

$$D_\infty = \eta \Delta \frac{\Lambda^2}{\Lambda^2 + \Delta^2} \coth(\beta \Delta / 2). \quad (3.54)$$

The function $f(t)$ also approaches (algebraically, not exponentially) a limiting value, which at high temperatures is typically much smaller than D_∞ (by a factor proportional to Λ).

In the limit that $\Delta \rightarrow 0$, we find

$$D_\infty \rightarrow 2\eta k_B T, \quad (3.55)$$

and, as mentioned previously, $\zeta(t)$ is zero in this limit. In this case the master equation takes the following simple form in the long-time limit:

$$\dot{\rho} = -2\eta k_B T [\hat{\sigma}_z, [\hat{\sigma}_z, \rho]]. \quad (3.56)$$

This describes dephasing of the spin in the x - y plane at rate $D_\infty/2$.

3.4.2 Quantum Brownian motion

Another important model for which the RWA cannot be used is quantum Brownian motion. In this case we have a single particle with mass M , with position and momentum operators \hat{X} and \hat{P} . It may be moving in some potential, and is coupled to an environment of simple harmonic oscillators. This is described by the Hamiltonian

$$\hat{H} = \frac{\hat{P}^2}{2M} + V(\hat{X}) + \sum_k \left(\frac{\hat{p}_k^2}{2m_k} + \frac{m_k \omega_k^2 \hat{q}_k^2}{2} \right) + \hat{X} \sum_k g_k \hat{q}_k. \quad (3.57)$$

The derivation of the perturbative master equation proceeds as in the case of the spin–boson model [PZ01]. It is only for simple potentials, such as the harmonic $V(\hat{X}) = M\Omega^2 \hat{X}^2/2$, that the evolution generated by \hat{H}_0 can be solved analytically. The derivation is much as in the spin–boson case, but, for dimensional correctness, we must replace η by $M\gamma$, where γ is a rate. The result is

$$\begin{aligned} \dot{\rho} = & -i[\hat{P}^2/(2M) + M\tilde{\Omega}(t)^2 \hat{X}^2/2, \rho] - i\gamma(t)[\hat{X}, \{\hat{P}, \rho\}] \\ & - D(t)[\hat{X}, [\hat{X}, \rho]] - f(t)[\hat{X}, [\hat{P}, \rho]]. \end{aligned} \quad (3.58)$$

Here $\tilde{\Omega}(t)$ is a shifted frequency and $\gamma(t)$ is a momentum-damping rate. $D(t)$ gives rise to diffusion in momentum and $f(t)$ to so-called anomalous diffusion.

If we again assume the Ohmic spectral density function (3.52) then we can evaluate these time-dependent coefficients. The coefficients all start at zero, and tend asymptotically to constants, with the same properties as in the spin–boson case. The shifted frequency $\tilde{\Omega}$ tends asymptotically to $\sqrt{\Omega - 2\gamma_\infty \Lambda}$, which is unphysical for Λ too large. In the high-temperature limit, $k_B T \gg \Omega$, with $\Lambda \gg \Omega$ one finds

$$D_\infty = M\gamma_\infty \Omega \frac{\Lambda^2}{\Lambda^2 + \Omega^2} \coth(\beta\Omega/2) \rightarrow 2\gamma_\infty k_B T M, \quad (3.59)$$

while $f(t)$ is negligible ($\propto \Lambda^{-1}$) compared with this.

Replacing the above time-dependent coefficients with their asymptotic values will be a bad approximation at short times, and indeed may well lead to nonsensical results (as will be discussed in Section 3.6). However, at long times it is reasonable to use the asymptotic values, giving the Markovian master equation

$$\dot{\rho} = -i[\hat{P}^2/(2M) + M\tilde{\Omega}_\infty^2 \hat{X}^2/2, \rho] - i\gamma_\infty[\hat{X}, \{\hat{P}, \rho\}] - 2\gamma_\infty k_B T M [\hat{X}, [\hat{X}, \rho]]. \quad (3.60)$$

Exercise 3.15 Show that this is identical with the Markovian master equation of Eq. (3.12) for this case.

The first irreversible term in Eq. (3.60) describes the loss, and the second the gain, of kinetic energy, as can be seen in the following exercise.

Exercise 3.16 Derive the equations of motion for the means and variances of the position and momentum using the high-temperature Brownian-motion master equation, Eq. (3.60). Thus show that momentum is damped exponentially at rate $2\gamma_\infty$, but that momentum

diffusion adds kinetic energy at rate $2\gamma_\infty k_B T$. Show that for $\tilde{\Omega}_\infty = 0$ the steady-state energy of the particle is $k_B T/2$, as expected from thermodynamics.

3.5 Fermionic reservoirs

In the previous examples the environment was taken to be composed of a very large (essentially infinite) number of harmonic oscillators. Such an environment is called *bosonic*, because the energy quanta of these harmonic oscillators are analogous to bosonic particles, with the associated commutation relations for the annihilation and creation operators (3.14). There are some very important physical situations in which the environment of a local system is in fact *fermionic*. An example is a local quantum dot (which acts something like a cavity for a single electron) coupled via tunnelling to the many electron states of a resistor. The annihilation and creation operators for fermionic particles, such as electrons, obey *anticommutation relations*

$$\{\hat{a}_k, \hat{a}_l^\dagger\} = \delta_{kl}, \quad (3.61)$$

$$\{\hat{a}_k, \hat{a}_l\} = 0. \quad (3.62)$$

The study of such systems is the concern of the rapidly developing field of *mesoscopic electronics* [Dat95, Imr97]. Unfortunately, perturbative master equations might not be appropriate in many situations when charged fermions are involved, since such systems are strongly interacting. However, there are some experiments for which a perturbative master equation is a good approximation. We now consider one of these special cases to illustrate some of the essential differences between bosonic and fermionic environments.

The concept of a mesoscopic electronic system emerged in the 1980s as experiments on small, almost defect-free, conductors and semiconductors revealed unexpected departures from classical current–voltage characteristics at low temperatures. The earliest of these results indicated quantized conductance. The classical description of conductance makes reference to random scattering of carriers due to inelastic collisions. However, in mesoscopic electronic systems, the mean free path for inelastic scattering may be longer than the length of the device. Such systems are dominated by *ballistic* behaviour in which conduction is due to the transport of single carriers, propagating in empty electron states above a filled Fermi sea, with only elastic scattering from confining potentials and interactions with magnetic fields. As Landauer [Lan88, Lan92] and Büttiker [Büt88] first made clear, conductance in such devices is determined not by inelastic scattering, but by the quantum-mechanical transmission probability, T , across device inhomogeneities. If a single ballistic channel supports a single transverse Fermi mode (which comprises two modes when spin is included), the transmission probability is $T \approx 1$. The resulting conductance of that channel is the reciprocal of the *quantum of resistance*. This is given by the Landauer–Büttiker theory as [Dat95]

$$R_Q = \frac{\pi \hbar}{e^2} \approx 12.9 \text{ k}\Omega. \quad (3.63)$$

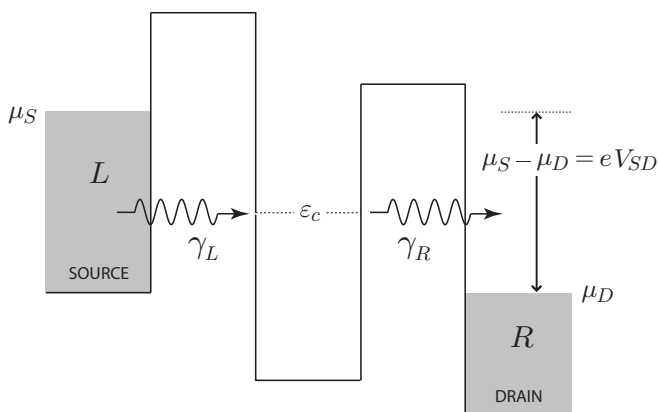


Fig. 3.1 A schematic representation of a quantum dot in the conduction band. Position runs from left to right and energy runs vertically. The quasibound state in the dot is labelled c . The grey regions labelled L and R represent metallic electronic states filled up to the local Fermi level. The difference in the Fermi levels between left and right is determined by the source–drain bias voltage as eV_{SD} .

A quantum dot is a three-dimensional confining potential for electrons or holes in a semiconductor, and can be fabricated in a number of ways [Tur95]. We will consider a very simple model in which the dot has only a single bound state for one electron. This is not as artificial as it may sound. Although a single quantum dot in fact contains a very large number of electrons, at low temperatures this system of electrons is close to the Fermi ground state. In a semiconductor dot the ground state is typically a filled valence band and an unoccupied conduction band. In a metallic dot (or grain as it sometimes called) the ground state is the conduction band filled up to the Fermi energy. At low temperatures and weak bias the current is carried by a few electrons near the Fermi energy and we are typically concerned only with *additional* electrons injected onto the dot. Because electrons are charged, large energy gaps can appear in the spectrum of multi-electron quantum dots, in addition to the quantization of energy levels due to confinement. This phenomenon is called *Coulomb blockade* [Kas93]. The Coulomb blockade energy required to add a single electron to a quantum dot is $e^2/(2C)$, where the capacitance C can be very small (less than 10^{-16} F) due to the small size of these systems. If the charging energy is large enough, compared with thermal energy, we can assume that only a single bound state for an additional electron is accessible in the quantum dot. Typically this would require a temperature below 1 K.

We also assume that the dot is coupled via tunnel junctions to two fermionic reservoirs; see Fig. 3.1. A tunnel junction is a region in the material from which charge carriers classically would be excluded by energy conservation. While propagating solutions of the Schrödinger equation cannot be found in such a region, exponentially decaying amplitudes can exist. We will assume that the region is not so extensive that all amplitudes decay to zero, but small enough for the coupling, due to the overlap of amplitudes inside and outside the region, to be small. In that case the coupling between propagating solutions on either side of the region can be treated perturbatively.

We assume that the reservoirs remain in the normal (Ohmic) conducting state. The total system is not in thermal equilibrium due to the bias voltage V_{SD} across the dot. However, the two reservoirs are held very close to thermal equilibrium at temperature T , but at *different* chemical potentials through contact to an external circuit via an *Ohmic contact*. We refer to the fermionic reservoir with the higher chemical potential as the *source* (also called the emitter) and the one with the lower chemical potential as the *drain* (also called the collector). The difference in chemical potentials is given by $\mu_S - \mu_D = eV_{SD}$. In this circumstance, charge may flow through the dot, and an external current will flow. The necessity to define a chemical potential is the first major difference between fermionic systems and the bosonic environments of quantum optics.

A perturbative master-equation approach to this problem is valid only if the resistance of the tunnel junction, R , is large compared with the quantum of resistance R_Q . The physical meaning of this condition is as follows. If for simplicity we denote the bias voltage of the junction as V , then the average current through the junction is V/R , so the tunnelling rate is $\Gamma = V/(eR)$. Thus the typical time between tunnelling events is $\Gamma^{-1} = eR/V$. Now, if the lifetime of the quasibound state is τ , then, by virtue of the time–energy uncertainty relation discussed in Section 3.3.1, there is an uncertainty in the energy level of order \hbar/τ . If the external potential is to control the tunnelling then this energy uncertainty must remain less than eV . Thus the lifetime must be at least of order $\hbar/(eV)$. If we demand that the lifetime be much less than the time between tunnelling events, so that the events do not overlap in time, we thus require $\hbar/(eV) \ll eR/V$. This gives the above relation between R and the quantum of resistance.

The total Hamiltonian of a system composed of the two Fermi reservoirs, connected by two tunnel barriers to a single Fermi bound state, is (with $\hbar = 1$)

$$\begin{aligned} \hat{H}_{\text{QD+leads}} = & \sum_k \varepsilon_k^S \hat{a}_k^\dagger \hat{a}_k + \varepsilon_c \hat{c}^\dagger \hat{c} + \sum_p \varepsilon_p^D \hat{b}_p^\dagger \hat{b}_p \\ & + \sum_k (T_k^S \hat{c}^\dagger \hat{a}_k + T_k^{S*} \hat{a}_k^\dagger \hat{c}) + \sum_p (T_p^D \hat{b}_p^\dagger \hat{c} + T_p^{D*} \hat{c}^\dagger \hat{b}_p). \end{aligned} \quad (3.64)$$

Here $a_k(a_k^\dagger)$, $c(c^\dagger)$ and $b_p(b_p^\dagger)$ are the fermion annihilation (creation) operators of electrons in the source (S) reservoir, in the central quantum dot and in the drain (D) reservoir, respectively. Because of the fermion anticommutation relations, the dot is described by just two states.

Exercise 3.17 Show from Eqs. (3.61) and (3.62) that the eigenvalues for the fermion number operator $\hat{a}_l^\dagger \hat{a}_l$ are 0 and 1, and that, if the eigenstates are $|0\rangle$ and $|1\rangle$, respectively, then $\hat{a}_l^\dagger |0\rangle = |1\rangle$.

The first three terms in Eq. (3.64) comprise \hat{H}_0 . The energy of the bound state without bias is ε_0 , which under bias becomes $\varepsilon_c = \varepsilon_0 - \alpha eV$, where α is a structure-dependent coefficient. The single-particle energies in the source and drain are, respectively, $\varepsilon_k^S = k^2/(2m)$ and $\varepsilon_p^D = p^2/(2m) - eV$. The energy reference is at the bottom of the conduction

band of the source reservoir. Here, and below, we are assuming spin-polarized electrons so that we do not have to sum over the spin degree of freedom.

The fourth and fifth terms in the Hamiltonian describe the coupling between the quasi-bound electrons in the dot and the electrons in the reservoir. The tunnelling coefficients T_k^S and T_p^D depend upon the profile of the potential barrier between the dot and the reservoirs, and upon the bias voltage. We will assume that at all times the two reservoirs remain in their equilibrium states despite the tunnelling of electrons. This is a defining characteristic of a reservoir, and comes from assuming that the dynamics of the reservoirs are much faster than those of the quasibound quantum state in the dot.

In the interaction frame the Hamiltonian may be written as

$$\hat{V}(t) = \sum_{j=1}^2 \hat{c}^\dagger \hat{\Upsilon}_j(t) e^{i\varepsilon_c t} + \hat{c} \hat{\Upsilon}_j^\dagger(t) e^{-i\varepsilon_c t}, \quad (3.65)$$

where the reservoir operators are given by

$$\hat{\Upsilon}_1(t) = \sum_k T_k^S \hat{a}_k e^{-i\varepsilon_k^S t}, \quad \hat{\Upsilon}_2(t) = \sum_p T_p^D \hat{b}_p e^{-i\varepsilon_p^D t}. \quad (3.66)$$

We now obtain an equation of motion for the state matrix ρ of the bound state in the dot by following the standard method in Section 3.2. The only non-zero reservoir correlation functions we need to compute are

$$I_{jN}(t) = \int_0^t dt_1 \langle \Upsilon_j^\dagger(t) \Upsilon_j(t_1) \rangle e^{-i\varepsilon_c(t-t_1)}, \quad (3.67)$$

$$I_{jA}(t) = \int_0^t dt_1 \langle \Upsilon_j(t_1) \Upsilon_j^\dagger(t) \rangle e^{-i\varepsilon_c(t-t_1)}. \quad (3.68)$$

Here N and A stand for normal (annihilation operators after creation operators) and antinormal (vice versa) ordering of operators – see Section A.5. In order to illustrate the important differences between the fermionic case and the bosonic case discussed previously, we will now explicitly evaluate the first of these correlation functions, $I_{1N}(t)$.

Using the definition of the reservoir operators and the assumed thermal Fermi distribution of the electrons in the source, we find

$$I_{1N}(t) = \sum_k \bar{n}_k^S |T_k^S|^2 \int_0^t dt_1 \exp[i(\varepsilon_k^S - \varepsilon_c)(t - t_1)]. \quad (3.69)$$

Since the reservoir is a large system, we can introduce a density of states $\rho(\omega)$ as usual and replace the sum over k by an integral to obtain

$$I_{1N}(t) = \int_0^\infty d\omega \rho(\omega) \bar{n}^S(\omega) |T^S(\omega)|^2 \int_{-t}^0 d\tau e^{-i(\omega - \varepsilon_c)\tau}, \quad (3.70)$$

where we have also changed the variable of time integration. The dominant term in the frequency integration will come from frequencies near ε_c because the time integration is

significant at that point. For fermionic reservoirs, the expression for the thermal occupation number is [Dat95]

$$\bar{n}^S(\omega) = [1 + e^{(\omega - \omega_f)/k_B T}]^{-1}, \quad (3.71)$$

where ω_f is the Fermi energy (recall that $\hbar = 1$). We assume that the bias is such that the quasibound state of the dot is below the Fermi level in the source. This implies that near $\omega = \varepsilon_c$, and at low temperatures, the average occupation of the reservoir state is very close to unity [Dat95].

Now we make the Markov approximation to derive an autonomous master equation as in Section 3.2. On extending the limits of integration from $-t$ to $-\infty$ in Eq. (3.70) as explained before, I_{1N} may be approximated by the constant

$$I_{1N}(t) \approx \pi \rho(\varepsilon_c) |T_S(\varepsilon_c)|^2 \equiv \gamma_L/2. \quad (3.72)$$

This defines the effective rate γ_L of injection of electrons from the source (the left reservoir in Fig. 3.1) into the quasibound state of the dot. This rate will have a complicated dependence on the bias voltage through both ε_c and the coupling coefficients $|T_S(\omega)|$, which can be determined by a self-consistent band calculation. We do not address this issue; we simply seek the noise properties as a function of the rate constants.

By evaluating all the other correlation functions under similar assumptions, we find that the quantum master equation for the state matrix representing the dot state in the interaction frame is given by

$$\frac{d\rho}{dt} = \frac{\gamma_L}{2} (2\hat{c}^\dagger \rho \hat{c} - \hat{c} \hat{c}^\dagger \rho - \rho \hat{c} \hat{c}^\dagger) + \frac{\gamma_R}{2} (2\hat{c} \rho \hat{c}^\dagger - \hat{c}^\dagger \hat{c} \rho - \rho \hat{c}^\dagger \hat{c}), \quad (3.73)$$

where γ_L and γ_R are constants determining the rate of injection of electrons from the source into the dot and from the dot into the drain, respectively.

From this master equation it is easy to derive the following equation for the mean occupation number $\langle n(t) \rangle = \text{Tr}[\hat{c}^\dagger \hat{c} \rho(t)]$:

$$\frac{d\langle n \rangle}{dt} = \gamma_L (1 - \langle n \rangle) - \gamma_R \langle n \rangle. \quad (3.74)$$

Exercise 3.18 Show this, and show that the steady-state occupancy of the dot is $\langle n \rangle_{ss} = \gamma_L/(\gamma_L + \gamma_R)$.

The effect of Fermi statistics is evident in Eq. (3.74). If there is an electron on the dot, $\langle n \rangle = 1$, and the occupation of the dot can decrease only by emission of an electron into the drain at rate γ_R .

It is at this point that we need to make contact with measurable quantities. In the case of electron transport, the measurable quantities reduce to current $I(t)$ and voltage $V(t)$. The measurement results are a time series of currents and voltages, which exhibit both systematic and stochastic components. Thus $I(t)$ and $V(t)$ are classical conditional stochastic processes, driven by the underlying quantum dynamics of the quasibound state on the dot.

The reservoirs in the Ohmic contacts play a key role in defining the measured quantities and ensuring that they are ultimately classical stochastic processes. Transport through the dot results in charge fluctuations in either the left or the right channel. These fluctuations decay extremely rapidly, ensuring that the channels remain in thermal equilibrium with the respective Ohmic contacts. For this to be possible, charge must be able to flow into and out of the reservoirs from an external circuit.

If a single electron tunnels out of the dot into the drain between time t and $t + dt$, its energy is momentarily above the Fermi energy. This electron scatters very strongly from the electrons in the drain and propagates into the right Ohmic contact, where it is perfectly absorbed. The nett effect is a small current pulse in the external circuit of total charge $e_L = eC_R/(C_L + C_R)$. Here $C_{L/R}$ is the capacitance between the dot and the L/R reservoir, and we have ignored any parasitic capacitance between source and drain. This is completely analogous to perfect photodetection: a photon emitted from a cavity will be detected with certainty by a detector that is a perfect absorber. Likewise, when an electron in the right channel tunnels onto the dot, there is a rapid relaxation of this unfilled state back to thermal equilibrium as an electron is emitted from the right Ohmic contact into the depleted state of the source. This again results in a current pulse carrying charge $e_R = e - e_L$ in the circuit connected to the Ohmic contacts.

The energy gained when one electron is emitted from the left reservoir is, by definition, the chemical potential of that reservoir, μ_L , while the energy lost when one electron is absorbed into the right reservoir is μ_R . The nett energy transferred between reservoirs is $\mu_L - \mu_R$. This energy is supplied by the external voltage, V , and thus $\mu_L - \mu_R = eV$. On average, in the steady state, the same current flows in the source and drain:

$$J_{ss} \equiv e_L \gamma_L (1 - \langle n \rangle_{ss}) + e_R \gamma_R \langle n \rangle_{ss} \quad (3.75)$$

$$= e \gamma_L (1 - \langle n \rangle_{ss}) = e \gamma_R \langle n \rangle_{ss} \quad (3.76)$$

$$= e \frac{\gamma_L \gamma_R}{\gamma_L + \gamma_R}. \quad (3.77)$$

Exercise 3.19 *Verify the identity of these expressions.*

From this we see that the average tunnelling rate of the device, Γ as previously defined, is given by

$$\Gamma = \left(\frac{1}{\gamma_L} + \frac{1}{\gamma_R} \right)^{-1}. \quad (3.78)$$

Typical values for the tunnelling rates achievable in these devices are indicated by results from an experiment by Yacoby *et al.* [YHMS95] in which single-electron transmission through a quantum dot was measured. The quantum dot was defined by surface gates on a GaAs/AlGaAs two-dimensional electron gas. The quantum dot was $0.4 \mu\text{m}$ wide and $0.5 \mu\text{m}$ long and had an electron temperature of 100 mK . They measured a tunnelling rate of order 0.3 GHz .

Box 3.2 Quantum dynamical semigroups

Formally solving the master equation for the state matrix defines a map from the state matrix at time 0 to a state matrix at *later* times t by \mathcal{N}_t : $\rho(0) \rightarrow \rho(t) = \mathcal{N}_t \rho(0)$ for all times $t \geq 0$. This dynamical map must be completely positive (see Box 1.3). More formally, we require a *quantum dynamical semigroup* [AL87], which is a family of completely positive maps \mathcal{N}_t for $t \geq 0$ such that

- $\mathcal{N}_t \mathcal{N}_s = \mathcal{N}_{t+s}$
- $\text{Tr}[(\mathcal{N}_t \rho) \hat{A}]$ is a continuous function of t for any state matrix ρ and Hermitian operator \hat{A} .

The family forms a semigroup rather than a group because there is not necessarily any inverse. That is, \mathcal{N}_t is not necessarily defined for $t < 0$.

These conditions formally capture the idea of Markovian dynamics of a quantum system. (Note that there is no implication that all open-system dynamics must be Markovian.) From these conditions it can be shown that there exists a superoperator \mathcal{L} such that

$$\frac{d\rho(t)}{dt} = \mathcal{L}\rho(t), \quad (3.79)$$

where \mathcal{L} is called the generator of the map \mathcal{N}_t . That is,

$$\rho(t) = \mathcal{N}_t \rho(0) = e^{\mathcal{L}t} \rho(0). \quad (3.80)$$

Moreover, this \mathcal{L} must have the Lindblad form.

3.6 The Lindblad form and positivity

We have seen a number of examples in which the dynamics of an open quantum system can be described by an autonomous differential equation (a time-independent master equation) for the state matrix of the system. What is the most general form that such an equation can take such that the solution is always a valid state matrix? This is a dynamical version of the question answered in Box 1.3 of Chapter 1, which was as follows: what are the physically allowed operations on a state matrix? In fact, the question can be formulated in a way that generalizes the notion of operations to a *quantum dynamical semigroup* – see Box. 3.2

It was shown by Lindblad in 1976 [Lin76] that, for a Markovian master equation $\dot{\rho} = \mathcal{L}\rho$, the generator of the quantum dynamics must be of the form

$$\mathcal{L}\rho = -i[\hat{H}, \rho] + \sum_{k=1}^K \mathcal{D}[\hat{L}_k]\rho, \quad (3.81)$$

for \hat{H} Hermitian and $\{\hat{L}_j\}$ arbitrary operators. Here \mathcal{D} is the superoperator defined earlier in Eq. (3.29). For mathematical rigour [Lin76], it is also required that $\sum_{k=1}^K \hat{L}_k^\dagger \hat{L}_k$ be a bounded operator, but that is often not satisfied by the operators we use, so this requirement is usually ignored. This form is known as the *Lindblad form*, and the operators $\{\hat{L}_k\}$

are called Lindblad operators. The superoperator \mathcal{L} is sometimes called the *Liouvillian* superoperator, by analogy with the operator which generates the evolution of a classical probability distribution on phase space, and the term Lindbladian is also used.

Each term in the sum in Eq. (3.81) can be regarded as an *irreversible channel*. It is important to note, however, that the decomposition of the generator into the Lindblad form is not unique. We can reduce the ambiguity by requiring that the operators $\hat{L}_1, \hat{L}_2, \dots, \hat{L}_k$ be linearly independent. We are still left with the possibility of redefining the Lindblad operators by an arbitrary $K \times K$ unitary matrix T_{kl} :

$$\hat{L}_k \rightarrow \sum_{l=1}^K T_{kl} \hat{L}_l. \quad (3.82)$$

In addition, \mathcal{L} is invariant under c-number shifts of the Lindblad operators, accompanied by a new term in the Hamiltonian:

$$\hat{L}_k \rightarrow \hat{L}_k + \chi_k, \quad \hat{H} \rightarrow \hat{H} - \frac{i}{2} \sum_{k=1}^K (\chi_k^* \hat{L}_k - \text{H.c.}). \quad (3.83)$$

Exercise 3.20 Verify the invariance of the master equation under (3.82) and (3.83).

In the case of a single irreversible channel, it is relatively simple to evaluate the completely positive map $\mathcal{N}_t = \exp(\mathcal{L}t)$ formally as

$$\mathcal{N}_t = \sum_{m=0}^{\infty} \mathcal{N}_t^{(m)}, \quad (3.84)$$

where the operations $\mathcal{N}^{(m)}(t)$ are defined by

$$\begin{aligned} \mathcal{N}_t^{(m)} = & \int_0^t dt_m \int_0^{t_m} dt_{m-1} \cdots \int_0^{t_2} dt_1 \mathcal{S}(t - t_m) \mathcal{X} \\ & \times \mathcal{S}(t_m - t_{m-1}) \mathcal{X} \cdots \mathcal{S}(t_2 - t_1) \mathcal{X} \mathcal{S}(t_1), \end{aligned} \quad (3.85)$$

with $\mathcal{N}_t^{(0)} = \mathcal{S}(t)$. Here the superoperators \mathcal{S} and \mathcal{X} are defined by

$$\mathcal{S}(\tau) = \mathcal{J} \left[e^{-\tau(\hat{H} + \hat{L}^\dagger \hat{L}/2)} \right], \quad (3.86)$$

$$\mathcal{X} = \mathcal{J}[\hat{L}], \quad (3.87)$$

where the superoperator \mathcal{J} is as defined in Eq. (1.80).

Exercise 3.21 Verify the above expression for \mathcal{N}_t by calculating \mathcal{N}_0 and $\dot{\rho}(t)$, where $\rho(t) = \mathcal{N}_t \rho(0)$. Also verify that \mathcal{N}_t is a completely positive map, as defined in Chapter 1.

As we will see in Chapter 4, Eq. (3.85) can be naturally interpreted in terms of a stochastic evolution consisting of periods of smooth evolution, described by $\mathcal{S}(\tau)$, interspersed with jumps, described by \mathcal{X} .

Most of the examples of open quantum systems that we have considered above led, under various approximations, to a Markov master equation of the Lindblad form. However, as

the example of Brownian motion (Section 3.4.2) showed, this is not always the case. It turns out that the time-dependent Brownian-motion master equation (3.58) does preserve positivity. It is only when making the approximations leading to the time-independent, but non-Lindblad, equation (3.60) that one loses positivity. Care must be taken in using master equations such as this, which are not of the Lindblad form, because there are *necessarily* initial states yielding time-evolved states that are non-positive (i.e. are not quantum states at all). Thus autonomous non-Lindblad master equations *must* be regarded as approximations, but, on the other hand, the fact that one has derived a Lindblad-form master equation does not mean that one has an exact solution. The approximations leading to the high-temperature spin-boson master equation (3.56) may be no more valid than those leading to the high-temperature Brownian-motion master equation (3.60), for example. Whether or not a given open system is well approximated by Markovian dynamics can be determined only by a detailed study of the physics.

3.7 Decoherence and the pointer basis

3.7.1 Einselection

We are now in a position to state, and address, one of the key problems of quantum measurement theory: what defines the measured observable? Recall the binary system and binary apparatus introduced in Section 1.2.4. For an arbitrary initial system (S) state, and appropriate initial apparatus (A) state, the final combined state after the measurement interaction is

$$|\Psi'\rangle = \sum_{x=0}^1 s_x |x\rangle |y := x\rangle, \quad (3.88)$$

where $|x\rangle$ and $|y\rangle$ denote the system and apparatus in the *measurement* basis. A measurement of the apparatus in this basis will yield $Y = x$ with probability $|s_x|^2$, that is, with exactly the probability that a direct projective measurement of a physical quantity of the form $\hat{C} = \sum_x c(x) |x\rangle_S \langle x|$ on the system would have given. On the other hand, as discussed in Section 1.2.6, one could make a measurement of the apparatus in some other basis. For example, measurement in a complementary basis $|p\rangle_A$ yields no information about the system preparation at all.

In general one could read out the apparatus in the arbitrary orthonormal basis

$$|\phi_0\rangle = \alpha^* |0\rangle + \beta^* |1\rangle, \quad (3.89)$$

$$|\phi_1\rangle = \beta |0\rangle - \alpha |1\rangle, \quad (3.90)$$

where $|\alpha|^2 + |\beta|^2 = 1$. The state after the interaction between the system and the apparatus can now equally well be written as

$$|\Psi'\rangle = d_0 |\psi_0\rangle_S \otimes |\phi_0\rangle_A + d_1 |\psi_1\rangle_S \otimes |\phi_1\rangle_A, \quad (3.91)$$

where $d_0|\psi_0\rangle_S = \alpha s_0|0\rangle + \beta s_1|1\rangle$ and $d_1|\psi_1\rangle_S = \beta^* s_0|0\rangle - \alpha^* s_1|1\rangle$. Note that $|\psi_0\rangle$ and $|\psi_1\rangle$ are *not orthogonal* if $|\phi_0\rangle$ and $|\phi_1\rangle$ are different from $|0\rangle$ and $|1\rangle$.

Exercise 3.22 Show that this is true except for the special case in which $|s_0| = |s_1|$.

It is apparent from the above that there is only one basis (the measurement basis) in which one should measure the apparatus in order to make an effective measurement of the system observable \hat{C} . Nevertheless, measuring in other bases is equally permitted by the formalism, and yields different sorts of information. This does not seem to accord with our intuition that a particular measurement apparatus is constructed, often at great effort, to measure a particular system quantity. The flaw in the argument, however, is that it is often not possible on physical grounds to read out the apparatus in an arbitrary basis. Instead, there is a preferred apparatus basis, which is determined by the nature of the apparatus and its environment. This has been called the *pointer basis* [Zur81]. For a well-constructed apparatus, the pointer basis will correspond to the measurement basis as defined above.

The pointer basis of an apparatus is determined by how it is built, without reference to any intended measured system to which it may be coupled. One expects the measurement basis of the apparatus, $|0\rangle, |1\rangle$, to correspond to two macroscopic *classically distinguishable* states of a particular degree of freedom of the apparatus. This degree of freedom could, for example, be the position of a pointer, whence the name ‘pointer basis’. An apparatus for which the pointer could be in a superposition of two distinct macroscopic states does not correspond to our intuitive idea of a pointer. Thus we expect that the apparatus can never enter a superposition of two distinct pointer states as Eq. (3.89) would require.

This is a kind of selection rule, called *einselection* (environmentally induced selection) by Zurek [Zur82]. In essence it is justified by an apparatus–environment interaction that very rapidly couples the pointer states to orthogonal environment (E) states:

$$|y\rangle|z := 0\rangle \rightarrow |y\rangle|z := y\rangle_E, \quad (3.92)$$

where here $|z\rangle$ denotes an environment state. This is identical in form to the original system–apparatus interaction. However, the crucial point is that now the total state is

$$|\Psi''\rangle = \sum_{x=0}^1 s_x |x\rangle |y := x\rangle |z := x\rangle. \quad (3.93)$$

If we consider using a different basis $\{|\phi_0\rangle, |\phi_1\rangle\}$ for the apparatus, we find that it is not possible to write the total state in the form of Eq. (3.93). That is,

$$|\Psi''\rangle \neq \sum_{x=0}^1 d_x |\psi_x\rangle_S |\phi_x\rangle_A |\theta_x\rangle_E, \quad (3.94)$$

for any coefficients d_x and states for the system and environment.

Exercise 3.23 Show that this is true except for the special case in which $|s_0| = |s_1|$.

Note that einselection does not solve the quantum measurement problem in that it does not explain how just one of the elements of the superposition in Eq. (3.93) appears to become real, with probability $|s_x|^2$, while the others disappear. The solutions to that problem are outside the scope of this book. What the approach of Zurek and co-workers achieves is to explain why, for macroscopic objects like pointers, some states are preferred over others in that they are (relatively) unaffected by decoherence. Moreover, they have argued plausibly that these states have classical-like properties, such as being localized in phase space. These states are not necessarily orthogonal states, as in the example above, but they are practically orthogonal if they correspond to distinct measurement outcomes [ZHP93].

3.7.2 A more realistic model

The above example is idealized in that we considered only two possible environment states. In reality the pointer may be described by continuous variables such as position. In this case, it is easy to see how physical interactions lead to an approximate process of einselection in the position basis. Most interactions depend upon the position of an object, and the position of a macroscopic object such as a pointer will almost instantaneously become correlated with many degrees of freedom in the environment, such as thermal photons, dust particles and so on. This process of decoherence rapidly destroys any coherence between states of macroscopically different position, but these states of relatively well-defined position are themselves little affected by the decoherence process (as expressed ideally in Eq. (3.92)).

Decoherence in this pointer basis can be reasonably modelled using the Brownian-motion master equation introduced in Section 3.4.2. In this situation, the dominant term in the master equation is the last one (momentum diffusion), so we describe the evolution of the apparatus state by

$$\dot{\rho} = -\gamma\lambda_T^{-2}[\hat{X}, [\hat{X}, \rho]]. \quad (3.95)$$

Here we have used γ for γ_∞ , and λ_T is the thermal de Broglie wavelength, $(2Mk_B T)^{-1/2}$. It is called this because the thermal equilibrium state matrix for a free particle, in the position basis

$$\rho(x, x') = \langle x | \rho | x' \rangle, \quad (3.96)$$

has the form $\rho(x, x') \propto \exp[-(x - x')^2/(4\lambda_T^2)]$. That is, the characteristic coherence length of the quantum ‘waves’ representing the particle (first introduced by de Broglie) is λ_T . In this position basis the above master equation is easy to solve:

$$\rho(x, x'; t) = \exp[-\gamma t(x - x')^2/\lambda_T^2]\rho(x, x'; 0). \quad (3.97)$$

Exercise 3.24 *Show this. Note that this does not give the thermal equilibrium distribution in the long-time limit because the dissipation and free-evolution terms have been omitted.*

Let the initial state for the pointer be a superposition of two states, macroscopically different in position, corresponding to two different pointer readings. Let $2s$ be the separation

of the states, and σ their width. For $s \gg \sigma$, the initial state matrix can be well approximated by

$$\rho(x, x'; 0) = (1/2)[\psi_-(x) + \psi_+(x)][\psi_-^*(x') + \psi_+^*(x')], \quad (3.98)$$

where

$$\psi_{\pm}(x) = (2\pi\sigma^2)^{-1/4} \exp[-(x \mp s)^2/(2\sigma^2)]. \quad (3.99)$$

That is, $\rho(x, x'; 0)$ is a sum of four equally weighted bivariate Gaussians, centred in (x, x') -space at $(-s, -s)$, $(-s, s)$, $(s, -s)$ and (s, s) . But the effect of the decoherence (3.95) on these four peaks is markedly different. The off-diagonal ones will decay rapidly, on a time-scale

$$\tau_{\text{dec}} = \gamma^{-1} \left(\frac{\lambda_T}{2s} \right)^2. \quad (3.100)$$

For $s \gg \lambda_T$, as will be the case in practice, this decoherence time is much smaller than the dissipation time,

$$\tau_{\text{diss}} = \gamma^{-1}. \quad (3.101)$$

The latter will also correspond to the time-scale on which the on-diagonal peaks in $\rho(x, x')$ change shape under Eq. (3.97), provided that $\sigma \sim \lambda_T$. This seems a reasonable assumption, since one would wish to prepare a well-localized apparatus (small σ), but if $\sigma \ll \lambda_T$ then it would have a kinetic energy much greater than the thermal energy $k_B T$ and so would dissipate energy at rate γ anyway.

The above analysis shows that, under reasonable approximations, the coherences (the off-diagonal terms) in the state matrix decay much more rapidly than the on-diagonal terms change. Thus the superposition is transformed on a time-scale t , such that $\tau_{\text{dec}} \ll t \ll \tau_{\text{diss}}$, into a mixture of pointer states:

$$\rho(x, x'; t) \approx (1/2)[\psi_-(x)\psi_-^*(x') + \psi_+(x)\psi_+^*(x)]. \quad (3.102)$$

Moreover, for macroscopic systems this time-scale is very short. For example, if $s = 1$ mm, $T = 300$ K, $M = 1$ g and $\gamma = 0.01$ s⁻¹, one finds (upon restoring \hbar where necessary) $\tau_{\text{dec}} \sim 10^{-37}$ s, an extraordinarily short time. On such short time-scales, it could well be argued that the Brownian-motion master equation is not valid, and that a different treatment should be used (see for example Ref. [SHB03]). Nevertheless, this result can be taken as indicative of the fact that there is an enormous separation of time-scales between that on which the pointer is reduced to a mixture of classical states and the time-scale on which those classical states evolve.

3.8 Preferred ensembles

In the preceding section we argued that the interaction of a macroscopic apparatus with its environment preserves classical states and destroys superpositions of them. From the simple model of apparatus–environment entanglement in Eq. (3.92), and from the solution

to the (cut-down) Brownian-motion master equation (3.97), it is seen that the state matrix becomes diagonal in this pointer basis. Moreover, from Eq. (3.92), the environment carries the information about which pointer state the system is in. Any additional evolution of the apparatus (such as that necessary for it to measure the system of interest) could cause transitions between pointer states, but again this information would also be carried in the environment so that at all times an observer could know where the apparatus is pointing, so to speak.

It would be tempting to conclude from the above examples that all one need do to find out the pointer basis for a given apparatus is to find the basis which diagonalizes its state once it has reached equilibrium with its environment. However, this is *not* the case, for two reasons. The first reason is that the states forming the diagonal basis are not necessarily states that are relatively unaffected by the decoherence process. Rather, as mentioned above, the latter states will in general be non-orthogonal. In that case the preferred representation of the equilibrium state matrix

$$\rho_{ss} = \sum_k \wp_k \hat{\pi}_k \quad (3.103)$$

will be in terms of an ensemble $E = \{\wp_k, \hat{\pi}_k\}$ of pure states, with positive weights \wp_k , represented by non-orthogonal projectors: $\hat{\pi}_j \hat{\pi}_k \neq \delta_{jk} \hat{\pi}_k$. The second reason, which is generally ignored in the literature on decoherence and the pointer basis, is that the mere fact that the state of a system becomes diagonal in some basis, through entanglement with its environment, does not mean that by observing the environment one can find the system to be always in one of those diagonal states. Once again, it may be that one has to consider non-orthogonal ensembles, as in Eq. (3.103), in order to find a set of states that allows a classical description of the system. By this we mean that the system can be always known to be in one of those states, but to make transitions between them.

The second point above is arguably the more fundamental one for the idea that decoherence explains the emergence of classical behaviour. That is, the basic idea of einselection is that there is a preferred ensemble for ρ_{ss} for which an ignorance interpretation holds. With this interpretation of Eq. (3.103) one would claim that the system ‘really’ is in one of the pure states $\hat{\pi}_k$, but that one happens to be ignorant of which $\hat{\pi}_k$ (i.e. which k) pertains. The weight \wp_k would be interpreted as the probability that the system has state $\hat{\pi}_k$. For this to hold, it is necessary that in principle an experimenter could know *which* state $\hat{\pi}_k$ the system is in at all times by performing continual measurements on the environment with which the system interacts. The pertinent index k would change stochastically such that the proportion of time for which the system has state $\hat{\pi}_k$ is \wp_k . This idea was first identified in Ref. [WV98]. The first point in the preceding paragraph then says that the states in the preferred ensemble should also be robust in the face of decoherence. For example, if the decoherence is described by a Lindbladian \mathcal{L} then one could use the criterion adopted in Ref. [WV98]. This is that the average fidelity

$$F(t) = \sum_k \wp_k \text{Tr}[\hat{\pi}_k \exp(\mathcal{L}t) \hat{\pi}_k] \quad (3.104)$$

should have a characteristic decay time that is as long as possible (and, for macroscopic systems, one hopes that this is much longer than that of a randomly chosen ensemble).

In the remainder of this section we are concerned with elucidating when an ignorance interpretation of an ensemble representing ρ_{ss} is possible. As well as being important in understanding the role of decoherence, it is also relevant to quantum control, as will be discussed in Chapter 6. Let us restrict the discussion to Lindbladians having a unique stationary state defined by

$$\mathcal{L}\rho_{ss} = 0. \quad (3.105)$$

Also, let us consider only *stationary ensembles* for ρ_{ss} . Clearly, once the system has reached steady state such a stationary ensemble will represent the system *for all times* t . Then, as claimed above, it can be proven that for some ensembles (and, in particular, often for the orthogonal ensemble) there is no way for an experimenter continually to measure the environment so as to find out which state the system is in. We say that such ensembles are not *physically realizable* (PR). However, there are other stationary ensembles that *are* PR.

3.8.1 Quantum steering

To appreciate physical realizability of ensembles, it is first necessary to understand a phenomenon discovered by Schrödinger [Sch35a] and described by him as ‘steering’³ (we will call it quantum steering). This phenomenon was rediscovered (and generalized) by Hughston, Jozsa and Wootters [HJW93]. Consider a system with state matrix ρ that is mixed solely due to its entanglement with a second system, the environment. That is, there is a pure state $|\Psi\rangle$ in a larger Hilbert space of system plus environment such that

$$\rho = \text{Tr}_{\text{env}}[|\Psi\rangle\langle\Psi|]. \quad (3.106)$$

This purification always exists, as discussed in Section A.2.2. Then, for any ensemble $\{(\hat{\pi}_k, \wp_k)\}_k$ that represents ρ , it is possible to measure the environment such that the system state is collapsed into one of the pure states $\hat{\pi}_k$ with probability \wp_k . This is sometimes known as the Schrödinger–HJW theorem.

Quantum steering gives rigorous meaning to the ignorance interpretation of any particular ensemble. It says that there will be a way to perform a measurement on the environment, without disturbing the system state on average, to obtain exactly the information as to which state the system is ‘really’ in. Of course, the fact that one can do this for any ensemble means that no ensemble can be fundamentally preferred over any other one, as a representation of ρ at *some particular time* t . To say that an ensemble is PR, however, requires justifying the ignorance interpretation at *all times* (after the system has reached steady state). We now establish the conditions for an ensemble to be PR.

³ Schrödinger introduced this as an evocative term for the Einstein–Podolsky–Rosen effect [EPR35] involving entangled states. For a completely general formulation of steering in quantum information terms, see Refs. [WJD07, JWD07].

3.8.2 Conditions for physical realizability

According to quantum steering, it is always possible to realize a given ensemble at some particular time t by measuring the environment. This may involve measuring parts of the environment that interacted with the system an arbitrarily long time ago, but there is nothing physically impossible in doing this. Now consider the future evolution of a particular system state $\hat{\pi}_k$ following this measurement. At time $t + \tau$, it will have evolved to $\rho_k(t + \tau) = \exp(\mathcal{L}\tau)\hat{\pi}_k$. This is a mixed state because the system has now become re-entangled with its environment.

The system state can be repurified by making another measurement on its environment. However, if the same ensemble is to remain as our representation of the system state then the pure system states obtained as a result of this measurement at time $t + \tau$ must be contained in the set $\{\hat{\pi}_j : j\}$. Because of quantum steering, this will be possible if and only if $\rho_k(t + \tau)$ can be represented as a mixture of these states. That is, for all k there must exist a probability distribution $\{w_{jk}(\tau) : j\}$ such that

$$\exp(\mathcal{L}\tau)\hat{\pi}_k = \sum_j w_{jk}(\tau)\hat{\pi}_j. \quad (3.107)$$

If $w_{jk}(\tau)$ exists then it is the probability that the measurement at time $t + \tau$ yields the state $\hat{\pi}_j$.

Equation (3.107) is a necessary but not sufficient criterion for the ensemble $\{(\hat{\pi}_j, \wp_j) : j\}$ to be PR. We also require that the weights be stationary. That is, for all j and all τ ,

$$\wp_j = \sum_k \wp_k w_{jk}(\tau). \quad (3.108)$$

Multiplying both sides of Eq. (3.107) by \wp_k , and summing over k , then using Eq. (3.108) and Eq. (3.103) gives $e^{\mathcal{L}\tau}\rho_{ss} = \rho_{ss}$, as required from the definition of ρ_{ss} .

One can analyse these conditions further to obtain simple criteria that can be applied in many cases of interest [WV01]. In particular, we will return to them in Chapter 6. For the moment, it is sufficient to prove that there are some ensembles that are PR and some that are not. This is what was called in Ref. [WV01] the *preferred-ensemble fact* (the ‘preferred’ ensembles are those that are physically realizable). Moreover, for some systems the orthogonal ensemble is PR and for others it is not. The models we consider are chosen for their simplicity (they are two-level systems), and are not realistic models for the decoherence of a macroscopic apparatus.

3.8.3 Examples

First we consider an example in which the orthogonal ensemble is PR: the high temperature spin–boson model. In suitably scaled time units, the Lindbladian in Eq. (3.56) is $\mathcal{L} = \mathcal{D}[\hat{\sigma}_z]$. In this example, there is no unique stationary state, but all stationary states are of the form

$$\rho_{ss} = \wp_- |\sigma_z := -1\rangle\langle\sigma_z := -1| + \wp_+ |\sigma_z := 1\rangle\langle\sigma_z := 1|. \quad (3.109)$$

Exercise 3.25 *Show this.*

The orthogonal ensemble thus consists of the $\hat{\sigma}_z$ eigenstates with weights \wp_{\pm} . To determine whether this ensemble is PR, we must consider the evolution of its members under the Lindbladian. It is trivial to show that $\mathcal{L}|\sigma_z := \pm 1\rangle\langle\sigma_z := \pm 1| = 0$ so that these states do not evolve at all. In other words, they are perfectly robust, with $w_{jk}(\tau) = \delta_{jk}$ in Eq. (3.107). It is easy to see that Eq. (3.108) is also satisfied, so that the orthogonal ensemble is PR.

Next we consider an example in which the orthogonal ensemble is not PR: the driven, damped two-level atom. In the zero-detuning and zero-temperature limit, the Lindbladian is defined by

$$\mathcal{L}\rho = -i\frac{\Omega}{2}[\hat{\sigma}_x, \rho] + \gamma\mathcal{D}[\hat{\sigma}_-]\rho. \quad (3.110)$$

The general solution of the corresponding Bloch equations is

$$x(t) = ue^{-(\gamma/2)t}, \quad (3.111)$$

$$y(t) = c_+e^{\lambda_+t} + c_-e^{\lambda_-t} + y_{ss}, \quad (3.112)$$

$$z(t) = c_+\frac{\gamma - 4i\tilde{\Omega}}{4\Omega}e^{\lambda_+t} + c_-\frac{\gamma + 4i\tilde{\Omega}}{4\Omega}e^{\lambda_-t} + z_{ss}, \quad (3.113)$$

with eigenvalues defined by

$$\lambda_{\pm} = -\frac{3}{4}\gamma \pm i\tilde{\Omega} \quad (3.114)$$

and c_{\pm} are constants given by

$$c_{\pm} = \frac{1}{8i\tilde{\Omega}}[\mp 4\Omega(w - z_{ss}) \pm (\gamma \pm 4i\tilde{\Omega})(v - y_{ss})], \quad (3.115)$$

where u , v and w are used to represent the initial conditions of x , y and z . A modified Rabi frequency has been introduced,

$$\tilde{\Omega} = \sqrt{\Omega^2 - (\gamma/4)^2}, \quad (3.116)$$

which is real for $\Omega > \gamma/4$ and imaginary for $\Omega < \gamma/4$. The steady-state solutions are $x_{ss} = 0$, $y_{ss} = 2\Omega\gamma/(\gamma^2 + 2\Omega^2)$ and $z_{ss} = -\gamma^2/(\gamma^2 + 2\Omega^2)$, as shown in Exercise 3.10.

Exercise 3.26 *Derive the above solution, using standard techniques for linear differential equations.*

In the Bloch representation, the diagonal states of ρ_{ss} are found by extending the stationary Bloch vector forwards and backwards to where it intersects the surface of the Bloch sphere. That is, the two pure diagonal states are

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{\pm} = \begin{pmatrix} 0 \\ \pm 2\Omega \\ \mp \gamma \end{pmatrix} (4\Omega^2 + \gamma^2)^{-1/2}. \quad (3.117)$$

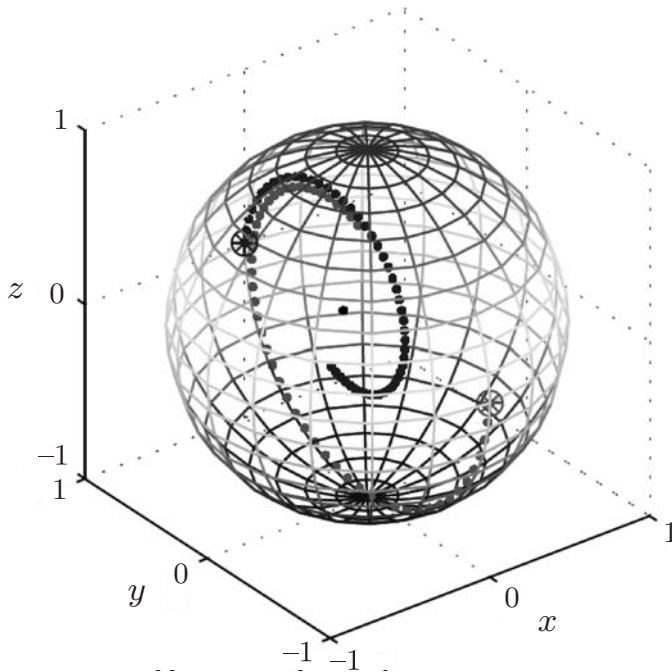


Fig. 3.2 Dynamics of two states on the Bloch sphere according to the master equation (3.110), for $\Omega = 10\gamma$, with points every $0.1\gamma^{-1}$. The initial states are those that diagonalize the stationary Bloch sphere, which are close to $y = \pm 1$. The stationary state is the dot close to the centre of the Bloch sphere.

Using these as initial conditions, it is easy to prove that, for general t ,

$$\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix}_{\pm} \neq w_{\pm+}(t) \begin{pmatrix} u \\ v \\ w \end{pmatrix}_{+} + w_{\pm-}(t) \begin{pmatrix} u \\ v \\ w \end{pmatrix}_{-} \quad (3.118)$$

for any weights $w_{\pm+}(t)$, $w_{\pm-}(t)$. That is, the diagonal states evolve into states that are not mixtures of the original diagonal states, so it is not possible for an observer to know at all times that the system is in a diagonal state. The orthogonal ensemble is not PR. This is illustrated in Fig. 3.2.

There are, however, *non-orthogonal* ensembles that *are* PR for this system. Moreover, there is a PR ensemble with just two members, like the orthogonal ensemble. This is the ensemble $\{(\hat{\pi}_{+}, 1/2), (\hat{\pi}_{-}, 1/2)\}$, where this time the two states have the Bloch vectors

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{\pm} = \begin{pmatrix} \pm\sqrt{1 - y_{ss}^2 - z_{ss}^2} \\ y_{ss} \\ z_{ss} \end{pmatrix}. \quad (3.119)$$

Using these as initial conditions, we find

$$\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix}_{\pm} = \begin{pmatrix} u_{\pm} e^{-\gamma t/2} \\ y_{ss} \\ z_{ss} \end{pmatrix}. \quad (3.120)$$

Obviously this *can* be written as a positively weighted sum of the two initial Bloch vectors, and averaging over the two initial states will give a sum that remains equal to the stationary Bloch vector. That is, the two conditions (3.107) and (3.108) are satisfied, and this ensemble is PR.

Exercise 3.27 *Prove the above by explicitly constructing the necessary weights $w_{\pm+}(t)$ and $w_{\pm-}(t)$.*

These results are most easily appreciated in the $\Omega \gg \gamma$ limit. Then the stationary solution is an almost maximally mixed state, displaced slightly from the centre of the Bloch sphere along the y axis. The diagonal states then are close to $\hat{\sigma}_y$ eigenstates, while the states in the PR ensemble are close to $\hat{\sigma}_x$ eigenstates. In this limit the master-equation evolution (3.110) is dominated by the Hamiltonian term, which causes the Bloch vector to rotate around the $\hat{\sigma}_x$ axis. Thus, the y eigenstates are rapidly rotated away from their original positions, so this ensemble is neither robust nor PR, but the x eigenstates are not rotated at all, and simply decay at rate $\gamma/2$ towards the steady state, along the line joining them. Thus this ensemble is PR. Moreover, it can be shown [WB00] that this is the most robust ensemble according to the fidelity measure Eq. (3.104), with a characteristic decay time (half-life) of $2 \ln 2/\gamma$. These features are shown in Fig. 3.3.

The existence of a PR ensemble in this second case (where the simple picture of a diagonal pointer basis fails) is not happenstance. For any master equation there are in fact infinitely many PR ensembles. Some of these will be robust, and thus could be considered pointer bases, and some will not. A full understanding of how PR ensembles arise will be reached in Chapter 4, where we consider the conditional dynamics of a continuously observed open system.

3.9 Decoherence in a quantum optical system

3.9.1 Theoretical analysis

In recent years the effects of decoherence have been investigated experimentally, most notably in a quantum optical (microwave) cavity [BHD⁺96]. To appreciate this experiment, it is necessary to understand the effect of damping of the electromagnetic field in a cavity at zero temperature on a variety of initial states. This can be described by the interaction-frame master equation, Eq. (3.38):

$$\dot{\rho} = \gamma \mathcal{D}[\hat{a}]\rho. \quad (3.121)$$

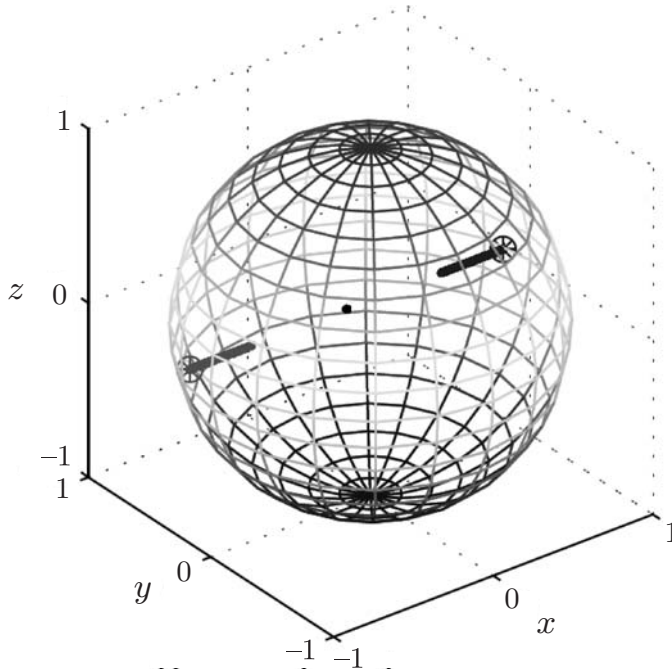


Fig. 3.3 Dynamics of two states on the Bloch sphere according to the master equation (3.110), for $\Omega = 10\gamma$, with points every $0.1\gamma^{-1}$. The initial states are the two non-orthogonal states $\hat{\pi}_{\pm}$ defined in Eq. (3.119), which are close to $x = \pm 1$. The stationary state is the dot close to the centre of the Bloch sphere.

If we use the solution given in Eq. (3.85) we find that the general solution can be written as a Kraus sum,

$$\rho(t) = \sum_{m=0}^{\infty} \hat{M}_m(t) \rho(0) \hat{M}_m^{\dagger}(t), \quad (3.122)$$

where

$$\hat{M}_m(t) = \frac{(1 - e^{-\gamma t})^{m/2}}{\sqrt{m!}} e^{-\gamma t \hat{a}^{\dagger} \hat{a}/2} \hat{a}^m. \quad (3.123)$$

We can regard this as an expansion of the state matrix in terms of the number of photons *lost* from the cavity in time t .

Exercise 3.28 Prove Eq. (3.122) by simplifying Eq. (3.85) using the property that $[\hat{a}^{\dagger} \hat{a}, \hat{a}^{\dagger}] = \hat{a}^{\dagger}$.

Equation (3.122) can be solved most easily in the number-state basis. However, it is rather difficult to prepare a simple harmonic oscillator in a number eigenstate. We encounter simple harmonic oscillators regularly in classical physics; springs, pendula, cantilevers etc. What type of state describes the kinds of motional states in which such oscillators are

typically found? We usually identify simple harmonic motion by observing oscillations. In the presence of friction oscillatory motion will decay. To observe a sustained oscillation, we need to provide a driving force to the oscillator. This combination of driving and friction reaches a steady state of coherent oscillation. In classical physics the resulting motion will have a definite energy, so one might expect that this would be a means of preparing a quantum oscillator in an energy eigenstate. However, a number state is actually time-independent, so this cannot be so. Quantum mechanically, the state produced by this mechanism does not have a definite energy. For weakly damped oscillators (as in quantum optics), it is actually a coherent state, as shown in Exercise 3.13. For the reasons just described, the coherent state is regarded as the most classical state of motion for a simple harmonic oscillator. It is often referred to as a *semiclassical* state. Another reason why coherent states are considered classical-like is their robustness with respect to the decoherence caused by damping.

Exercise 3.29 From Eq. (3.122) show that, for a damped harmonic oscillator in the interaction frame, a coherent state simply decays exponentially. That is, if $|\psi(0)\rangle = |\alpha\rangle$ then $|\psi(t)\rangle = |\alpha e^{-\gamma t/2}\rangle$.

Hint: Consider the effect of $\hat{M}_m(t)$ on a coherent state, using the fact that $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ and also using the number-state expansion for $|\alpha\rangle$.

Suppose we somehow managed to prepare a cavity field in a superposition of two coherent states,

$$|\psi(0)\rangle = N(|\alpha\rangle + |\beta\rangle), \quad (3.124)$$

where the normalization constant is $N^{-1} = \sqrt{2 + 2\text{Re}\langle\alpha|\beta\rangle}$. If $|\alpha - \beta| \gg 1$ then this corresponds to a superposition of macroscopically different fields. Such a superposition is often called a *Schrödinger-cat* state, after the thought experiment invented by Schrödinger which involves a superposition of a live cat and a dead cat [Sch35b].

We now show that such a superposition is very fragile with respect to even a very small amount of damping. Using the solution (3.122), the state will evolve to

$$\begin{aligned} \rho(t) \propto & |\alpha(t)\rangle\langle\alpha(t)| + |\beta(t)\rangle\langle\beta(t)| \\ & + C(\alpha, \beta, t)|\alpha(t)\rangle\langle\beta(t)| + C^*(\alpha, \beta, t)|\beta(t)\rangle\langle\alpha(t)|, \end{aligned} \quad (3.125)$$

where $\alpha(t) = \alpha e^{-\gamma t/2}$, $\beta(t) = \beta e^{-\gamma t/2}$ and

$$C(\alpha, \beta, t) = \exp\left\{-\frac{1}{2} \left[|\alpha(t)|^2 + |\beta(t)|^2 - 2\alpha(t)\beta^*(t) \right] (1 - e^{\gamma t}) \right\}. \quad (3.126)$$

Exercise 3.30 Show this, by the same method as in Exercise 3.29.

The state (3.125) is a superposition of two damped coherent states with amplitudes $\alpha(t)$ and $\beta(t)$ with a suppression of coherence between the states through the factor $C(\alpha, \beta, t)$. Suppose we now consider times much shorter than the inverse of the amplitude decay rate, $\gamma t \ll 1$. The coherence-suppression factor is then given by

$$C(\alpha, \beta, t) \approx \exp(-|\alpha - \beta|^2 \gamma t/2). \quad (3.127)$$

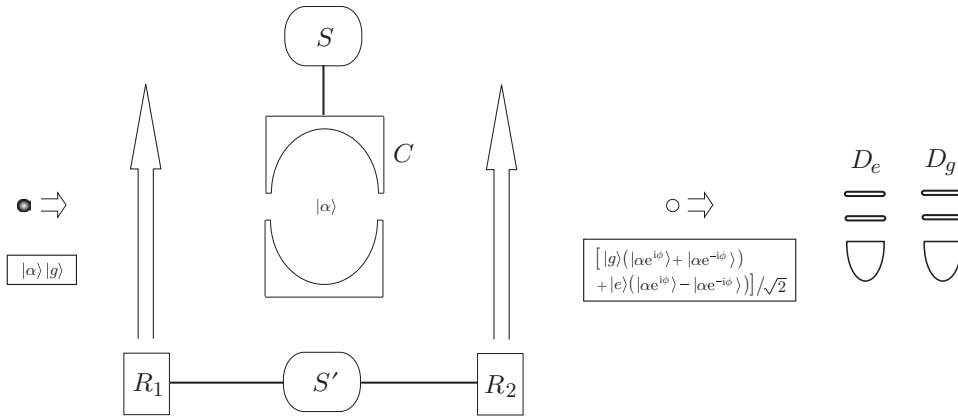


Fig. 3.4 A schematic diagram of the experiment performed by the Haroche group to investigate the decoherence of oscillator coherent states. The atom is prepared in an appropriate Rydberg state. The cavities R_1 and R_2 each apply a $\pi/2$ pulse. The interaction with the cavity field in C produces superpositions of coherent states. The final ionization detectors determine the atomic state of the atom. Figure 2 adapted with permission from M. Brune *et al.*, *Phys. Rev. Lett.* **77**, 4887, (1996). Copyrighted by the American Physical Society.

We thus see that at the very beginning the coherence does not simply decay at the same rate as the amplitudes, but rather at a decay rate that depends quadratically on the difference between the amplitudes of the initial superposed states. This is qualitatively the same as was seen for Brownian motion in Section 3.7.2. For macroscopically different states ($|\alpha - \beta| \gg 1$) the decoherence is very rapid. Once the coherence between the two states has become very small we can regard the state as a statistical mixture of the two coherent states with exponentially decaying coherent amplitudes. The quantum character of the initial superposition is rapidly lost and for all practical purposes we may as well regard the initial state as a classical statistical mixture of the two ‘pointer states’. For this reason it is very hard to prepare an oscillator in a Schrödinger-cat state. However, the decoherence we have described has been observed experimentally for $|\alpha - \beta| \sim 1$.

3.9.2 Experimental observation

The experimental demonstration of the fast decay of coherence for two superposed coherent states was first performed by the Haroche group in Paris using the cavity QED system of Rydberg atoms in microwave cavities [BHD⁺96]. The experiment is based on Ramsey fringe interferometry (see Box 1.4). A schematic diagram of the experiment is shown in Fig. 3.4.

A two-level atomic system with ground state $|g\rangle$ and excited state $|e\rangle$ interacts with a cavity field in C . This cavity field is well detuned from the atomic resonance. The ground and excited states of the atom correspond to Rydberg levels with principal quantum numbers 50 and 51. Such highly excited states have very large dipole moments and can

thus interact very strongly with the cavity field even though it is well detuned from the cavity resonance. The effect of the detuned interaction is to change the phase of the field in the cavity. However, the sign of the phase shift is opposite for each of the atomic states. Using second-order perturbation theory, an effective Hamiltonian for this interaction can be derived:

$$\hat{H}_C = \chi \hat{a}^\dagger \hat{a} \hat{\sigma}_z, \quad (3.128)$$

where $\hat{\sigma}_z = |e\rangle\langle e| - |g\rangle\langle g|$, and $\chi = |\Omega|^2/(2\delta)$, where Ω is the single-photon Rabi frequency and $\delta = \omega_a - \omega_c$ is the atom–cavity detuning. Thus decreasing the detuning increases χ (which is desirable), but the detuning cannot be decreased too much or the description in terms of this effective interaction Hamiltonian becomes invalid.

Assume to begin that the cavity fields R_1 and R_2 in Fig. 3.4 above are resonant with the atomic transition. Say the cavity C is initially prepared in a weakly coherent state $|\alpha\rangle$ (in the experiment $|\alpha| = 3.1$) and the atom in the state $(|g\rangle + |e\rangle)/\sqrt{2}$, using a $\pi/2$ pulse in cavity R_1 . Then in time τ the atom–cavity system will evolve under the Hamiltonian (3.128) to

$$|\psi(\tau)\rangle = \frac{1}{\sqrt{2}}(|g\rangle|\alpha e^{i\phi}\rangle + |e\rangle|\alpha e^{-i\phi}\rangle), \quad (3.129)$$

where $\phi = \chi\tau/2$.

Exercise 3.31 *Verify this.*

The state in Eq. (3.129) is an entangled state between a two-level system and an oscillator. Tracing over the atom yields a field state that is an equal mixture of two coherent states separated in phase by 2ϕ .

To obtain a state that correlates the atomic energy levels with coherent superpositions of coherent states, the atom is subjected to another $\pi/2$ pulse in cavity R_2 . This creates the final state

$$|\psi\rangle_{\text{out}} = \frac{1}{\sqrt{2}}[|g\rangle(|\alpha e^{i\phi}\rangle + |\alpha e^{-i\phi}\rangle) + |e\rangle(|\alpha e^{i\phi}\rangle - |\alpha e^{-i\phi}\rangle)]. \quad (3.130)$$

If one now determines that the atom is in the state $|g\rangle$ at the final ionization detectors, the conditional state of the field is

$$|\psi^g\rangle_{\text{out}} = N_+(|\alpha e^{i\phi}\rangle + |\alpha e^{-i\phi}\rangle), \quad (3.131)$$

where N_+ is a normalization constant. Likewise, if the atom is detected in the excited state,

$$|\psi^e\rangle_{\text{out}} = N_- (|\alpha e^{i\phi}\rangle - |\alpha e^{-i\phi}\rangle). \quad (3.132)$$

These conditional states are superpositions of coherent states.

In the preceding discussion we ignored the cavity decay since this is small on the time-scale of the interaction between a single atom and the cavity field. In order to see the effect of decoherence, one can use the previous method to prepare the field in a coherent superposition of coherent states and then let it evolve for a time T so that there is a significant probability that at least one photon is lost from the cavity. One then needs to probe the

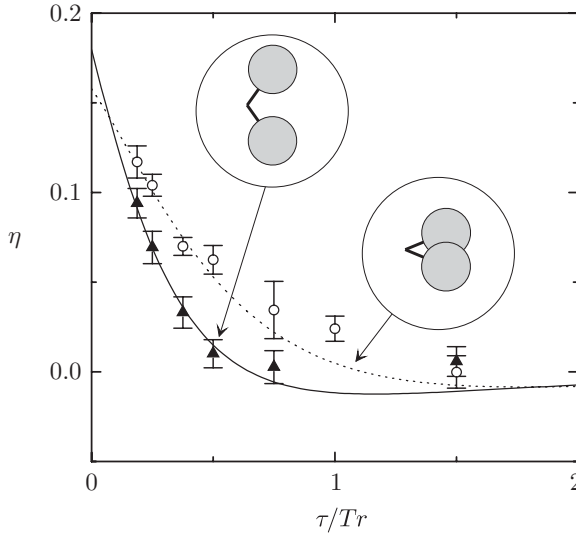


Fig. 3.5 A plot of the two-atom correlation η versus the delay time between successive atoms for two different values of the conditional phase shift. Figure 5(b) adapted with permission from M. Brune *et al.*, *Phys. Rev. Lett.* **77**, 4887, (1996). Copyrighted by the American Physical Society.

decohered field state. It is impossible to measure directly the state of a microwave cavity field at the quantum level because of the low energy of microwave photons compared with optical photons. Instead the Haroche team used a second atom as a probe for the field state. They then measured the state of the second atom, obtaining the conditional probabilities $p(e|g)$ and $p(e|e)$ (where the conditioning label refers to the result of the first atom measurement). Since the respective conditional field states after the first atom are different, these probabilities should be different. The extent of the difference is given by

$$\eta = p(e|e) - p(e|g). \quad (3.133)$$

From the result (3.125), after a time τ the two conditional states will have decohered to

$$\begin{aligned} \rho_{\text{out}}^g(\tau) \propto & (|\alpha_\tau e^{i\phi}\rangle\langle\alpha_\tau e^{i\phi}| + |\alpha_\tau e^{-i\phi}\rangle\langle\alpha_\tau e^{-i\phi}|) \\ & \pm (C(\tau)|\alpha_\tau e^{i\phi}\rangle\langle\alpha_\tau e^{-i\phi}| + C(\tau)^*|\alpha_\tau e^{-i\phi}\rangle\langle\alpha_\tau e^{i\phi}|), \end{aligned} \quad (3.134)$$

where $\alpha_\tau < \alpha$ due to decay in the coherent amplitude and $|C(\tau)| < 1$ due to the decay in the coherences as before. In the limit $C(\tau) \rightarrow 0$, these two states are indistinguishable and so $\eta \rightarrow 0$. Thus, by repeating a sequence of double-atom experiments, the relevant conditional probabilities may be sampled and a value of η as a function of the delay time can be determined. (In the experiment, an extra averaging was performed to determine η , involving detuning the cavities R_1 and R_2 from atomic resonance ω_0 by a varying amount Δ .)

In Fig. 3.5 we reproduce the results of the experimental determination of η for two different values of the conditional phase shift, ϕ , as a function of the delay time τ in units

of cavity relaxation lifetime $T_r = 1/\gamma$. As expected, the correlation signal decays to zero. Furthermore, it decays to zero more rapidly for larger conditional phase shifts. That is to say, it decays to zero more rapidly when the superposed states are further apart in phase-space. The agreement with the theoretical result is very good.

3.10 Other examples of decoherence

3.10.1 Quantum electromechanical systems

We now consider a simple model of a measured system in which the apparatus undergoes decoherence due to its environment. In the model the measured system is a two-level system (with basis states $|0\rangle$ and $|1\rangle$) while the apparatus is a simple harmonic oscillator, driven on resonance by a classical force. The coupling between the two-level system and the oscillator is assumed to change the frequency of the oscillator. The effective Hamiltonian for the system plus apparatus in the interaction frame is

$$\hat{H} = \epsilon(\hat{a}^\dagger + \hat{a}) + \chi \hat{a}^\dagger \hat{a} \hat{\sigma}_z, \quad (3.135)$$

where ϵ is the strength of the resonant driving force and χ is the strength of the coupling between the oscillator and the two-level system. The irreversible dynamics of the apparatus is modelled using the weak-damping, zero-temperature master equation of Eq. (3.121), giving the master equation

$$\dot{\rho} = -i\epsilon[\hat{a} + \hat{a}^\dagger, \rho] - i\chi[\hat{a}^\dagger \hat{a} \hat{\sigma}_z, \rho] + \gamma \mathcal{D}[\hat{a}]\rho. \quad (3.136)$$

There are numerous physical problems that could be described by this model. It could represent a two-level electric dipole system interacting with an electromagnetic cavity field that is far detuned, as can occur in cavity QED (see the preceding Section 3.9.2) and circuit QED (see the following Section 3.10.2). Another realization comes from the rapidly developing field of quantum electromechanical systems, as we now discuss.

Current progress in the fabrication of nano-electromechanical systems (NEMSs) will soon yield mechanical oscillators with resonance frequencies close to 1 GHz, and quality factors Q above 10^5 [SR05]. (The quality factor is defined as the ratio of the resonance frequency ω_0 to the damping rate γ .) At that scale, a NEMS oscillator becomes a quantum electromechanical system (QEMS). One way to define the quantum limit is for the thermal excitation energy to be less than the energy gap between adjacent oscillator energy eigenstates: $\hbar\omega_0 > k_B T$. This inequality would be satisfied by a factor of two or so with a device having resonance frequency $\omega_0 = 1 \times 2\pi$ GHz and temperature of $T_0 = 20$ mK.

In this realization, the two-level system or qubit could be a solid-state double-well structure with a single electron tunnelling between the wells (quantum dots). We will model this as an approximate two-state system. It is possible to couple the quantum-electromechanical oscillator to the charge state of the double dot via an external voltage gate. A possible device is shown in Fig. 3.6. The two wells are at different distances from the voltage gate and this distance is modulated as the oscillator moves. The electrostatic energy

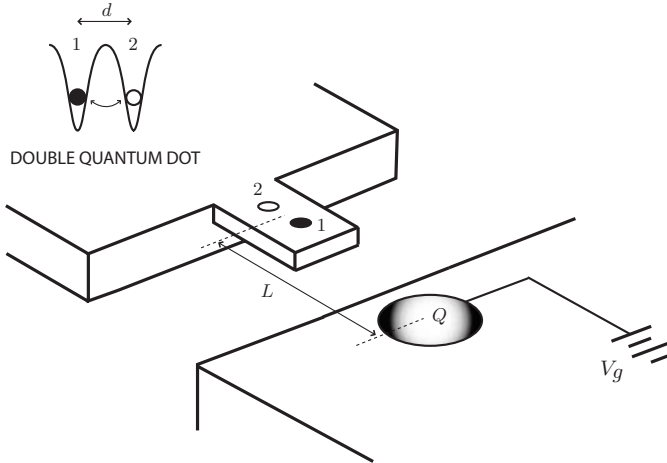


Fig. 3.6 A possible scheme for coupling a single-electron double-dot system to a nano-mechanical resonator. The double dot is idealized as a double-well potential for a single electron.

of the system depends on which well is occupied by the electron and on the square of the oscillator displacement. This leads to a shift in the frequency of the oscillator that depends on the location of the electron [CR98]. Currently such nano-mechanical electrometers are strongly dominated by thermal fluctuations and the irreversible dynamics are not well described by the decay term in Eq. (3.136). However, if quality factors and resonance frequencies continue to increase, these devices should enter a domain of operation where this description is acceptable.

At any time the state of the system plus apparatus may be written as

$$\rho(t) = \rho_{00} \otimes |0\rangle\langle 0| + \rho_{11} \otimes |1\rangle\langle 1| + \rho_{10} \otimes |1\rangle\langle 0| + \rho_{10}^\dagger \otimes |0\rangle\langle 1|, \quad (3.137)$$

where ρ_{ij} is an operator that acts only in the oscillator Hilbert space. If we substitute this into Eq. (3.136), we find the following equations:

$$\dot{\rho}_{00} = -i\epsilon[\hat{a} + \hat{a}^\dagger, \rho_{00}] + i\chi[\hat{a}^\dagger \hat{a}, \rho_{00}] + \gamma \mathcal{D}[\hat{a}]\rho_{00}, \quad (3.138)$$

$$\dot{\rho}_{11} = -i\epsilon[\hat{a} + \hat{a}^\dagger, \rho_{11}] - i\chi[\hat{a}^\dagger \hat{a}, \rho_{11}] + \gamma \mathcal{D}[\hat{a}]\rho_{11}, \quad (3.139)$$

$$\dot{\rho}_{10} = -i\epsilon[\hat{a} + \hat{a}^\dagger, \rho_{10}] - i\chi\{\hat{a}^\dagger \hat{a}, \rho_{10}\} + \gamma \mathcal{D}[\hat{a}]\rho_{10}, \quad (3.140)$$

where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ as usual. On solving these equations for the initial condition of an arbitrary qubit state $c_0|0\rangle + c_1|1\rangle$ and the oscillator in the ground state, we find that the combined state of the system plus apparatus is

$$\begin{aligned} \rho(t) = & |c_0|^2 |\alpha_-(t)\rangle\langle \alpha_-(t)| \otimes |0\rangle\langle 0| + |c_1|^2 |\alpha_+(t)\rangle\langle \alpha_+(t)| \otimes |1\rangle\langle 1| \\ & + [c_0 c_1^* C(t) |\alpha_+(t)\rangle\langle \alpha_-(t)| \otimes |1\rangle\langle 0| + \text{H.c.}], \end{aligned} \quad (3.141)$$

where $|\alpha_{\pm}(t)\rangle$ are coherent states with amplitudes

$$\alpha_{\pm}(t) = \frac{-i\epsilon}{\gamma/2 \pm i\chi} [1 - e^{-(\gamma/2 \pm i\chi)t}]. \quad (3.142)$$

The coherence factor $C(t)$ has a complicated time dependence, but tends to zero as $t \rightarrow \infty$. Thus the two orthogonal states of the measured qubit become classically correlated with different coherent states of the apparatus. The latter are the pointer basis states of the apparatus, and may be approximately orthogonal. Even if they are not orthogonal, it can be seen that the qubit state becomes diagonal in the eigenbasis of $\hat{\sigma}_z$.

For short times $C(t)$ decays as an exponential of a quadratic function of time. Such a quadratic dependence is typical for coherence decay in a measurement model that relies upon an initial build up of correlations between the measured system and the pointer degree of freedom. For long times ($\gamma t \gg 1$), the coherence decays exponentially in time: $C(t) \sim e^{-\Gamma t}$. The rate of decoherence is

$$\Gamma = \frac{2\epsilon^2\gamma\chi^2}{(\gamma^2/4 + \chi^2)^2}. \quad (3.143)$$

This qubit decoherence rate can be understood as follows. The long-time solution of Eq. (3.141) is

$$\rho_{\infty} = |c_0|^2 |\alpha_{-}\rangle\langle\alpha_{-}| \otimes |0\rangle\langle 0| + |c_1|^2 |\alpha_{+}\rangle\langle\alpha_{+}| \otimes |1\rangle\langle 1| \quad (3.144)$$

with $\alpha_{\pm} = -i\epsilon(\gamma/2 \pm i\chi)^{-1}$.

Exercise 3.32 Verify by direct substitution that this is a steady-state solution of the master equation (3.136).

The square separation $S = |\alpha_{-} - \alpha_{+}|^2$ between the two possible oscillator amplitudes in the steady state is given by

$$S = \frac{4\epsilon^2\chi^2}{(\gamma^2/4 + \chi^2)^2}. \quad (3.145)$$

Thus the long-time decoherence rate is $\Gamma = S\gamma/2$. This is essentially the rate at which information about which oscillator state is occupied (and hence which qubit state is occupied) is leaking into the oscillator's environment through the damping at rate γ . If $S \gg 1$, then the decoherence rate is much faster than the rate at which the oscillator is damped.

3.10.2 A superconducting box

The international effort to develop a quantum computer in a solid-state system is driving a great deal of fundamental research on the problem of decoherence. Recent experiments have begun to probe the mechanisms of decoherence in single solid-state quantum devices, particularly superconducting devices. In this section we will consider the physical mechanisms of decoherence in these devices and recent experiments. A superconducting box or *Cooper-pair box* (CPB) is essentially a small island of superconducting material separated

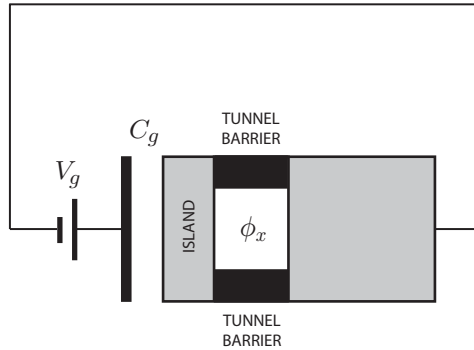


Fig. 3.7 A Cooper-pair box system. A superconducting metallic island is connected to a Cooper pair reservoir by a split tunnel junction, threaded by a magnetic flux ϕ_x . A DC bias gate with voltage V_g can make it energetically favourable for one or more Cooper-pairs to tunnel onto the island.

by a tunnel barrier from a reservoir of Cooper pairs. A Cooper pair (CP) is a pair of electrons bound together due to complex interactions with the lattice of the superconducting material [Coo56, BCS57]. Although electrons are fermions, a pair of electrons acts like a boson, and so can be described similarly to photons, using number states $|N\rangle$ for $N \in \mathbb{N}$.

A schematic representation of a CPB is shown in Fig. 3.7. The box consists of a small superconducting metallic island with oxide barrier tunnel junctions insulating it from the Cooper-pair reservoir. As the voltage V_g on the bias gate is changed, one or more Cooper pairs may tunnel onto the island. The tunnelling rate is determined by the Josephson energy E_J of the junction. This can be changed by adjusting the magnetic flux ϕ_x threading the loop: a so-called split-junction CPB.

In the experiment of Schuster *et al.* [SWB⁺05] the CPB was placed inside a superconducting co-planar microwave LC -resonator. The resonator supports a quantized mode of the electromagnetic field, while the CPB acts like an atomic system. Thus the term ‘circuit QED’ (as opposed to the ‘cavity QED’ of Section 3.9.2) is used for these systems. The coupling between the CPB and the microwave field is given by

$$\begin{aligned} \hat{H} = & \hbar\omega_r\hat{a}^\dagger\hat{a} - \frac{E_J}{2} \sum_N (|N\rangle\langle N+1| + |N+1\rangle\langle N|) \\ & + 4E_C \sum_N (N - \hat{n}_g)^2 |N\rangle\langle N|. \end{aligned} \quad (3.146)$$

In the first term, $\omega_r = \sqrt{LC}$ is the frequency and \hat{a} the annihilation operator for the microwave resonator field (note that in this section we are not setting $\hbar = 1$). The second term is the Josephson tunnelling term, with Josephson frequency E_J/\hbar . The third term is the coupling between the field and the CPB, in which $E_C = e^2/(2C_\Sigma)$ and $\hat{n}_g = C_g\hat{V}_g/(2e)$. Here C_Σ is the capacitance between the island and the rest of the circuit, C_g is the capacitance between the CPB island and the bias gate for the island, and \hat{V}_g is the operator for the total voltage applied to the island by the bias gate. This voltage can be split as $\hat{V}_g = V_g^{(0)} + \hat{v}$,

where $V_g^{(0)}$ is a DC field and \hat{v} is the microwave field in the cavity, which is quantized. It is related to the cavity annihilation operator by

$$\hat{v} = (\hat{a} + \hat{a}^\dagger)\sqrt{\hbar\omega_r/(2C)}. \quad (3.147)$$

We can thus write

$$\hat{n}_g = n_g^{(0)} + \delta\hat{n}_g; \quad \delta\hat{n}_g(t) = [C_g/(2e)]\hat{v}(t). \quad (3.148)$$

For $\delta\hat{n}_g$ small, we can choose the bias $n_g^{(0)}$ such that the CPB never has more than one CP on it at any time. That is, we can restrict the Hilbert space to the $N \in \{0, 1\}$ subspace, and write the Hamiltonian as

$$\hbar\omega_r\hat{a}^\dagger\hat{a} - 2E_C(1 - 2n_g^{(0)})\hat{\sigma}_z - \frac{E_J}{2}\hat{\sigma}_z - 4E_C\delta\hat{n}_g(t)(1 - 2n_g^{(0)} - \hat{\sigma}_x). \quad (3.149)$$

Here (differing from the usual convention) we have defined $\hat{\sigma}_x = |0\rangle\langle 0| - |1\rangle\langle 1|$ and $\hat{\sigma}_z = |1\rangle\langle 0| + |0\rangle\langle 1|$. If one chooses to operate at the charge-degeneracy point, $n_g^{(0)} = 1/2$, the Hamiltonian takes the form

$$\hat{H} = \hbar\omega_r\hat{a}^\dagger\hat{a} + \hbar\omega_a\hat{\sigma}_z/2 - \hbar g(\hat{a} + \hat{a}^\dagger)\hat{\sigma}_x, \quad (3.150)$$

where

$$g = e\frac{C_g}{C_\Sigma}\sqrt{\frac{\omega_r}{\hbar LC}}, \quad \omega_a = \frac{E_J}{\hbar}. \quad (3.151)$$

Defining $\hat{H}_0 = \hbar\omega_a(\hat{a}^\dagger\hat{a} + \hat{\sigma}_z/2)$, we move to an interaction frame with respect to this Hamiltonian, and make a rotating-wave approximation as usual. The new Hamiltonian is

$$\hat{V} = \hbar\Delta\hat{a}^\dagger\hat{a} + \hbar g(\hat{a}\hat{\sigma}_+ + \hat{a}^\dagger\hat{\sigma}_-), \quad (3.152)$$

with $\Delta = \omega_r - \omega_a$ the detuning between the circuit frequency and the CPB tunnelling frequency. It is assumed to be small compared with ω_a . We can, however, still consider a detuning that is large compared with g . Treating the second term in Eq. (3.152) as a perturbation on the first term, it is possible to show using second-order perturbation theory that Eq. (3.152) may be approximated by the effective Hamiltonian

$$\hat{V}_{\text{eff}} = \hbar\Delta\hat{a}^\dagger\hat{a} + \hbar\chi\hat{a}^\dagger\hat{a}\hat{\sigma}_z, \quad (3.153)$$

where $\chi = g^2/\Delta$. Moving frames again to the cavity resonance, and including a resonant microwave driving field ϵ , gives a Hamiltonian with the same form as Eq. (3.135).

Schuster *et al.* [SWB⁺05] recently implemented this system experimentally and measured the measurement-induced qubit dephasing rate given in Eq. (3.143). In their experiment, $\Delta/(2\pi) = 100$ MHz, $g/(2\pi) = 5.8$ MHz and the cavity decay rate was $\gamma/(2\pi) = 0.8$ MHz. Schoelkopf's team used a second probe microwave field tuned to the CPB resonance to induce coherence in the qubit basis. The measurement-induced decoherence time then appears as a broadening of the spectrum representing the response of the qubit to the probe. This spectrum is related to the norm squared of the Fourier transform of the coherence function in time. The results are found to be in good agreement with the theory

presented here for small χ . Although the decay of coherence is exponential for long times with rate (3.143), for short times the decoherence is quadratic in time. This is manifested experimentally in the line shape of the probe absorption spectrum: the line shape deviates from the usual Lorentzian shape (corresponding to exponential decay) in its wings.

3.11 Heisenberg-picture dynamics

We saw in Section 1.3.2 that quantum dynamics, and even quantum measurement, can be formulated in the Heisenberg picture. It is thus not surprising that there is a Heisenberg-picture formulation for master equations. This formulation is sometimes called the quantum stochastic differential-equation technique, or the quantum Langevin approach [GC85] (after Paul Langevin, who developed the corresponding theory of classical stochastic differential equations early in the twentieth century [Lan08]). In this section we will develop the Heisenberg-picture description for a system coupled to a bosonic (harmonic-oscillator) bath. We will show how the Markovian limit can be elegantly formulated in the Heisenberg picture, and used to derive a Lindblad-form master equation.

Consider the interaction-frame coupling Hamiltonian in the rotating-wave approximation (3.24) derived in Section 3.3.1

$$\hat{V}_{\text{IF}}(t) = -i[\hat{b}(z := -t)\hat{c}^\dagger - \hat{b}^\dagger(z := -t)\hat{c}], \quad (3.154)$$

where

$$\hat{b}(z) = \gamma^{-1/2} \sum_k g_k \hat{b}_k e^{+i\delta_k z}, \quad (3.155)$$

where δ_k is the detuning of the bath mode k from the system, γ is the dissipation rate, and, as in the example of Section 3.3.1, $i\hat{c}$ is the system lowering operator multiplied by $\sqrt{\gamma}$.

We use z , rather than t , as the argument of \hat{b} for two reasons. The first is that $\hat{b}(z := -t)$ is *not* at this stage a Heisenberg-picture operator. Rather, the interaction Hamiltonian is time-dependent because we are working in the interaction frame, and the operator $\hat{b}(z)$ is defined simply to make $\hat{V}_{\text{IF}}(t)$ simple in form. The second reason is that in some quantum-optical situations, such as the damping of a cavity mode at a single mirror, it is possible to consider the electromagnetic field modes which constitute the bath as being functions of one spatial direction only. On defining the speed of light *in vacuo* to be unity, and the origin as the location of the mirror, we have that, at time $t = 0$, $\hat{b}(z)$ relates to the bath at position $|z|$ away from the mirror. For $z < 0$ it represents a property of the incoming field, and for $z > 0$ it represents a property of the outgoing field. That is, $\hat{b}(z := -t)$ represents the field that will interact (for $t > 0$) or has interacted (for $t < 0$) with the system at time t . An explanation of this may be found in many textbooks, such as that of Gardiner and Zoller [GZ04].

Now, in the limit of a continuum bath as considered in Section 3.3.1, we find that

$$[\hat{b}(z), \hat{b}^\dagger(z')] = \gamma^{-1} \Gamma(z - z'). \quad (3.156)$$

In order to derive a Markovian master equation, it was necessary to assume that $\Gamma(\tau)$ was sharply peaked at $\tau = 0$. Ignoring the Lamb shift in Eq. (3.30), and taking the Markovian limit, we obtain

$$[\hat{b}(z), \hat{b}^\dagger(z')] = \delta(z - z'). \quad (3.157)$$

Physically, this result cannot be exact because the bath modes all have positive frequency. Also, one must be careful using this result because of the singularity of the δ -function. Nevertheless, it is the result that must be used to obtain a strict correspondence with a Markovian master equation.

Before moving to the Heisenberg picture, it is useful to define the unitary operator for an infinitesimal evolution generated by Eq. (3.154):

$$\hat{U}(t + dt, t) = \exp\left[\hat{c} d\hat{B}_{z:=-t}^\dagger - \hat{c}^\dagger d\hat{B}_{z:=-t}\right]. \quad (3.158)$$

Here we have defined a new infinitesimal operator,

$$d\hat{B}_z = \hat{b}(z)dt. \quad (3.159)$$

The point of defining this infinitesimal is that, although it appears to be of order dt , because of the singularity of the commutation relation (3.157), it is actually of order \sqrt{dt} . This can be seen by calculating its commutation relations

$$[d\hat{B}_z, d\hat{B}_z^\dagger] = dt, \quad (3.160)$$

where we have used the heuristic equation $\delta(0)dt = 1$. This can be understood by thinking of dt as the smallest unit into which time can be divided. Then the discrete approximation to a δ -function is a function which is zero everywhere except for an interval of size dt around zero, where it equals $\delta(0) = 1/dt$ (so that its area is unity). Because $d\hat{B}_z$ is of order \sqrt{dt} , it is necessary to expand $\hat{U}(t + dt, t)$ to second rather than first order in its argument. That is,

$$\begin{aligned} \hat{U}(t + dt, t) = & \hat{1} + \left(\hat{c} d\hat{B}_{z:=-t}^\dagger - \hat{c}^\dagger d\hat{B}_{z:=-t} \right) - \frac{1}{2} \hat{c}^\dagger \hat{c} dt - \frac{1}{2} \{ \hat{c}^\dagger, \hat{c} \} d\hat{B}_{z:=-t}^\dagger d\hat{B}_{z:=-t} \\ & + \frac{1}{2} \hat{c}^2 \left(d\hat{B}_{z:=-t}^\dagger \right)^2 + \frac{1}{2} (\hat{c}^\dagger)^2 \left(d\hat{B}_{z:=-t} \right)^2. \end{aligned} \quad (3.161)$$

Exercise 3.33 Show this, using Eq. (3.160).

3.11.1 Quantum Langevin equations

To obtain the Heisenberg-picture dynamics of the system, one might think that all one need do is to write down the usual Heisenberg equations of motion (in the interaction frame) generated by the Hamiltonian (3.154). That is, for an arbitrary system operator \hat{s} ,

$$\frac{d\hat{s}(t)}{dt} = [\hat{b}(z := -t, t)\hat{c}^\dagger(t) - \hat{b}^\dagger(z := -t, t)\hat{c}(t), \hat{s}(t)], \quad (3.162)$$

where now $\hat{b}(z, t)$ is also time-dependent through the evolution of $\hat{b}_k(t)$ in the Heisenberg picture. However, because of the singularity of the commutation relation (3.157), the situation is not so simple. The approach we will follow is different from that in most texts. It has the advantage of being simple to follow and of having a close relation to an analogous approach in classical Markovian stochastic differential equations. For a detailed discussion, see Appendix B.

In our approach, to find the correct Heisenberg equations one proceeds as follows (note that all unitaries are in the interaction frame as usual):

$$\hat{s}(t + dt) = \hat{U}^\dagger(t + dt, t_0) \hat{s}(t_0) \hat{U}(t + dt, t_0) \quad (3.163)$$

$$= \hat{U}^\dagger(t, t_0) \hat{U}^\dagger(t + dt, t) \hat{s}(t_0) \hat{U}(t + dt, t) \hat{U}(t, t_0) \quad (3.164)$$

$$= \hat{U}_{\text{HP}}^\dagger(t + dt, t) \hat{s}(t) \hat{U}_{\text{HP}}(t + dt, t), \quad (3.165)$$

where $\hat{s}(t) = \hat{U}^\dagger(t, t_0) \hat{s}(t_0) \hat{U}(t, t_0)$ and

$$\hat{U}_{\text{HP}}(t + dt, t) \equiv \hat{U}^\dagger(t, t_0) \hat{U}(t + dt, t) \hat{U}(t, t_0). \quad (3.166)$$

Here we are (just for the moment) using the subscript HP to denote that Eq. (3.166) is obtained by replacing the operators appearing in $\hat{U}(t + dt, t)$ by their Heisenberg-picture versions at time t . If we were to expand the exponential in $\hat{U}_{\text{HP}}(t + dt, t)$ to first order in its argument, we would simply reproduce Eq. (3.162). As motivated above, this will not work, and instead we must use the second-order expansion as in Eq. (3.161). First we define

$$d\hat{B}_{\text{in}}(t) \equiv d\hat{B}_{z:=-t}(t), \quad (3.167)$$

and $\hat{b}_{\text{in}}(t)$ similarly. These are known as *input field operators*. Note that as usual the t -argument on the right-hand side indicates that here $d\hat{B}_{z:=-t}$ is in the Heisenberg picture. Because of the bath commutation relation (3.157), this operator is unaffected by any evolution prior to time t , since $d\hat{B}_{\text{in}}(t)$ commutes with $d\hat{B}_{\text{in}}^\dagger(t')$ for non-equal times. Thus we could equally well have defined

$$d\hat{B}_{\text{in}}(t) \equiv d\hat{B}_{z:=-t}(t'), \quad \forall t' \leq t. \quad (3.168)$$

In particular, if $t' = t_0$, the initial time for the problem, then $d\hat{B}_{\text{in}}(t)$ is the same as the Schrödinger-picture operator $d\hat{B}_{z:=-t}$ appearing in $\hat{U}(t + dt, t)$ of Eq. (3.158).

If the bath is initially in the vacuum state, this leads to a significant simplification, as we will now explain. Ultimately we are interested in calculating the average of system (or bath) operators. In the Heisenberg picture, such an average is given by

$$\langle \hat{s}(t) \rangle = \text{Tr}[\hat{s}(t) \rho_S \otimes \rho_B] = \text{Tr}_S[\langle \mathbf{0} | \hat{s}(t) | \mathbf{0} \rangle \rho_S], \quad (3.169)$$

where $|\mathbf{0}\rangle$ is the vacuum bath state and ρ_S is the initial system state. Since $d\hat{B}_{\text{in}}(t)|\mathbf{0}\rangle = 0$ for all t , any expression involving $d\hat{B}_{\text{in}}(t)$ and $d\hat{B}_{\text{in}}^\dagger(t)$ that is in normal order (see Section A.5) will contribute nothing to the average. Thus it is permissible to drop all normally ordered terms in Eq. (3.161) that are of second order in $d\hat{B}_{\text{in}}(t)$. That is to say, we can drop all

second-order terms in $d\hat{B}_{\text{in}}(t)$ in Eq. (3.161) because we have already used

$$d\hat{B}_{\text{in}}(t)d\hat{B}_{\text{in}}^\dagger(t) = [d\hat{B}_{\text{in}}(t), d\hat{B}_{\text{in}}^\dagger(t)] + d\hat{B}_{\text{in}}^\dagger(t)d\hat{B}_{\text{in}}(t) = dt \quad (3.170)$$

to obtain the non-zero second-order term $-\frac{1}{2}\hat{c}^\dagger\hat{c} dt$ in Eq. (3.161).

Although they do not contribute to $\langle d\hat{s}(t) \rangle$, first-order terms in the input field operator must be kept because they will in general contribute (via a non-normally ordered product) to the change in an operator product such as $\langle d(\hat{r}\hat{s}) \rangle$. That is because, not surprisingly, one must consider *second-order* corrections to the usual product rule:

$$d(\hat{r}\hat{s}) = (d\hat{r})\hat{s} + \hat{r}(d\hat{s}) + (d\hat{r})(d\hat{s}). \quad (3.171)$$

One thus obtains from Eq. (3.165) the following Heisenberg equation of motion in the interaction frame:

$$d\hat{s} = dt \left(\hat{c}^\dagger\hat{s}\hat{c} - \frac{1}{2}\{\hat{c}^\dagger\hat{c}, \hat{s}\} + i[\hat{H}, \hat{s}] \right) - [d\hat{B}_{\text{in}}^\dagger(t)\hat{c} - \hat{c}^\dagger d\hat{B}_{\text{in}}(t), \hat{s}]. \quad (3.172)$$

Here we have dropped the time arguments from all operators except the input bath operators. We have also included a system Hamiltonian \hat{H} , as could arise from having a non-zero \hat{V}_S , or a Lamb-shift term, as discussed in Section 3.3.1. Remember that we are still in the interaction frame – \hat{H} here is not the same as the $\hat{H} = \hat{H}_0 + \hat{V}$ for the system plus environment with which we started the calculation.

We will refer to Eq. (3.172) as a quantum Langevin equation (QLE) for \hat{s} . The operator \hat{s} may be a system operator or it may be a bath operator. Because $\hat{b}_{\text{in}}(t)$ is the bath operator *before* it interacts with the system, it is independent of the system operator $\hat{s}(t)$. Hence for system operators one can derive

$$\left\langle \frac{d\hat{s}}{dt} \right\rangle = \langle (\hat{c}^\dagger\hat{s}\hat{c} - \frac{1}{2}\hat{c}^\dagger\hat{c}\hat{s} - \frac{1}{2}\hat{s}\hat{c}^\dagger\hat{c}) + i[\hat{H}, \hat{s}] \rangle. \quad (3.173)$$

Although the noise terms in (3.172) do not contribute to Eq. (3.173), they are necessary in order for Eq. (3.172) to be a valid Heisenberg equation of motion. If they are omitted then the operator algebra of the system will not be preserved.

Exercise 3.34 *Show this. For specificity, consider the case $\hat{c} = \sqrt{\gamma}\hat{a}$, where \hat{a} is an annihilation operator, and show that, unless these terms are included, $[\hat{a}(t), \hat{a}^\dagger(t)]$ will not remain equal to unity.*

The master equation. Note that Eq. (3.173) is Markovian, depending only on the average of system operators at the same time. Therefore, it should be derivable from a Markovian evolution equation for the system in the Schrödinger picture. That is to say, there should exist a master equation for the system state matrix such that

$$\langle \dot{\hat{s}}(t) \rangle = \text{Tr}[\hat{s}\dot{\rho}(t)]. \quad (3.174)$$

Here, the placement of the time argument indicates the picture (Heisenberg or Schrödinger). By inspection of Eq. (3.173), the corresponding master equation is

$$\dot{\rho} = \mathcal{D}[\hat{c}]\rho - i[\hat{H}, \rho]. \quad (3.175)$$

As promised, this is of the Lindblad form.

3.11.2 Generalization for a non-vacuum bath

The above derivation relied upon the assumption that the bath was initially in the vacuum state $|0\rangle$. However, it turns out that there are other bath states for which it is possible to derive a Markovian QLE and hence a Markovian master equation. This generalization includes a bath with thermal noise and a bath with so-called broad-band squeezing. Instead of the equation $d\hat{B}_{\text{in}}(t)d\hat{B}_{\text{in}}^\dagger(t) = dt$, with all other second-order products ignorable and all first-order terms being zero on average, we have in the general case

$$d\hat{B}_{\text{in}}^\dagger(t)d\hat{B}_{\text{in}}(t) = N dt, \quad (3.176)$$

$$d\hat{B}_{\text{in}}(t)d\hat{B}_{\text{in}}^\dagger(t) = (N + 1)dt, \quad (3.177)$$

$$d\hat{B}_{\text{in}}(t)d\hat{B}_{\text{in}}(t) = M dt, \quad (3.178)$$

$$\langle d\hat{B}_{\text{in}}(t) \rangle = \beta dt, \quad (3.179)$$

while Eq. (3.160) still holds. The parameter N is positive, while M and β are complex, with M constrained by

$$|M|^2 \leq N(N + 1). \quad (3.180)$$

This type of input field is sometimes called a white-noise field, because the bath correlations are δ -correlated in time. That is, they are flat (like the spectrum of white light) in frequency space. A thermal bath is well approximated by a white-noise bath with $M = 0$ and $N = \{\exp[\hbar\omega_0/(k_B T)] - 1\}^{-1}$, where ω_0 is the frequency of the system's free oscillation. Only a pure squeezed (or vacuum) bath attains the equality in Eq. (3.180).

Using these rules in expanding the unitary operator in Eq. (3.165) gives the following general QLE for a white-noise bath:

$$\begin{aligned} d\hat{s} = i dt [\hat{H}, \hat{s}] + \frac{1}{2} \{ & (N + 1)(2\hat{c}^\dagger \hat{s} \hat{c} - \hat{s} \hat{c}^\dagger \hat{c} - \hat{c}^\dagger \hat{c} \hat{s}) + N(2\hat{c} \hat{s} \hat{c}^\dagger - \hat{s} \hat{c} \hat{c}^\dagger - \hat{c} \hat{c}^\dagger \hat{s}) \\ & + M[\hat{c}^\dagger, [\hat{c}^\dagger, \hat{s}]] + M^*[\hat{c}, [\hat{c}, \hat{s}]] \} dt - [d\hat{B}_{\text{in}}^\dagger \hat{c} - \hat{c}^\dagger d\hat{B}_{\text{in}}, \hat{s}]. \end{aligned} \quad (3.181)$$

Here we have dropped time arguments but are still (obviously) working in the Heisenberg picture.

Exercise 3.35 Derive Eq. (3.181).

The corresponding master equation is evidently

$$\begin{aligned} \dot{\rho} = & (N+1)\mathcal{D}[\hat{c}]\rho + N\mathcal{D}[\hat{c}^\dagger]\rho + \frac{M}{2}[\hat{c}^\dagger, [\hat{c}^\dagger, \rho]] + \frac{M^*}{2}[\hat{c}, [\hat{c}, \rho]] \\ & - i[\hat{H} + i(\beta^*\hat{c} - \beta\hat{c}^\dagger), \rho]. \end{aligned} \quad (3.182)$$

Note that the effect of the non-zero mean field (3.179) is simply to add a driving term to the existing system Hamiltonian \hat{H} . Although not obviously of the Lindblad form, Eq. (3.182) can be written in that form, with three irreversible terms, as long as Eq. (3.180) holds.

Exercise 3.36 Show this.

Hint: Define N' such that $|M|^2 = N'(N'+1)$ and consider three Lindblad operators proportional to \hat{c} , \hat{c}^\dagger and $[\hat{c}(N' + M^* + 1) - \hat{c}^\dagger(N' + M)]$.

3.12 Further reading

There is a large and growing literature on describing the evolution of open quantum systems, both with and without the Markovian assumption. For a review, see the book by Breuer and Petruccione [BP02]. One of the interesting developments since that book was published is the derivation [PV05] of a Markovian master equation for Brownian motion starting from Einstein's original concept of Brownian motion. That is, instead of considering a particle coupled to a bath of harmonic oscillators, a massive particle is made to suffer collisions by being immersed in a bath of less massive particles in thermal equilibrium. Building on the work of Diósi [Dió93], Petruccione and Vacchini [PV05] have rigorously derived a *Lindblad*-form master equation that involves diffusion in position as well as momentum.

As we have discussed, the Lindblad form is the only form of a Markovian master equation that corresponds to a completely positive map for the state. The question of which *non-Markovian* master equations give rise to completely positive evolution has recently been addressed by Andersson, Cresser and Hall [ACH07]. They consider time-local non-Markovian master equations; that is, master equations with time-dependent coefficients such as those we discussed in Section 3.4. For finite-dimensional systems, they show how the state map for any time may be constructed from the master equation, and give a simple test for complete positivity. Conversely, they show that any continuous time-dependent map can be turned into a master equation.

In this chapter we have discussed master equations for systems that can exchange excitations with both fermionic and bosonic baths. However, when presenting the Heisenberg-picture dynamics (quantum Langevin equations) we considered only the case of a bosonic bath. The reason is that there is an important technical issue due to the anticommutation relations between the fermionic driving field and those system operators which can change the number of fermions within the system. This problem has been addressed in a recent paper by Gardiner [Gar04].

The decoherence ‘programme’ described briefly in Section 3.7 has been reviewed recently by Zurek, one of its chief proponents [Zur03]. For an excellent discussion of

some of the conceptual issues surrounding decoherence and the quantum measurement problem, see the recent review by Schlosshauer [Sch04]. For an extensive investigation of physically realizable ensembles and robustness for various open quantum systems see Refs. [WV02a, WV02b, ABJW05]. Finally, we note that an improved version of the Schrödinger-cat decoherence experiment of Section 3.9.2 has been performed, also by the Haroche group. The new results [DDS⁺08] allow reconstruction of the whole quantum state (specifically, its Wigner function – see Section A.5), showing the rapid vanishing of its nonclassical features under damping.