

Graduate course on open quantum systems
Third term 2004
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1 Introduction

1.1 Preliminaries

General and background reading:

1. *The theory of open quantum systems*, H.-P. Breuer and F. Petruccione (Oxford 2002). The most complete book overall for the course, strong on the formal mathematical aspects and very detailed (especially in its treatment of non-Markovian effects). It can be hard going at times, but generally repays the effort. Be careful not to lose the wood for the trees!
2. *Quantum Noise* (2nd Ed.), C.W. Gardiner and P. Zoller (Springer 2000). As its title suggests, strong on the stochastic treatment of open systems. Especially strong on applications to quantum optics.
3. *Quantum Computation and Quantum Information*, M.A. Nielsen and I.L. Chuang (Cambridge, 2000). This book is becoming the ‘bible’ of the emerging field of quantum information. It is extremely well written and an excellent background read. Unfortunately for us, its treatment of open systems follows the ‘quantum operations’ approach, in which only the end result of interactions with the environment is considered (rather than the process by which this occurs) so it fails to cover large parts of our material.
4. Lecture notes for Physics 229: Quantum Information and Computation, J. Preskill (1998, available on-line at <http://www.theory.caltech.edu/people/preskill/ph229/>). In all but name another excellent book on quantum information. Takes a slightly more ‘physics’ approach than Nielsen & Chuang.

1.2 Closed and open systems.

1.2.1 Closed systems

Described by a single wavefunction Ψ depending on a well-defined set of variables $\{X_i\}$. Hamiltonian evolution under the influence of a well-defined (though possibly time-dependent) Hamiltonian:

$$i\hbar\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle \quad (1)$$

Time-dependence of \hat{H} assumed to come from outside the system, for example through a classically varying electric or magnetic field.

Resulting evolution is unitary:

$$|\Psi(t)\rangle = \hat{U}(t, t_0)|\Psi(t_0)\rangle, \quad \hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{1} \quad (2)$$

with

$$\hat{U}(t, t_0) = \hat{T} \exp \left[\frac{-i}{\hbar} \int_{t_0}^t dt' \hat{H}(t') \right] \quad (3)$$

where \hat{T} is the time-ordering operator, ordering earliest times to the right and later times to the left:

$$\hat{T} \exp \left[\frac{-i}{\hbar} \int_{t_0}^t dt' \hat{H}(t') \right] = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}(t') - \frac{1}{\hbar^2} \int_{t_0}^t dt'' \int_{t_0}^{t'} dt' \hat{H}(t'') \hat{H}(t') + O(t - t_0)^3. \quad (4)$$

For the simplest case of a time-independent Hamiltonian $\hat{H}(t) = \hat{H}$:

$$\hat{U}(t, t_0) = \exp[-i\hat{H}(t - t_0)/\hbar]. \quad (5)$$

Examples:

- Isolated atom;
- Electron in free space (isolated spin);
- An entire solid (as far as internal phenomena of solid-state physics are concerned);
- The universe (presumably?).

1.2.2 Open system

Open to influence from some ‘environment’, which may in turn be influenced by what the ‘system’ is doing.

Examples:

- Atom in presence of electromagnetic field, or collisions with other atoms or molecules;
- Electron in a solid interacting with other excitations;
- One small region of space within a solid, such as a point or line defect;
- A cat.

The aim of this course is to extract the quantum mechanical laws governing the behaviour of such systems. In (most of) this course we shall assume that the entire system still follows the conventional Schrödinger equation, and pursue the consequences for the behaviour of one part of it.

Nevertheless, one consequence is that in certain circumstances an object begins to behave ‘classically’ as a result of its coupling to the environment, even when its own intrinsic dynamics is quantum. Many (although not all) workers in the field believe that this explains how it is that the macroscopic classical limit arises out of quantum mechanics.

This course is topical because of the many experiments that now seek to probe quantum behaviour in larger and more complex systems, for example in the fields of superconductivity and superfluidity, ultra-cold atoms and molecules, and quantum information processing.

1.3 The density operator.

The density operator is a generalization of the wavefunction to include the possibility of uncertainty in its preparation. If we know only that the system is described by an ensemble of quantum states $\{|\Psi_n\rangle\}$ with probabilities $\{p_n\}$ then the appropriate density operator is

$$\hat{\rho}(t) = \sum_n p_n |\Psi_n(t)\rangle \langle \Psi_n(t)|. \quad (6)$$

It will become particularly important for the treatment of open systems, but note it still has significance even for a closed system: if I give you a closed quantum system and tell you the range of possible preparations and the associated probabilities, then the appropriate description of the system is through the density operator.

Some properties of $\hat{\rho}$:

- $\hat{\rho}$ looks like an operator. Hence in any set of basis states that are complete for a given problem it can be represented as a matrix—the density matrix. (I shall probably use the terms density matrix and density operator more-or-less interchangeably in the course.) If the complete set of basis states $\{|i\rangle\}$ is orthonormal, we can write

$$\hat{\rho} = \sum_{ij} |i\rangle \langle i|\hat{\rho}|j\rangle \langle j| \equiv \sum_{ij} |i\rangle \rho_{ij} \langle j| \quad \text{with} \quad \rho_{ij} = \langle i|\hat{\rho}|j\rangle. \quad (7)$$

- The density operator is Hermitian: $\hat{\rho}^\dagger = \hat{\rho}$.
- Since the operator is Hermitian, it has real eigenvalues. If the states $\{|\Psi_n\rangle\}$ are orthonormal, these eigenvalues are just the p_n . The eigenvalues must therefore lie between 0 and 1.
- Assuming the states $|\Psi_n\rangle$ are properly normalized, and that the probabilities p_n sum to one, the density operator is normalized so

$$\text{Tr}[\hat{\rho}] = \sum_i \langle i|\hat{\rho}|i\rangle = \sum_n p_n \sum_i |\langle i|\Psi_n\rangle|^2 = \sum_n p_n = 1. \quad (8)$$

(This is equivalent to saying the eigenvalues must sum to one, as one would guess from the previous point.)

- If and only if the density operator represents a pure state ($p_n = 1$ for some n , with all the other p_n zero), it is idempotent (i.e. is a projector onto that particular pure state):

$$\hat{\rho}^2 = \hat{\rho} \quad (\text{for pure states}). \quad (9)$$

- The expectation value of any operator can be calculated if $\hat{\rho}$ is known:

$$\begin{aligned} \langle \hat{O} \rangle &= \sum_n p_n \langle \Psi_n | \hat{O} | \Psi_n \rangle \\ &= \sum_{ij} \sum_n \langle \Psi_n | i \rangle \langle i | \hat{O} | j \rangle \langle j | \Psi_n \rangle \\ &= \sum_{ij} O_{ij} \rho_{ji} = \text{Tr}[\hat{O} \hat{\rho}]. \end{aligned} \quad (10)$$

- More generally, the probability of any outcome of any measurement can be obtained from $\hat{\rho}$: the probability of a measurement outcome corresponding to a projection into a state $|e_i\rangle$ is

$$\text{Tr}[|e_i\rangle \langle e_i| \hat{\rho}]. \quad (11)$$

- There are in general many different ways to decompose a given $\hat{\rho}$ into quantum states according into equation (6). However, because $\hat{\rho}$ itself determines the distribution of results of all measurements, there is no way to distinguish between these different decompositions.
- The diagonal matrix element ρ_{ii} play the role of probabilities to find the system in state $|i\rangle$; the off-diagonal elements ρ_{ij} are often described as *coherences* between states i and j .

The time-dependence of the density operator in a closed system:

$$\begin{aligned} \partial_t \hat{\rho} &= \sum_n p_n (\partial_t |\Psi_n(t)\rangle) \langle \Psi_n(t)| + |\Psi_n(t)\rangle (\partial_t \langle \Psi_n(t)|) \\ &= \frac{1}{i\hbar} \sum_n p_n \hat{H} |\Psi_n(t)\rangle \langle \Psi_n(t)| - \frac{1}{i\hbar} \sum_n p_n |\Psi_n(t)\rangle \langle \Psi_n(t)| \hat{H} \\ &= \frac{1}{i\hbar} [\hat{H}, \hat{\rho}]. \end{aligned} \quad (12)$$

Note this looks like (but is **not** the same as) the equation for the time-dependence of an operator \hat{O} in the Heisenberg representation:

$$\frac{d\hat{O}}{dt} = \frac{\partial\hat{O}}{\partial t} + \frac{1}{i\hbar}[\hat{O}, \hat{H}] \quad (13)$$

Equation (12) holds in the *Schrödinger* representation, where the wavefunctions are time-dependent but the operators are not.

The solution to equation (12) may be formally written

$$\hat{\rho}(t) = \hat{U}(t, t_0)\hat{\rho}(t_0)[\hat{U}(t, t_0)]^\dagger. \quad (14)$$

1.3.1 Example: density operator for a single spin.

For a single $S = 1/2$ spin, there is a two-dimensional state space $|\uparrow\rangle, |\downarrow\rangle$. Therefore the density matrix is a 2×2 matrix. Given that it must be normalized and Hermitian, the density matrix must take the form

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + \alpha_z & \alpha_x + i\alpha_y \\ \alpha_x - i\alpha_y & 1 - \alpha_z \end{pmatrix}. \quad (15)$$

In terms of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (16)$$

this becomes

$$\rho = \frac{1}{2}[\hat{1} + \vec{\alpha} \cdot \vec{\sigma}]. \quad (17)$$

The eigenvalues are then $(1 \pm |\vec{\alpha}|)/2$, so for physical states we require $0 \leq |\vec{\alpha}| \leq 1$.

This leads to the *Bloch sphere* representation of the density matrix, in which a particular density matrix is represented by the vector $\vec{\alpha}$. The centre of the sphere ($\vec{\alpha} = 0$) corresponds to the completely disordered density matrix $\hat{\rho} = \hat{1}/2$; the surface of the sphere ($|\vec{\alpha}| = 1$) corresponds to the pure states with different spin orientations. The direction of the vector $\vec{\alpha}$ corresponds to the direction of the expectation value of the spin.

1.4 Direct-sum problems

Suppose our entire system has two sets of configurations available to it. which are alternatives: sometimes it is in the region of interest (let us call this the *system* region S), sometimes it is in another (complementary) set of states (the *environment* region). Examples:

- Single particle scattering from a potential of finite range, where only the region around the defect is of interest;
- Two spins in which only the states $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ having total spin $M_s = 0$ are of interest;

Mathematically we express this by saying that the total Hilbert space for the system is a direct sum of system and environment parts:

$$\mathcal{H} = \mathcal{H}_S \oplus \mathcal{H}_E. \quad (18)$$

Let us define a projection operator \hat{P} which projects onto S , and a complementary projection operator $\hat{Q} = \hat{1} - \hat{P}$. In terms of a basis set for the system, this means we can divide the basis into ‘system’ and ‘environment’ parts; we can therefore represent a wavefunction $|\Psi\rangle$ in terms

on a ‘system’ part $\hat{P}|\Psi\rangle$ and an ‘environment’ part $\hat{Q}|\Psi\rangle$. One convenient way of writing this is in the column vector form

$$\Psi = \begin{pmatrix} \Psi_S \\ \Psi_E \end{pmatrix} \quad (19)$$

The density matrix can then be written in block form:

$$\rho = \begin{pmatrix} \rho_{SS} & \rho_{SE} \\ \rho_{ES} & \rho_{EE} \end{pmatrix} \quad (20)$$

Then $\rho_{SS} = \hat{P}\hat{\rho}\hat{P}$ contains the information about the system within the system subspace. Note that it is *not* normalized:

$$\text{Tr}[\rho_{SS}] \leq 1. \quad (21)$$

This reflects the fact that the system does not spend all its time in the S subspace.

It can be used to evaluate the expectation value or distribution of measurement results for any operator that acts only within S .

1.5 Direct-product problems

Now suppose we can instead divide our system into two *distinguishable* parts, system S and environment E , such that we must always specify the coordinates of both parts in order to give a complete description of the system.

Examples:

- An electron (S) interacting with electromagnetic field modes (E);
- Two spins, one of which is the system (S) and the other is the environment (E);
- A spin (S) interacting with lattice vibrations (E).

The Hilbert space is now a direct product of system and environment parts:

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E. \quad (22)$$

This means that, if $\{|i\rangle_S\}$ is a basis set for S and $\{|j\rangle_E\}$ is a basis set for E , then a complete basis set for the whole system is

$$\{|i, j\rangle\} = \{|i\rangle_S |j\rangle_E\}. \quad (23)$$

A wavefunction $|\Psi\rangle$ could therefore be represented as

$$|\Psi\rangle = \sum_{ij} |i\rangle_S |j\rangle_E \langle j|_E \langle i|_S |\Psi\rangle = \sum_{ij} c_{ij} |i\rangle_S |j\rangle_E, \quad (24)$$

and a density matrix (or indeed any other operator) would have matrix elements

$$\rho_{ij, i'j'} = \langle i|_S \langle j|_E \hat{\rho} |j'\rangle_E |i'\rangle_S. \quad (25)$$

There is now no way of finding a single wavefunction to describe the state of the interesting (S) part of the system, since there is no consistent way to get rid of the extra information describing the E part, and the state of the S system depends upon it. However we can define a suitable density matrix, called the **reduced density matrix** ρ_S , to describe the state of the S subsystem; it is obtained by tracing out (summing over the diagonal elements of) the environment.

$$\rho_{Sii'} \equiv \sum_j \rho_{ij, i'j}, \quad (26)$$

or

$$\hat{\rho}_S = \text{Tr}_E[\hat{\rho}]. \quad (27)$$

We can see why this works by extending some operator \hat{O}_S acting over the sub-system into an operator acting over the whole ($S + E$) system in the form $\hat{O}_S \otimes \hat{1}_E$. Then

$$\langle \hat{O}_S \otimes \hat{1}_E \rangle = \text{Tr}[\hat{O}_S \otimes \hat{1}_E \hat{\rho}] = \text{Tr}_E[\hat{O}_S \hat{\rho}_S]. \quad (28)$$

In other words, the expectation value is obtained by following the standard procedure of equation (10), but using the reduced density matrix rather than the full density matrix. Hence *the reduced density matrix encodes all the accessible information about the S subsystem.*

2 Handling direct-sum systems

Further reading:

- My DPhil thesis (1989) and/or three related papers:
 - A.J. Fisher *J. Phys. C* **21** 3229–3249 (1988);
 - A.J. Fisher *J. Phys.: Condens. Matt.* **1** 3883–3895 (1989);
 - A.J. Fisher *J. Phys.: Condens. Matt.* **2** 6079–6082 (1990);
- J.E. Inglesfield, *J. Phys. C* **14** 3795–3806 (1981);
- G.A. Baraff and M. Schlüter, *J. Phys. C* **19** 4383–4391 (1986).

2.1 Time-independent embedding

2.1.1 Embedding the wavefunction

The Schrödinger equation for a time-independent direct-sum system is

$$\begin{pmatrix} E - \hat{H}_{SS} & -\hat{H}_{SE} \\ -\hat{H}_{ES} & E - \hat{H}_{EE} \end{pmatrix} \begin{pmatrix} \psi_S \\ \psi_E \end{pmatrix} \quad (29)$$

or

$$(E - \hat{H}_{SS} - \hat{H}_{SE}(E - \hat{H}_{EE})^{-1}\hat{H}_{ES})\psi_S = 0. \quad (30)$$

This says that the effect of the environment on the system can be replaced by the inclusion of an extra (energy-dependent) term in the Hamiltonian—the *embedding potential*.

$$\hat{\Sigma}(E) = \hat{H}_{SE}(E - \hat{H}_{EE})^{-1}\hat{H}_{ES}. \quad (31)$$

The system wavefunction ψ_S is then an eigenfunction of $E - \hat{H}_{SS} - \hat{\Sigma}$ with zero eigenvalue.

2.1.2 Embedding the Green operator

In the energy domain, the Green operator G for the whole system satisfies

$$\hat{G}(E) = (E - \hat{H})^{-1} \quad \text{or} \quad (E - \hat{H})\hat{G}(E) = \hat{1}. \quad (32)$$

It has a number of useful properties. For example, its Fourier transform in the time domain gives the time evolution operator for the system:

$$\hat{G}_r(\tau) = \int \frac{d\omega}{2\pi} \hat{G}(\hbar\omega + i\eta) \exp(-i\omega\tau) = -\frac{i}{\hbar} \theta(\tau) \exp(-i\hat{H}\tau/\hbar) = -\frac{i}{\hbar} \theta(\tau) \hat{U}(0, \tau), \quad (33)$$

where η is a positive infinitesimal and r stands for ‘retarded’. It is a true Green function for the Schrödinger equation, in that

$$(i\hbar\partial_t - \hat{H})\hat{G}_r(t - t') = \hat{1}\delta(t - t'). \quad (34)$$

Note also that poles in G correspond to eigenfunctions of \hat{H} , and its imaginary part is related to the density of states operator $\delta(E - \hat{H})$:

$$\delta(E - \hat{H}) = -\frac{1}{\pi} \Im \hat{G}(E + i\eta). \quad (35)$$

A continuum of states corresponds to a branch cut along the real energy axis. Note G by itself contains no information about the probability of occupancy of these states.

The embedding potential can also be applied to calculate G within the system subspace:

$$[E - \hat{H}_{SS} - \hat{H}_{SE}(E - \hat{H}_{EE})^{-1}\hat{H}_{ES}]\hat{G}_{SS} = (E - \hat{H}_{SS} - \hat{\Sigma})\hat{G}_{SS} = 0. \quad (36)$$

The residue of the pole in \hat{G}_{SS} corresponding to the appearance of a zero eigenvalue in $E - \hat{H}_{SS} - \hat{\Sigma}$ is then

$$R = \frac{1}{1 - \langle \psi_S | \frac{\partial \hat{\Sigma}}{\partial E} | \psi_S \rangle}, \quad (37)$$

where $|\psi_S\rangle$ is the eigenket corresponding to equation (30). The physical interpretation of this is that R is the fraction of the time the system spends in the S region when it is in the eigenstate ψ_S .

2.2 Time-dependent embedding

We can also do embedding in the time domain. Suppose for simplicity the Hamiltonian remains time-independent in the Schrödinger representation. Then the time-dependent S.E. becomes

$$\left[i\hbar\partial_t - \begin{pmatrix} \hat{H}_{SS} & \hat{H}_{SE} \\ \hat{H}_{ES} & \hat{H}_{EE} \end{pmatrix} \right] \begin{pmatrix} \Psi_S(t) \\ \Psi_E(t) \end{pmatrix} = 0. \quad (38)$$

From this we can obtain

$$i\hbar\partial_t \Psi_S(t) = \hat{H}_{SS}\Psi_S(t) + \int_{-\infty}^t dt' \hat{H}_{SE}\mathcal{G}(t-t')\hat{H}_{ES}\Psi_S(t')dt'. \quad (39)$$

Here \mathcal{G} is a retarded Green's function for the isolated environment (i.e. in the absence of any coupling to the system):

$$[i\hbar\partial_t - \hat{H}_{EE}]\mathcal{G}(t-t') = \hat{1}_{EE}\delta(t-t'). \quad (40)$$

The second term on the right is our first example of a *memory kernel*; its non-locality in time is a consequence of the energy-dependence of the embedding potential, and expresses the environment's memory of the previous state of the system.

2.3 The embedding potential in real space

The embedding potential is closely related to the boundary conditions the wavefunction has to obey in real space. Let's divide space into two parts, I and II, and we are interested in the wave function only within region I. Suppose it is known that a wavefunction $\psi(r)$ has to satisfy the time-independent Schrödinger equation (in atomic units) in some external region (region II). Then it can be shown (Inglesfield 1981) that the normal derivative at a point r_s on the surface S separating I and II obeys

$$\frac{\partial\psi(r_s)}{\partial n_s} = \int d^2r'_s \Sigma(r_s, r'_s)\psi(r'_s). \quad (41)$$

The nonlocal, energy-dependent operator Σ , which is defined on the surface S , is a real-space version of the embedding potential. (We don't have time to make this analogy explicit—see Fisher (1988) for more details.) Σ can be calculated from *any* Green's function G_0 obeying

$$[E - (-\frac{1}{2}\nabla_r^2 + V(r))]G_0(r, r') = \delta^3(r - r') \quad r, r' \in \text{II}. \quad (42)$$

Specifically,

$$\Sigma(r_s, r'_s) = G_0^{-1}(r_s, r'_s) + \frac{1}{2} \int d^2 r''_s G_0^{-1}(r_s, r''_s) \frac{\partial}{\partial n''_s} G_0(r''_s, r'_s), \quad (43)$$

where G_0^{-1} is the *surface* inverse of G_0 :

$$\int_S d^2 r''_s G_0^{-1}(r_s, r''_s) G_0(r''_s, r'_s) = \delta^2(r_s - r'_s). \quad (44)$$

Things look particularly simple if G_0 obeys the von Neumann boundary condition $\partial G_0 / \partial n = 0$ on S , in which case

$$\Sigma(r_s, r'_s) = G_0^{-1}(r_s, r'_s). \quad (45)$$

It is also possible to find a simple form if G_0 obeys the Dirichlet boundary condition $G_0 = 0$ on S ; in this case

$$\Sigma(r_s, r'_s) = -\frac{1}{4} \frac{\partial^2}{\partial n \partial n'} G_0(r_s, r'_s). \quad (46)$$

2.4 The embedding potential and scattering theory

Suppose we have some reference Hamiltonian, \hat{H}_0 , and that the true Hamiltonian \hat{H} differs from \hat{H}_0 by a perturbation \hat{V} which is non-zero only in the system region S . Suppose \hat{H}_0 is easily soluble, so we know the corresponding Green operator \hat{G}_0 . For example, \hat{H}_0 might correspond to a problem with a high degree of symmetry, such as

- A particle propagating in a vacuum;
- A perfectly ordered crystal.

Since the embedding potential $\hat{\Sigma} = \hat{H}_{SE}(E - \hat{H}_{EE})^{-1}\hat{H}_{ES}$ is independent of \hat{H}_{SS} , it is the same for both Hamiltonians, \hat{H} and \hat{H}_0 . We can therefore calculate it once and for all from the easily-found Green operator \hat{G}_0 :

$$\hat{G}_{0SS} = (E - \hat{H}_{0SS} - \hat{\Sigma})^{-1} \Rightarrow \hat{\Sigma} = E - \hat{H}_{0SS} - \hat{G}_{0SS}^{-1}. \quad (47)$$

In other words, Σ can be calculated if we can solve *any* problem with the same environment as the one we are interested in (Baraff and Schlüter 1986).

We can easily use equation (47) to make contact with another familiar way of solving this sort of problem. We could write the full Green operator \hat{G} corresponding to the Hamiltonian we are really interested in, \hat{H} , as

$$\hat{G}^{-1} = E - \hat{H}_0 - \hat{V} = \hat{G}_0^{-1} - \hat{V}. \quad (48)$$

Re-arranging gives Dyson's equation

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}. \quad (49)$$

Writing this out in the matrix system+environment representation gives

$$\begin{pmatrix} \hat{G}_{SS} & \hat{G}_{SE} \\ \hat{G}_{ES} & \hat{G}_{EE} \end{pmatrix} = \begin{pmatrix} \hat{G}_{0SS} & \hat{G}_{0SE} \\ \hat{G}_{0ES} & \hat{G}_{0EE} \end{pmatrix} + \begin{pmatrix} \hat{G}_{0SS} & \hat{G}_{0SE} \\ \hat{G}_{0ES} & \hat{G}_{0EE} \end{pmatrix} \begin{pmatrix} \hat{V}_{SS} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{G}_{SS} & \hat{G}_{SE} \\ \hat{G}_{ES} & \hat{G}_{EE} \end{pmatrix} \quad (50)$$

Picking out the SS block of this expression gives

$$\hat{G}_{SS} = \hat{G}_{0SS} + \hat{G}_{0SS} \hat{V}_{SS} \hat{G}_{SS}. \quad (51)$$

The significance of this is that Dyson's equation can be solved entirely within the system subspace, without worrying about the environment.

However, inserting equation (47) into equation (36) gives

$$\hat{G}_{SS}^{-1} = E - \hat{H}_{SS} - (E - \hat{H}_{0SS} - \hat{G}_{0SS}^{-1}) = \hat{G}_{0SS}^{-1} - \hat{V}_{SS}, \quad (52)$$

which rearranges exactly to the system part of the Dyson equation (51). The embedding potential therefore contains exactly the same information as standard scattering theory, but expressed in a different form.

2.5 Descriptions of many-particle systems

This is all very well if we want to consider a single particle which can either be 'here' (in S) or 'there' (in E). In the next lecture we will look at a problem (electron-molecule scattering) which fits nicely into this mould—but frequently we have many particles, any one of which can enter or leave the system. Suppose the particles are indistinguishable (bosons or fermions). Then we can describe them in two different ways.

2.5.1 The many-particle wavefunction

For an N -particle system, the wavefunction is a function of all N particle coordinates:

$$\Psi = \Psi(r_1, \dots, r_N), \quad (53)$$

with the symmetry condition

$$\Psi(r_1, \dots, r_i, \dots, r_j, \dots, r_N) = (-1)^\zeta \Psi(r_1, \dots, r_j, \dots, r_i, \dots, r_N), \quad (54)$$

and $\zeta = +1$ for fermions and $\zeta = -1$ for bosons.

Suppose we define our system S and environment E in terms of the location of individual particles. The many-particle Hilbert space is *no longer* a direct sum of system and environment parts; if we wanted to write it as a direct sum, we would have to distinguish cases in which there were zero, one, two, and so on up to N particles in the system, with the remainder in the environment. This is a mess!

2.5.2 The occupation-number representation

Suppose each of our particles can sit in any one of M states $\{|\phi_i\rangle\}$. These could be, for example

- Orbitals with a particular spin localized on or near a particular atom (in solid-state physics); or
- Positions in a discretized version of real space.

Let's assume for convenience these states are orthogonal (though that is not essential, so long as they are linearly independent). Then we can construct a complete basis set for the N -particle system from the symmetrized products:

$$|i_1, \dots, i_N\rangle = \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \phi_{i_1}(r_1) & \dots & \phi_{i_1}(r_N) \\ \dots & \dots & \dots \\ \phi_{i_N}(r_1) & \dots & \phi_{i_N}(r_N) \end{vmatrix} \quad (\text{fermions}) \quad (55)$$

$$= \frac{1}{\sqrt{N!}} \text{perm} \begin{vmatrix} \phi_{i_1}(r_1) & \dots & \phi_{i_1}(r_N) \\ \dots & \dots & \dots \\ \phi_{i_N}(r_1) & \dots & \phi_{i_N}(r_N) \end{vmatrix} \quad (\text{bosons}). \quad (56)$$

We can alternatively specify each $|i_1, \dots, i_N\rangle$ by the *occupation number* n_j of each state ϕ_j : this is simply the number of times state j appears in the set $\{i_1, \dots, i_N\}$. For fermions the occupation number must be 0 or 1; for bosons it can be any integer.

Let us divide the single-particle basis set into two subsets, corresponding to the system S and the environment E . Now the problem has a direct *product* structure: to specify a configuration of the system (one of the basis kets $\{|i_1, \dots, i_N\rangle\}$) we have to specify the values of the occupation numbers for both the system region and the environment region. If we know there are exactly N particles in the system, there is a constraint on the occupation numbers that

$$\sum_{i \in S} n_i + \sum_{j \in E} n_j = N. \quad (57)$$

However, if the system is very large then it generally makes no difference whether we work at fixed N or at fixed chemical potential; in that case, no constraint on the occupation numbers is necessary.

3 Handling direct-product systems

Reading:

- Nielsen & Chuang Chapter 8;
- Preskill Chapter 3.

3.1 Statistical mechanics: the conditional free energy

At equilibrium, we are used to the idea that we can concentrate on a small number of ‘relevant’ or ‘slow’ degrees of freedom (comparable to the variables describing our ‘system’); conventionally, the values of these quantities are used to define macrostates of a system. In classical statistical mechanics we can then define an effective free energy, which is a function of the N_S system variables $\{X_S, P_S\}$:

$$F_{\text{eff}}(X_S, P_S) = -k_B T \log \left[\frac{1}{h^{N_E}} \int d^{N_E} X_E d^{N_E} P_E \exp[-\beta H(X_S, P_S, X_E, P_E)] \right], \quad (58)$$

where $\{X_E, P_E\}$ are the (classical) degrees of freedom of the environment, and we suppose that there are N_E environmental degrees of freedom in all. The quantity thus defined has the property that the partition function is

$$Z = \frac{1}{h^{N_S}} \int d^{N_S} X_S d^{N_S} P_S \exp[-\beta F_{\text{eff}}(X_S, P_S)], \quad (59)$$

and therefore $\exp[-\beta F_{\text{eff}}(X_S, P_S)]/Z$ has the natural interpretation of a probability distribution function on the system variables.

The corresponding quantum expression is

$$Z = \text{Tr}_S[\exp(-\beta \hat{F}_{\text{eff}})], \quad (60)$$

where the system operator \hat{F}_{eff} is defined in terms of the overall (system + environment) Hamiltonian \hat{H} by

$$\hat{F}_{\text{eff}} = -k_B T \log \left[\text{Tr}_E[\exp(-\beta \hat{H})] \right]. \quad (61)$$

The system density matrix is then

$$\hat{\rho}_S = \frac{1}{Z} \exp[-\beta \hat{F}_{\text{eff}}]. \quad (62)$$

3.2 Quantum operations

Now we focus on the *evolution* of the system, rather than on its behaviour at equilibrium. If we make some general unitary operation \hat{U} on the system and its environment, what is its effect on the system? First suppose that the overall density operator is initially a direct product $\hat{\rho}_S \otimes \hat{\rho}_E$. (This is a significant approximation—we’ll come back to it later.) Let $\{|e_k\rangle\}$ be an orthonormal basis for the environment, and let $\hat{\rho}_E = |e_0\rangle\langle e_0|$ (i.e., suppose that the environment is in the pure state $|e_0\rangle$). This sounds like a further approximation, but in fact isn’t; suppose we had an environmental density operator corresponding to the mixed state

$$\hat{\rho}_E = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad (63)$$

where the N states $\{\psi_i\}$ are not necessarily orthogonal but are normalized, and $\sum_i p_i = 1$. Then we can always introduce an additional ‘far environment’, F , with an orthonormal set of at least N states $\{|f_i\rangle\}$. The following pure state of the combined $E + F$ system,

$$|\Psi\rangle = \sum_i \sqrt{p_i} |\psi_i\rangle |f_i\rangle, \quad (64)$$

has the property that its reduced density matrix in the original environment is

$$\text{Tr}_F[|\Psi\rangle\langle\Psi|] = \sum_{ij} \sqrt{p_i p_j} |\psi_i\rangle\langle\psi_j| \text{Tr}_F[|f_i\rangle\langle f_j|] = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \hat{\rho}_E, \quad (65)$$

and it is therefore indistinguishable (as far as any measurement within E only is concerned) from the original density matrix $\hat{\rho}_E$. This is referred to as a ‘purification’ of $\hat{\rho}_E$. For the moment we will suppose this has been done, and the original environment E replaced by a new, bigger, environment (which we will still, however label as E) in a pure state.

Now apply \hat{U} to

$$\mathcal{E}(\hat{\rho}_S) = \text{Tr}_E[\hat{U}(\hat{\rho}_S \otimes \hat{\rho}_E)\hat{U}^\dagger] \quad (66)$$

$$= \sum_k \langle e_k | \hat{U}(\hat{\rho}_S \otimes |e_0\rangle\langle e_0|) \hat{U}^\dagger |e_k\rangle \quad (67)$$

$$= \sum_k \hat{E}_k \hat{\rho}_S \hat{E}_k^\dagger, \quad (68)$$

where

$$E_k \equiv \langle e_k | \hat{U} |e_0\rangle. \quad (69)$$

Note that

$$\text{Tr}_S[\mathcal{E}(\hat{\rho})] = \text{Tr}_S \left[\sum_k E_k \hat{\rho} E_k^\dagger \right] = \text{Tr}_S \left[\sum_k E_k^\dagger E_k \hat{\rho} \right] = 1 \quad (70)$$

for any $\hat{\rho}$, so it follows that

$$\sum_k E_k^\dagger E_k = \hat{1}_S. \quad (71)$$

What sort of thing is \mathcal{E} ? It is more general than an ordinary operator, because it acts on density *operators* of the system, not on states of it. Hence it is called a **super-operator** (Preskill) or a **quantum operation** (Nielsen and Chuang).

3.2.1 The requirements for a quantum operation

It is clear from the way \mathcal{E} was introduced that any quantum operation ought generally to have certain properties.

1. It should *preserve the normalization* of the state:

$$\text{Tr}[\mathcal{E}(\hat{\rho})] = 1 \quad \text{if} \quad \text{Tr}\hat{\rho} = 1. \quad (72)$$

2. It should be *linear*:

$$\mathcal{E}\left(\sum_i p_i \hat{\rho}_i\right) = \sum_i p_i \mathcal{E}(\hat{\rho}_i). \quad (73)$$

3. It is *completely positive*: if we choose any possible environment E and any possible density joint density matrix $\hat{\rho}$ of the system and environment, then the result of the composite operation $(\mathcal{I} \otimes \mathcal{E})\hat{\rho}$ is another positive operator. (This requirement includes, but is more general than, the requirement that $\mathcal{E}(\hat{\rho}_S)$ be positive for any system density matrix $\hat{\rho}_S$.)

Most generally, a quantum operation is simply *defined* as a map from density operators to other density operators satisfying these conditions.

3.2.2 The Kraus representation theorem

It turns out that any quantum operation satisfying the conditions in §3.2.1 can be expressed in the form

$$\mathcal{E}(\hat{\rho}) = \sum_k \hat{E}_k \hat{\rho} \hat{E}_k^\dagger, \quad (74)$$

with

$$\sum_k \hat{E}_k^\dagger \hat{E}_k = \hat{1}. \quad (75)$$

The formula (74) is known as the *Kraus representation* or *operator-sum representation* of the quantum operation; the operators $\{\hat{E}_k\}$ known as the *Kraus operators*. Proof: see Preskill §3.3, or Nielsen and Chuang §8.2.4.

3.3 Examples

3.3.1 Unitary evolution

Unitary evolution of the system by itself trivially has the form of a quantum operation:

$$\hat{\rho}_S \rightarrow \hat{U}_S \hat{\rho}_S \hat{U}_S^\dagger, \quad (76)$$

with

$$\hat{U}_S^\dagger \hat{U}_S = \hat{1}_S. \quad (77)$$

3.3.2 Probabilistic unitary evolution

Suppose our system remains isolated, but its Hamiltonian is uncertain because of some (classical) random process. The result is that different Hamiltonians may be applied with probabilities p_i ; the resulting evolution is

$$\hat{\rho} \rightarrow \sum_i p_i \hat{U}_{Si} \hat{\rho}_S \hat{U}_{Si}^\dagger, \quad (78)$$

where \hat{U}_{Si} is the unitary evolution associated with Hamiltonian i . This has the form of a quantum operation with Kraus operators $\sqrt{p_i} \hat{U}_{Si}$.

3.3.3 Von Neumann measurements

Suppose we make a projective (von Neumann) measurement on our system. If the operator we measure is $\hat{O} = \sum_m o_m |m\rangle\langle m| \equiv \sum_m o_m \hat{P}_m$, then according to the standard von Neumann measurement postulate, result o_m is measured with probability $p_m = \langle m | \hat{\rho}_S | m \rangle = \text{Tr}_S[\hat{P}_m \hat{\rho}_S]$. In this event the state of the system is replaced by $\hat{P}_m \hat{\rho}_S \hat{P}_m^\dagger / p_m$.

We can therefore regard the whole measurement process as that of replacing

$$\rho_S \rightarrow \sum_m p_m \frac{\hat{P}_m \hat{\rho}_S \hat{P}_m^\dagger}{p_m} = \sum_m \hat{P}_m \hat{\rho}_S \hat{P}_m^\dagger, \quad (79)$$

where by construction $\sum_m \hat{P}_m \hat{P}_m^\dagger = \sum_i \hat{P}_m = \hat{1}_S$. The von Neumann measurement is therefore a special case of a quantum operation in which the Kraus operators are the projection operators \hat{P}_m .

3.3.4 POVMs

Now let's make it more general: allow the system *and* environment to interact by applying a unitary operator \hat{U} which simultaneously applies the operators \hat{M}_m to the system, and takes the environment from the fixed starting state $|e_0\rangle$ to some one particular environment state, say $|e_m\rangle$. Then

$$\hat{U}|\psi\rangle|e_0\rangle = \sum_m \hat{M}_m|\psi\rangle|e_m\rangle. \quad (80)$$

Normalization of this new state requires

$$\langle e_0|\langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle|e_0\rangle = \sum_m \langle\psi|\hat{M}_m^\dagger\hat{M}_m|\psi\rangle = 1. \quad (81)$$

If this is true for any ψ , we conclude that $\sum_m \hat{M}_m^\dagger\hat{M}_m = \hat{I}_S$. The operators $\hat{M}_m\hat{M}_m^\dagger$ are often said to form a **positive operator-valued measure** (POVM—see Nielsen& Chuang §§2.2.3–2.2.6, or Preskill §3.1).

Having ensured that the system and the environment are correlated in this way, we now measure the state of the *environment* (rather than of the system), using the operator $\hat{O} = \hat{I}_S \otimes \sum_m o_m|e_m\rangle\langle e_m| \equiv \sum_m o_m\hat{P}_m$. The probability of outcome m is

$$p_m = \langle e_0|\langle\psi|\hat{U}^\dagger(\hat{I}_S \otimes |e_m\rangle\langle e_m|)\hat{U}|\psi\rangle|e_0\rangle \quad (82)$$

$$= \sum_{m'm''} \langle e_{m'}|\langle\psi|\hat{M}_{m'}^\dagger(\hat{I}_S \otimes |e_m\rangle\langle e_m|)\hat{M}_{m''}|\psi\rangle|e_{m''}\rangle \quad (83)$$

$$= \sum_m \langle\psi|\hat{M}_m^\dagger\hat{M}_m|\psi\rangle, \quad (84)$$

and in this event the state of the whole system is

$$\frac{\hat{P}_m\hat{U}|\psi\rangle|e_0\rangle}{\sqrt{p_m}} = \frac{\hat{M}_m|\psi\rangle|e_m\rangle}{\sqrt{p_m}}. \quad (85)$$

The effect of the whole process on the reduced density matrix of the system is to take

$$\hat{\rho}_S \rightarrow \sum_m p_m \frac{\hat{M}_m\hat{\rho}_S\hat{M}_m^\dagger}{p_m} = \sum_m \hat{M}_m\hat{\rho}_S\hat{M}_m^\dagger. \quad (86)$$

The process of generalized measurement is therefore equivalent to a quantum operation in which the Kraus operators are the generalized measurement operators $\{\hat{M}_m\}$. Note this is more general than the case of a von Neumann measurement, because the operators \hat{M}_m need not be projectors.

3.4 Quantum channels

Finally let's see some examples of quantum operations on a single spin-1/2. These are often called 'quantum channels'—think of Alice transmitting a spin to Bob through a channel which may introduce noise or distortions by interaction with the environment.

3.4.1 The depolarizing channel

A process in which the density matrix is replaced by the completely mixed state $\hat{1}/2$ with probability p , and left unchanged with probability $(1-p)$. Hence

$$\mathcal{E}(\rho) = \frac{p}{2}\hat{1} + (1-p)\hat{\rho} = \frac{p'}{3}(\hat{\sigma}_x\hat{\rho}\hat{\sigma}_x + \hat{\sigma}_y\hat{\rho}\hat{\sigma}_y + \hat{\sigma}_z\hat{\rho}\hat{\sigma}_z) + (1-p')\hat{\rho}, \quad (87)$$

where $p' = 3p/4$. The depolarizing channel reduces the radius of the Bloch sphere by a factor $1 - p$, while preserving its shape. Its Kraus operators can be written

$$E_0 = \sqrt{1 - p'}\hat{1}; \quad E_1 = \sqrt{\frac{p'}{3}}\hat{\sigma}_x; \quad E_2 = \sqrt{\frac{p'}{3}}\hat{\sigma}_y; \quad E_3 = \sqrt{\frac{p'}{3}}\hat{\sigma}_z. \quad (88)$$

3.4.2 The bit-flip channel

This is a process in which the spin is flipped from up to down (or vice versa) using the operator $\hat{\sigma}_x$, with probability p :

$$\mathcal{E}(\hat{\rho}) = p\hat{\sigma}_x\hat{\rho}\hat{\sigma}_x + (1 - p)\hat{\rho}. \quad (89)$$

(Note I have interchanged p and $1 - p$ from the definition given by Nielsen & Chuang in their text, but agree with the definition used for their Figure 8.8.) Its effect is to leave the x -axis of the Bloch sphere unchanged, but to compress the y - and z -axes by a factor $1 - 2p$. Its Kraus operators can be written

$$E_0 = \sqrt{1 - p}\hat{1}; \quad E_1 = \sqrt{p}\hat{\sigma}_x. \quad (90)$$

3.4.3 The phase-flip channel

It is then easy to see that the operation

$$\mathcal{E}(\hat{\rho}) = p\hat{\sigma}_z\hat{\rho}\hat{\sigma}_z + (1 - p)\hat{\rho} \quad (91)$$

performs a corresponding compression of the Bloch sphere by a factor $1 - 2p$ in the the xy -plane. In the normal z basis, it therefore suppresses the off-diagonal matrix elements of $\hat{\rho}$ while leaving the diagonal ones unaltered. This is the type of process that contributes to T_2 -relaxation in spin resonance. Its Kraus operators can be written

$$E_0 = \sqrt{1 - p}\hat{1}; \quad E_1 = \sqrt{p}\hat{\sigma}_z. \quad (92)$$

In case you're wondering, the corresponding channel for applying $\hat{\sigma}_y$,

$$\mathcal{E}(\hat{\rho}) = p\hat{\sigma}_y\hat{\rho}\hat{\sigma}_y + (1 - p)\hat{\rho} \quad (93)$$

has the effect of compressing the xz -plane by a factor $1 - 2p$ and can be thought of as a combination of bit-flip and phase-flip, since $\hat{\sigma}_z\hat{\sigma}_x = i\hat{\sigma}_y$.

3.4.4 The amplitude-damping channel

Finally consider an operation which produces a 'downward' decay only, from $|\downarrow\rangle$ to $|\uparrow\rangle$, with probability p . (This would be a suitable model for spontaneous emission from an atom, or for a T_1 process in spin resonance at very low temperature.) Thus one of the Kraus operators ought to be

$$\hat{E}_1 = \sqrt{p} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad (94)$$

From the requirement that $\sum_k \hat{E}_k \hat{E}_k^\dagger = 1$, we see that a suitable Kraus operator to complete the set would be

$$\hat{E}_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1 - p} \end{pmatrix} \quad (95)$$

The effect on the Bloch sphere is to ‘squash’ it towards the North pole into an ellipsoid, so that in the z -direction its height is reduced by a factor $1 - p$, while its radius in the xy -plane is reduced by a factor $\sqrt{1 - p}$.

The introduction of ‘upward’ as well as ‘downward’ decay processes generalizes the channel so that it becomes appropriate for an environment at finite temperature (see Nielsen & Chuang §8.3.5).

4 The Markovian limit

Further reading:

- Preskill §3.5.
- Breuer & Petruccione Chapter 3 (especially §3.2).

To start with, let's define three timescales.

- τ_S , the characteristic timescale on which the system itself evolves;
- τ_E , the characteristic timescale on which the environment evolves and hence 'forgets' information about its initial state;
- τ_R , the rate at which the relaxation of the system as a result of its interaction with the environment occurs.

4.1 The Lindblad master equation.

The theory of quantum operations supposes that things just 'happen' to the system's density matrix—we don't ask why, or how fast. Now let's start looking at the dynamics, but let's do so on a timescale δt that has to satisfy two conditions.

- δt should be small compared with the characteristic timescale of the system—so the system density matrix only evolves 'a little bit' in this time interval (i.e. $\delta t \ll \tau_S$).
- But δt should also be long compared with the time over which the environment 'forgets' its information about the system (i.e. $\delta t \gg \tau_E$).

Since we are beyond the timescale τ_E , we might hope that the evolution of the system will depend only on the present system density matrix, and not on anything that has happened in the past. In that case the evolution through time δt should be described by a quantum operation on the current system density matrix. The idea is to look for a suitable quantum operation such that $\hat{\rho}_S$ should be altered only to order δt :

$$\hat{\rho}_S(\delta t) = \mathcal{E}(\hat{\rho}_S(0)) = \sum_k \hat{E}_k \hat{\rho}_S(0) \hat{E}_k^\dagger = \hat{\rho}_S(0) + O(\delta t). \quad (96)$$

Thus it follows that one of the Kraus operators, \hat{E}_0 say, must be $\hat{1}_S + O(\delta t)$, and the others must be $O(\sqrt{\delta t})$. So, let's write

$$\hat{E}_0 = \hat{1}_S + (\hat{K} - \frac{i}{\hbar} \hat{H}) \delta t, \quad (97)$$

$$\hat{E}_k = \sqrt{\delta t} \hat{L}_k, \quad k \geq 1. \quad (98)$$

Here \hat{K} and \hat{H} are Hermitian operators, but are otherwise arbitrary at this stage; the operators \hat{L}_k are also arbitrary and are known as **Lindblad operators** (note that they need be neither unitary nor Hermitian). However, the normalization condition on the Kraus operators requires

$$\sum_k \hat{E}_k^\dagger \hat{E}_k = \hat{1}_S \quad \Rightarrow \quad \hat{1}_S = \hat{1}_S + (2\hat{K} + \sum_k \hat{L}_k^\dagger \hat{L}_k) \delta t + O(\delta t)^2. \quad (99)$$

Hence

$$\hat{K} = -\frac{1}{2} \sum_k \hat{L}_k^\dagger \hat{L}_k, \quad (100)$$

and therefore

$$\hat{\rho}_S(\delta t) = [\hat{1}_S + \delta t(\hat{K} - \frac{i}{\hbar}\hat{H})]\hat{\rho}(0)[\hat{1}_S + \delta t(\hat{K} + \frac{i}{\hbar}\hat{H})] + \delta t \sum_k \hat{L}_k \hat{\rho}(0) \hat{L}_k^\dagger \quad (101)$$

$$= \hat{\rho}_S(0) - \left\{ \frac{i}{\hbar} [\hat{H}, \hat{\rho}_S(0)] + \sum_k \left[\hat{L}_k \hat{\rho}_S(0) \hat{L}_k^\dagger - \frac{1}{2} \{ \hat{\rho}_S(0), \hat{L}_k^\dagger \hat{L}_k \} \right] \right\} \delta t + O(\delta t)^2, \quad (102)$$

where $\{\hat{A}, \hat{B}\}$ represents the anti-commutator $\hat{A}\hat{B} + \hat{B}\hat{A}$. Taking the limit $\delta t \rightarrow 0$ we obtain the **Lindblad master equation**:

$$\frac{d\hat{\rho}_S}{dt} = \frac{1}{i\hbar} [\hat{H}, \hat{\rho}_S] + \sum_k \left[\hat{L}_k \hat{\rho}_S(0) \hat{L}_k^\dagger - \frac{1}{2} \{ \hat{\rho}_S(0), \hat{L}_k^\dagger \hat{L}_k \} \right]. \quad (103)$$

Note that:

- If there were no Lindblad operators (i.e., if there were only one Kraus operator in the decomposition (96), this formula would reduce to equation (12). We would then identify \hat{H} as the Hamiltonian of the (closed) system.
- However, there is in general no reason to suppose that the operator \hat{H} appearing in equation(103) is the Hamiltonian of the isolated system. Indeed, we shall see later that there are (potentially important) corrections to it that come from the interaction with the environment.
- Indeed, \hat{H} is not even unique; the equation of motion remains invariant under the changes

$$\hat{L}_k \rightarrow \hat{L}_k + l_k \hat{1}_S, \quad \hat{H} \rightarrow \hat{H} + \frac{1}{2i} \sum_k (l_k^* \hat{L}_k - l_k \hat{L}_k^\dagger) + b \hat{1}_S, \quad (104)$$

where $\{l_k\}$ and b are arbitrary scalars. The equation of motion also remains invariant under an arbitrary unitary transformation of the Lindblad operators:

$$\hat{L}_k \rightarrow \sum_j u_{kj} \hat{L}_j. \quad (105)$$

- The right-hand side of equation (103) is a linear functional of $\hat{\rho}_S$; it defines the Lindbladian super-operator \mathcal{L} through

$$\frac{d\hat{\rho}_S}{dt} = \mathcal{L}[\hat{\rho}_S]. \quad (106)$$

The formal solution to this can be written in the form of a time-evolution super-operator:

$$\hat{\rho}_S(t) = \mathcal{V}(T) \hat{\rho}_S(0) \equiv \hat{T}_{\leftarrow} \exp\left[\int_0^t \mathcal{L}(s) ds\right] \hat{\rho}_S(0). \quad (107)$$

Here \hat{T}_{\leftarrow} is the same entity we previously called \hat{T} : the time-ordering operator that puts earliest times to the right and latest times to the left. Provided the Lindbladian is time-independent, this can be simplified to

$$\hat{\rho}_S(t) = \exp(\mathcal{L}t) \hat{\rho}_S(0). \quad (108)$$

Note however that this is not a recipe for efficient practical calculations; if the dimension of the system's Hilbert space is N , a matrix representation for \mathcal{L} would contain $N^2 \times N^2$ elements; directly exponentiating it would therefore require $O(N^4)$ operations.

- The term involving the Lindblad operators on the RHS of equation (103) is known as the *dissipator*, written $\mathcal{D}[\hat{\rho}]$; thus we have

$$\mathcal{L}[\hat{\rho}_S] = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}_S] + \mathcal{D}[\hat{\rho}_S] \quad (109)$$

- This is all in the Schrödinger representation, where the wavefunction (or density matrix) is time-dependent but operators are not. An alternative way of representing the information is to transfer the time-dependence to the operators: we then require that the expectation value of any (system) operator \hat{O} be the same in either picture.

$$\text{Tr}_S[\hat{O}\hat{\rho}_S(t)] = \text{Tr}_S[\hat{O}(\mathcal{V}\hat{\rho}_S(0))] = \text{Tr}_S[(\mathcal{V}^\dagger(t)\hat{O})\hat{\rho}_S(0)] \equiv \text{Tr}_S[\hat{O}_H(t)\hat{\rho}_S(0)], \quad (110)$$

where $\mathcal{V}^\dagger(t) \equiv \hat{T}_{\leftarrow} \exp[\int_0^t \mathcal{L}^\dagger(s)ds]$, and the operator \hat{T}_{\leftarrow} orders in the opposite sense to normal (i.e. earliest times to the left). Note that \hat{O}_H obeys the equation of motion

$$\frac{d\hat{O}_H}{dt} = \mathcal{V}^\dagger(t)\mathcal{L}^\dagger(t)\hat{O}. \quad (111)$$

In the case of a time-independent Lindbladian things simplify once again, and

$$\hat{O}_H(t) = \exp[\mathcal{L}^\dagger t]\hat{O}, \quad \frac{d\hat{O}_H}{dt} = \mathcal{L}^\dagger(t)\hat{O}_H(t). \quad (112)$$

4.2 Example: spontaneous emission.

This is essentially the continuous version of the amplitude damping channel we discussed in §3.4.4. We take a two-level atom represented using the Pauli matrices, and assume we have a Hamiltonian

$$\hat{H} = -\frac{\hbar\omega_0}{2}\sigma_z \quad (113)$$

(where ω_0 is the energy difference between the ground and excited states, and the minus sign gives us the usual convention that $|\uparrow\rangle = |0\rangle$ is the ground state and $|\downarrow\rangle = |1\rangle$ the excited state) and a single Lindblad operator

$$\hat{L} = \sqrt{\Gamma} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \quad (114)$$

Thus

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = i\omega_0 \begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix} + \Gamma \begin{pmatrix} \rho_{11} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & -\rho_{11} \end{pmatrix}. \quad (115)$$

The solutions are

$$\begin{aligned} \rho_{00}(t) &= \rho_{00}(0) + \rho_{11}(0)[1 - \exp(-\Gamma t)]; & \rho_{11}(t) &= \rho_{11}(0) \exp(-\Gamma t); \\ \rho_{01}(t) &= \rho_{01}(0) \exp[(i\omega_0 - \Gamma/2)t]; & \rho_{10}(t) &= \rho_{10}(0) \exp[(-i\omega_0 - \Gamma/2)t]. \end{aligned} \quad (116)$$

Notice that the population in the excited state $|1\rangle$ decays exponentially with a time constant $T_1 = 1/\Gamma$, whereas the off-diagonal elements of the density matrix ('coherences') decay with a longer time constant $T_2 = 2/\Gamma$. (The fact that $T_1 = \frac{1}{2}T_2$ corresponds exactly to the fact that the xy -plane of the Bloch sphere is 'squashed' more slowly than the z -axis in the amplitude damping channel.)

4.3 Example: the Bloch equations in magnetic resonance for spin 1/2

A spin precessing in a static magnetic field (chosen to be in the z -direction) is described by a similar Hamiltonian

$$\hat{H} = -\frac{\hbar\omega_0}{2}\sigma_z, \quad (117)$$

where now $\omega_0 = \mu B$ is the Larmor frequency. However there are now three types of process we might want to describe with Lindblad operators:

$$\begin{aligned} \hat{L}_1 &= \sqrt{\Gamma_1}\sigma_+ = \sqrt{\Gamma_1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \\ \hat{L}_2 &= \sqrt{\Gamma_2}\sigma_- = \sqrt{\Gamma_2} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \\ \hat{L}_3 &= \sqrt{\Gamma_3}\sigma_z = \sqrt{\Gamma_3} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \quad (118)$$

\hat{L}_1 describes relaxation from $|1\rangle$ to $|0\rangle$ with the emission of energy (c.f. the amplitude damping channel); \hat{L}_2 describes the reverse relaxation from $|0\rangle$ to $|1\rangle$ with the absorption of energy; \hat{L}_3 describes pure dephasing processes which do not transfer energy between the spin and its environment (c.f. the phase-flip channel).

Thus the Lindblad equation becomes

$$\begin{aligned} \frac{\partial}{\partial t} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} &= i\omega_0 \begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix} + \Gamma_1 \begin{pmatrix} \rho_{11} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & -\rho_{11} \end{pmatrix} + \Gamma_2 \begin{pmatrix} -\rho_{00} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & \rho_{00} \end{pmatrix} \\ &+ \Gamma_3 \begin{pmatrix} 0 & -2\rho_{01} \\ -2\rho_{10} & 0 \end{pmatrix}. \end{aligned} \quad (119)$$

The solutions are now

$$\begin{aligned} \rho_{00}(t) &= \rho_{00}^{\text{eqm}} + (\rho_{00}(0) - \rho_{00}^{\text{eqm}}) \exp(-t/T_1); & \rho_{11}(t) &= \rho_{11}^{\text{eqm}} + (\rho_{11}(0) - \rho_{11}^{\text{eqm}}) \exp(-t/T_1); \\ \rho_{01}(t) &= \rho_{01}(0) \exp[(i\omega_0 - T_2^{-1})t]; & \rho_{10}(t) &= \rho_{10}(0) \exp[(-i\omega_0 - T_2^{-1})t], \end{aligned} \quad (120)$$

where the equilibrium populations ρ_{00}^{eqm} and ρ_{11}^{eqm} satisfy

$$\Gamma_1 \rho_{11}^{\text{eqm}} = \Gamma_2 \rho_{00}^{\text{eqm}}, \quad (121)$$

and the relaxation times T_1 and T_2 are now given by

$$T_1^{-1} = \Gamma_1 + \Gamma_2; \quad (122)$$

$$T_2^{-1} = 2\Gamma_3 + \frac{(\Gamma_1 + \Gamma_2)}{2}. \quad (123)$$

If the steady-state populations given by equation (121) are to correspond to the thermal equilibrium populations of the spin in an applied field, we must have the detailed balance condition

$$\frac{\Gamma_2}{\Gamma_1} = \exp(-\beta\hbar\omega_0). \quad (124)$$

We would expect (and will confirm later) that the \hat{L}_1 process involves the emission (spontaneous or stimulated) of phonons, and the \hat{L}_2 process comes from the absorption of phonons. Hence we expect

$$\Gamma_1 = \gamma[1 + n(\omega_0)]; \quad \Gamma_2 = \gamma n(\omega_0), \quad (125)$$

where $n(\omega)$ is the Bose occupation number

$$n(\omega) = \frac{1}{1 - \exp(-\beta\hbar\omega)}. \quad (126)$$

From this we deduce that

$$T_1^{-1} = \Gamma_1 + \Gamma_2 = \gamma[2n(\omega_0) + 1] = \gamma e^{\beta\hbar\omega_0} \coth\left(\frac{\beta\hbar\omega_0}{2}\right); \quad (127)$$

$$T_2^{-1} = 2\Gamma_3 + T_1^{-1}/2. \quad (128)$$

Note that T_2 may be much shorter than T_1 if the pure dephasing process is fast (i.e. if Γ_3 is large, as is frequently the case).

An alternative way of writing the equation of motion (119) is in terms of the components of the Bloch vector $\vec{\alpha}$:

$$\frac{d\alpha_z}{dt} = -\frac{(\alpha_z - \alpha_z^{\text{eqm}})}{T_1}; \quad (129)$$

$$\frac{d\alpha_x}{dt} = -\omega_0\alpha_y - \alpha_x/T_2; \quad (130)$$

$$\frac{d\alpha_y}{dt} = \omega_0\alpha_x - \alpha_y/T_2, \quad (131)$$

where the mean magnetization is $\alpha_z^{\text{eqm}} = \tanh(\beta\hbar\omega_0/2)$. This makes it explicit that the motion is a combination of free precession about the z -axis and relaxation towards the equilibrium magnetization $(0, 0, \alpha_z^{\text{eqm}})$. Note that equation (129) is essentially that written down by Marshall in his lecture to describe the decay of the net spin population (which he called $N_L - N_U$).

4.4 The Pauli master equation

The examples in sections §4.2 and §4.3 share the property that the equation of motion for the populations (diagonal elements of ρ) involve only other diagonal elements. This is generally true provided the following conditions are satisfied (as they are surprisingly often).

1. We choose a basis which diagonalizes \hat{H} ; in that case the Hamiltonian part of the evolution has no effect on the populations.
2. Each Lindblad operator has at most non-zero entry in each row and column—in other words, it connects each basis state to at most one other basis state. In that case the Lindblad operators contribute the following terms to the equation of motion for the diagonal element ρ_{nn} :

$$\partial_t \rho_{nn}(t) = \sum_k [(L_k)_{nm_k} \rho_{m_k m_k} (L_k^\dagger)_{m_k n} - |L_{k, nm_k}|^2 \rho_{nn}] = \sum_k |L_{k, nm_k}|^2 (\rho_{m_k m_k} - \rho_{nn}), \quad (132)$$

where it is assumed that Lindblad operator k couples state n only to state m_k .

The resulting set of equations for the populations $P(n, t) = \rho_{nn}(t)$ can be written in the more familiar form

$$\partial_t P(n, t) = \sum_m [W(n \leftarrow m)P(m, t) - W(m \leftarrow n)P(n, t)], \quad (133)$$

where

$$W(n \leftarrow m) = \sum_k |L_{k, nm_k}|^2 \delta_{m, m_k}. \quad (134)$$

Equation (133) is known as the **Pauli master equation**; it constitutes a set of purely classical kinetic equations describing the evolution of the populations of the system's quantum states.

4.5 The Markovian weak-coupling limit

This is all very well, but where might the dynamics described in the master equations actually come from in terms of microscopic interactions? We start by answering this in the simplest case, where the system is coupled weakly to the environment.

Further reading:

- Breuer & Petruccione §3.3.

4.5.1 The interaction representation

In any system where the Hamiltonian can be split into two parts

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad (135)$$

it is often convenient to partition similarly the time-dependence in such a way that the operators evolve with time according to the unperturbed Hamiltonian \hat{H}_0 (which we assume is time-independent):

$$\frac{d\hat{O}_I(t)}{dt} = \frac{1}{i\hbar}[\hat{O}_I(t), \hat{H}_0] \quad (136)$$

$$\hat{O}_I(t) = \exp(i\hat{H}_0 t/\hbar)\hat{O}_S \exp(-i\hat{H}_0 t/\hbar) \quad (137)$$

for an operator \hat{O} that has no intrinsic time-dependence, where $\hat{O}_S = \hat{O}_I(0)$ is the corresponding operator in the Schrödinger representation. Meanwhile the corresponding wavefunction obeys

$$\partial_t |\Psi_I(t)\rangle = \frac{1}{i\hbar} \hat{H}_{1I}(t) |\Psi_I(t)\rangle, \quad (138)$$

$$|\Psi_I(t)\rangle = \hat{U}_I(t, 0) |\Psi(0)\rangle, \quad (139)$$

$$\hat{U}_I(t, 0) = \hat{T}_{\leftarrow} \exp \left[\frac{-i}{\hbar} \int_0^t dt' \hat{H}_{1I}(t') \right]. \quad (140)$$

where $\hat{H}_{1I}(t)$ is the interaction representation form of \hat{H}_1 . Hence the density matrix obeys

$$\partial_t \hat{\rho}_I(t) = \frac{1}{i\hbar} [\hat{H}_{1I}(t), \hat{\rho}_I(t)], \quad (141)$$

$$\hat{\rho}_I(t) = \hat{U}_I(t, 0) \hat{\rho}(0) [\hat{U}_I(t, 0)]^\dagger. \quad (142)$$

4.5.2 The Redfield Equation

Write the Hamiltonian as

$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_I, \quad (143)$$

where only \hat{H}_I involves both the system and environment degrees of freedom. Work in the interaction representation with \hat{H}_I as the perturbation (so \hat{H}_0 corresponds to uncoupled system and environment). So the equation of motion of the density matrix in the interaction representation is

$$\frac{d\hat{\rho}(t)}{dt} = \frac{1}{i\hbar} [\hat{H}_I(t), \hat{\rho}(t)]. \quad (144)$$

(We suppress the subscript I for interaction representation quantities, as everything will be in the interaction representation until further notice.) This has formal solution

$$\hat{\rho}(t) = \hat{\rho}(0) + \frac{1}{i\hbar} \int_0^t ds [\hat{H}_I(s), \hat{\rho}(s)], \quad (145)$$

which gives

$$\frac{d\hat{\rho}(t)}{dt} = \frac{1}{i\hbar}[\hat{H}_I(t), \hat{\rho}(0)] - \frac{1}{\hbar^2} \int_0^t ds [\hat{H}_I(t), [\hat{H}_I(s), \hat{\rho}(s)]]. \quad (146)$$

Tracing over the environment gives

$$\frac{d\hat{\rho}_S(t)}{dt} = \frac{1}{i\hbar} \text{Tr}_E[\hat{H}_I(t), \hat{\rho}(0)] - \frac{1}{\hbar^2} \int_0^t ds \text{Tr}_E[\hat{H}_I(t), [\hat{H}_I(s), \hat{\rho}(s)]]. \quad (147)$$

(note the subscript S stands for ‘system’, not ‘Schrödinger’—we are still in the interaction representation). We now make

- **Assumption 1.** The first term on the RHS of (147) is zero. This is not really an assumption: we can always absorb terms into the system Hamiltonian \hat{H}_S so as to ensure that the mean value of the interaction Hamiltonian, averaged over the density matrix of the environment, is zero: $\text{Tr}_E[\hat{H}_I(t)\hat{\rho}(0)] = 0$.

More importantly, we also make

- **Assumption 2** (known as the Born Approximation in this literature). We suppose that the density matrix factors approximately at all times into $\hat{\rho}(t) = \hat{\rho}_S(t) \otimes \hat{\rho}_E$, where $\hat{\rho}_E$ is independent of time. This assumes weak system-environment coupling.

Assumptions 1 and 2 together enable us to write

$$\frac{d\hat{\rho}_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t ds \text{Tr}_E[\hat{H}_I(t), [\hat{H}_I(s), \hat{\rho}_S(s) \otimes \hat{\rho}_E]]. \quad (148)$$

We now make

- **Assumption 3** (Markovian approximation, first part). We suppose that the timescales over which the ‘memory’ represented by the integral in equation (148) is important are sufficiently short that the system density matrix is hardly different from its current value, so we can replace $\hat{\rho}_S(s) \rightarrow \hat{\rho}_S(t)$.

Hence

$$\frac{d\hat{\rho}_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t ds \text{Tr}_E[\hat{H}_I(t), [\hat{H}_I(s), \hat{\rho}_S(t) \otimes \hat{\rho}_E]]. \quad (149)$$

This is known as the **Redfield equation**. It is time-local (only involves $\hat{\rho}_S(t)$), but still contains an explicit reference to the ‘starting time’ at $t = 0$. This dependence on the past can be made explicit by substituting $s = t - s'$, in terms of which

$$\frac{d\hat{\rho}_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t ds' \text{Tr}_E[\hat{H}_I(t), [\hat{H}_I(t - s'), \hat{\rho}_S(t) \otimes \hat{\rho}_E]]. \quad (150)$$

Now we make further

- **Assumption 4** (Markovian approximation, second part). We suppose that we can extend the integral on the RHS of equation (150) to infinity without significantly altering the results.

Thus we have

$$\frac{d\hat{\rho}_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^\infty ds' \text{Tr}_E[\hat{H}_I(t), [\hat{H}_I(t - s'), \hat{\rho}_S(t) \otimes \hat{\rho}_E]]. \quad (151)$$

This equation is fully Markovian in the sense that it depends only on the current density matrix $\hat{\rho}_S(t)$ and contains no explicit reference to any other time.

Assumptions 3 and 4 correspond to requiring that the time be large compared with the timescale of the environment’s memory of what the system has done to it: $t \gg \tau_E$.

4.5.3 Correlation functions

To see what we've done, it helps to write equation (151) in terms of the **correlation functions** of the environment. First decompose the interaction Hamiltonian into

$$\hat{H}_I(t) = \sum_{\alpha} \hat{A}_{\alpha}(t) \otimes \hat{B}_{\alpha}(t), \quad (152)$$

where \hat{A} is a system operator, and \hat{B} is an environment operator. Note that, although it is not necessary for each individual \hat{A} and \hat{B} to be Hermitian, the Hermitian conjugate of each operator must also appear in the sum, so we can also write

$$\hat{H}_I(t) = \sum_{\alpha} \hat{A}_{\alpha}^{\dagger}(t) \otimes \hat{B}_{\alpha}^{\dagger}(t), \quad (153)$$

Now define the correlation function

$$C_{\alpha\beta}(s) \equiv \text{Tr}_E[\hat{B}_{\alpha}^{\dagger}(t)\hat{B}_{\beta}(t-s)\hat{\rho}_E] = \text{Tr}_E[\hat{B}_{\alpha}^{\dagger}(s)\hat{B}_{\beta}(0)\hat{\rho}_E], \quad (154)$$

where the second equality follows if the environment is stationary. Now we can rewrite equation (151) as

$$\begin{aligned} \frac{d\hat{\rho}_S(t)}{dt} &= \frac{1}{\hbar^2} \int_0^{\infty} ds' \text{Tr}_E[\hat{H}_I(t-s')\hat{\rho}_S(t) \otimes \hat{\rho}_E \hat{H}_I(t) - \hat{H}_I(t)\hat{H}_I(t-s')\hat{\rho}_S(t) \otimes \hat{\rho}_E] + \text{h.c.} \\ &= \frac{1}{\hbar^2} \int_0^{\infty} ds' \sum_{\alpha\beta} C_{\alpha\beta}(s) [\hat{A}_{\beta}(t-s)\hat{\rho}_S(t)\hat{A}_{\alpha}^{\dagger}(t) - \hat{A}_{\alpha}^{\dagger}(t)\hat{A}_{\beta}(t-s)\hat{\rho}_S(t)] + \text{h.c.} \end{aligned} \quad (155)$$

Now it's clear exactly which environmental timescales have to be short: the relevant τ_E is the time beyond which the correlation functions of the environmental operators that couple to the system decay.

To go further we need an explicit form for the time-dependence of the system operators \hat{A} . It turns out that different approximations are useful in the limit $\tau_S \ll \tau_R$ (good qubits) and $\tau_S \gg \tau_R$ (bad qubits).

4.6 Good qubits—the rotating wave approximation

If the system evolves very fast compared to any environmentally-induced relaxation, it makes sense to decompose the system operators into parts evolving with definite frequencies. Hence we write

$$\hat{A}_{\alpha}(t) = \sum_{\omega} e^{-i\omega t} \hat{A}_{\alpha}(\omega), \quad (156)$$

where

$$\hat{A}_{\alpha}(\omega) = \sum_{\epsilon, \epsilon' \text{ s.t. } \epsilon' - \epsilon = \hbar\omega} \Pi(\epsilon) \hat{A}_{\alpha} \Pi(\epsilon'), \quad (157)$$

where $\Pi(\epsilon)$ projects onto the eigenstates of \hat{H}_S having eigenvalue ϵ . A typical example would be in the spin system of §4.3, where we could put

$$\sigma_x(t) = e^{-i\omega_0 t} \sigma_+ + e^{i\omega_0 t} \sigma_-. \quad (158)$$

So, now we have

$$\begin{aligned} \frac{d\hat{\rho}_S(t)}{dt} &= \frac{1}{\hbar^2} \sum_{\omega\omega'} \int_0^{\infty} ds e^{i\omega s} \sum_{\alpha\beta} C_{\alpha\beta}(s) e^{i(\omega' - \omega)t} [\hat{A}_{\beta}(\omega)\hat{\rho}_S(t)\hat{A}_{\alpha}^{\dagger}(\omega') - \hat{A}_{\alpha}^{\dagger}(\omega')\hat{A}_{\beta}(\omega)\hat{\rho}_S(t)] + \text{h.c.} \\ &= \frac{1}{\hbar^2} \sum_{\omega\omega'} \Gamma_{\alpha\beta}(\omega) e^{i(\omega' - \omega)t} [\hat{A}_{\beta}(\omega)\hat{\rho}_S(t)\hat{A}_{\alpha}^{\dagger}(\omega') - \hat{A}_{\alpha}^{\dagger}(\omega')\hat{A}_{\beta}(\omega)\hat{\rho}_S(t)] + \text{h.c.}, \end{aligned} \quad (159)$$

where

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds e^{i\omega s} C_{\alpha\beta}(s) \quad (160)$$

is the *causal* (since it only involves $s > 0$) Fourier transform of the correlation function $C_{\alpha\beta}$. We now make

- **Approximation 5** (the Rotating Wave Approximation—RWA). This corresponds to saying that any term like $e^{i(\omega-\omega')t}$ averages to zero on the timescales relevant to relaxation processes, so we only need to keep terms with $\omega = \omega'$.

This assumption simplifies our expression to

$$\frac{d\hat{\rho}_S(t)}{dt} = \frac{1}{\hbar^2} \sum_\omega \sum_{\alpha\beta} \Gamma_{\alpha\beta}(\omega) [\hat{A}_\beta(\omega) \hat{\rho}_S(t) \hat{A}_\alpha^\dagger(\omega) - \hat{A}_\alpha^\dagger(\omega) \hat{A}_\beta(\omega) \hat{\rho}_S(t)] + \text{h.c.} \quad (161)$$

Now we split up $\Gamma_{\alpha\beta}$ as

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2} J_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega), \quad (162)$$

where $J_{\alpha\beta}(\omega)$ is the power spectrum of the correlations (i.e. the full Fourier transform of the correlation functions)

$$J_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega) = \int_{-\infty}^\infty ds e^{i\omega s} C_{\alpha\beta}(s), \quad (163)$$

and

$$S_{\alpha\beta}(\omega) = \frac{1}{2i} [\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}^*(\omega)]. \quad (164)$$

We then find

$$\begin{aligned} \frac{d\hat{\rho}_S(t)}{dt} = & \frac{1}{\hbar^2} \sum_\omega \sum_{\alpha\beta} \left\{ -i S_{\alpha\beta}(\omega) [\hat{A}_\alpha^\dagger(\omega) \hat{A}_\beta(\omega), \hat{\rho}_S(t)] \right. \\ & \left. + J_{\alpha\beta}(\omega) \left[\hat{A}_\beta(\omega) \hat{\rho}_S(t) \hat{A}_\alpha^\dagger(\omega) - \frac{1}{2} \{ \hat{A}_\alpha^\dagger(\omega) \hat{A}_\beta(\omega), \hat{\rho}_S(t) \} \right] \right\}. \end{aligned} \quad (165)$$

This is almost of Lindblad form, with a Hamiltonian term

$$\hat{H}_{LS} = \frac{1}{\hbar^2} \sum_\omega \sum_{\alpha\beta} S_{\alpha\beta}(\omega) \hat{A}_\alpha^\dagger(\omega) \hat{A}_\beta(\omega). \quad (166)$$

(The subscript *LS* shows that this Hamiltonian term plays a similar role to the Lamb shift in atomic physics.) The dissipator is

$$\mathcal{D}(\hat{\rho}_s(t)) = \frac{1}{\hbar^2} \sum_\omega \sum_{\alpha\beta} J_{\alpha\beta}(\omega) \left[\hat{A}_\beta(\omega) \hat{\rho}_S(t) \hat{A}_\alpha^\dagger(\omega) - \frac{1}{2} \{ \hat{A}_\alpha^\dagger(\omega) \hat{A}_\beta(\omega), \hat{\rho}_S(t) \} \right] \quad (167)$$

and may be put into conventional Lindblad form by diagonalising the matrix $J_{\alpha\beta}(\omega)$ for each value of ω .

4.7 The quantum optical master equation

A classic case where this approach is valid is for an atom (the system) coupled to electromagnetic field modes (the environment). In that case the environment is a set of harmonic oscillators:

$$\hat{H}_E = \sum_k \sum_\lambda \hbar\omega_k \hat{b}_\lambda^\dagger(k) \hat{b}_\lambda(k), \quad (168)$$

where λ labels one of the two transverse polarizations for wavevector k and $\hat{b}_\lambda(k)$ is an annihilation operator. The interaction Hamiltonian is (in the electric dipole approximation)

$$-\hat{\mathbf{D}} \cdot \hat{\mathbf{E}} = -i\hat{\mathbf{D}} \cdot \sum_k \sum_\lambda \sqrt{\frac{2\pi\hbar\omega_k}{V}} \mathbf{e}_\lambda(k) [\hat{b}_\lambda(k) - \hat{b}_\lambda^\dagger(k)], \quad (169)$$

where V is a normalization volume for the field modes and \mathbf{e}_λ is a unit polarization vector, We can decompose $\hat{\mathbf{D}}$ in the same manner as before:

$$\hat{\mathbf{D}}(t) = \sum_\omega e^{-i\omega t} \hat{A}(\omega). \quad (170)$$

The spectral correlation tensor is now

$$\Gamma_{ij}(\omega) = \frac{1}{\hbar^2} \int_0^\infty ds e^{i\omega s} \langle \hat{E}_i(t) \hat{E}_j(t-s) \rangle. \quad (171)$$

In thermal equilibrium (i.e. black-body radiation), we have

$$\Gamma_{ij}(\omega) = \delta_{ij} \left[\frac{1}{2} J(\omega) + iS(\omega) \right], \quad (172)$$

with

$$\begin{aligned} J(\omega) &= \frac{4\omega^3}{3\hbar c^3} [1 + n(\omega)]; \\ S(\omega) &= \frac{2}{3\pi\hbar c^3} \mathcal{P} \left[\int_0^\infty \omega_k^3 d\omega_k \left(\frac{1 + n(\omega_k)}{\omega - \omega_k} + \frac{n(\omega_k)}{\omega + \omega_k} \right) \right], \end{aligned} \quad (173)$$

where \mathcal{P} stands for a Cauchy principal value. Hence the Lamb shift Hamiltonian becomes

$$\hat{H}_{LS} = \sum_\omega \hbar S(\omega) \hat{A}^\dagger(\omega) \hat{A}(\omega), \quad (174)$$

and the dissipator is

$$\begin{aligned} \mathcal{D}(\hat{\rho}_S) &= \sum_{\omega>0} \frac{4\omega^3}{3\hbar c^3} [1 + n(\omega)] (\hat{A}(\omega) \hat{\rho}_S \hat{A}^\dagger(\omega) - \frac{1}{2} \{ \hat{A}^\dagger(\omega) \hat{A}(\omega), \hat{\rho}_S \}) \\ &\quad + \sum_{\omega<0} \frac{4\omega^3}{3\hbar c^3} n(\omega) (\hat{A}^\dagger(\omega) \hat{\rho}_S \hat{A}(\omega) - \frac{1}{2} \{ \hat{A}(\omega) \hat{A}^\dagger(\omega), \hat{\rho}_S \}), \end{aligned} \quad (175)$$

Note that in both equations (174) and (175) the frequency sums go over the (usually discrete) energy response of the system.

For a two-level atom (as in §4.2) with transition dipole \mathbf{d} , where we can write

$$\hat{\mathbf{D}}(t) = \mathbf{d}(\hat{\sigma}_+ e^{-i\omega_0 t} + \hat{\sigma}_- e^{+i\omega_0 t}), \quad (176)$$

we find that the dissipator contains two Lindblad operators:

$$\hat{L}_1 = |\mathbf{d}| \sqrt{\frac{4\omega_0^3}{3\hbar c^3}} [1 + n(\omega_0)] \hat{\sigma}_+; \quad \hat{L}_2 = |\mathbf{d}| \sqrt{\frac{4\omega_0^3}{3\hbar c^3}} n(\omega_0) \hat{\sigma}_-. \quad (177)$$

\hat{L}_1 produces decay from the excited state to the ground state, while \hat{L}_2 produces excitation. The rates of each process are precisely consistent with the values of the Einstein A and B coefficients. A very similar analysis can be made for the coupling to a phonon (rather than photon) bath in magnetic resonance—this justifies the assumed form (125).

4.8 Bad qubits—quantum Brownian motion

We now consider ‘bad’ qubits, where the system has very little chance to evolve before the interaction with the environment takes effect—in other words, where $\tau_S \gg \tau_R$.

First, we decompose the correlation functions in a different way to equation (162), as:

$$D_{\alpha\beta}(\tau) = i \langle [\hat{B}_\alpha(\tau), \hat{B}_\beta(0)] \rangle = i (C_{\alpha\beta}(\tau) - C_{\beta^\dagger\alpha^\dagger}(-\tau)) \quad (\text{the ‘dissipation kernel’}); \quad (178)$$

$$D_{\alpha\beta}^{(1)}(\tau) = \langle \{\hat{B}_\alpha(\tau), \hat{B}_\beta(0)\} \rangle = (C_{\alpha\beta}(\tau) + C_{\beta^\dagger\alpha^\dagger}(-\tau)) \quad (\text{the ‘noise kernel’}). \quad (179)$$

Here α^\dagger is the index labelling those operators \hat{A} and \hat{B} which are the Hermitian conjugates of \hat{A}_α and \hat{B}_α . Hence

$$C_{\alpha\beta}(\tau) = \frac{1}{2} [D_{\alpha\beta}^{(1)}(\tau) - iD_{\alpha\beta}(\tau)]; \quad (180)$$

$$C_{\beta^\dagger\alpha^\dagger}(-\tau) = [C_{\alpha\beta}(\tau)]^* = \frac{1}{2} [D_{\alpha\beta}^{(1)}(\tau) + iD_{\alpha\beta}(\tau)]. \quad (181)$$

Note that **if** the operators are Hermitian, then $\alpha^\dagger = \alpha$, and both D and $D^{(1)}$ are real:

$$D_{\alpha\beta} = i(C_{\alpha\beta}(\tau) - (C_{\alpha\beta}(\tau))^*) = -2\Im C_{\alpha\beta}(\tau); \quad (182)$$

$$D_{\alpha\beta}^{(1)}(\tau) = (C_{\alpha\beta}(\tau) + C_{\beta\alpha}(-\tau)) = 2\Re C_{\alpha\beta}(\tau). \quad (183)$$

Substituting in equation (151), we find

$$\begin{aligned} \frac{d\hat{\rho}_S(t)}{dt} &= \frac{1}{\hbar^2} \int_0^\infty ds \sum_{\alpha\beta} C_{\alpha\beta}(s) [\hat{A}_\beta(t-s) \hat{\rho}_S(t) \hat{A}_\alpha^\dagger(t) - \hat{A}_\alpha^\dagger(t) \hat{A}_\beta(t-s) \hat{\rho}_S(t) +] + \text{h.c.} \\ &= \frac{1}{2\hbar^2} \int_0^\infty ds \sum_{\alpha\beta} \left[D_{\alpha\beta}^{(1)}(s) [\hat{A}_\alpha^\dagger(t), [\hat{\rho}_S(t), \hat{A}_\beta(t-s)]] + iD_{\alpha\beta}(s) [\hat{A}_\alpha^\dagger(t), \{\hat{\rho}_S(t), \hat{A}_\beta(t-s)\}] \right]. \end{aligned} \quad (184)$$

In order to go from the first line to the second, we have grouped together the terms from operators $\alpha\beta$ with those in the Hermitian conjugate part from $\alpha^\dagger\beta^\dagger$.

Now, rather than make the decomposition (156) and use Approximation 5, we make instead

- **Approximation 5’**: since the system evolves very little during the time over which the environment influences it, we write

$$\hat{A}_\beta(t-s) \approx \hat{A}_\beta(t) - s\dot{\hat{A}}_\beta(t), \quad (185)$$

where

$$\dot{\hat{A}}_\beta(t) = \frac{1}{i\hbar} [\hat{A}_\beta(t), \hat{H}_S(t)] \quad (186)$$

(remember we are in the interaction representation).

Using this, we find

$$\begin{aligned} \frac{d\hat{\rho}_S(t)}{dt} &= \frac{1}{2\hbar^2} \int_0^\infty ds \sum_{\alpha\beta} \left[D_{\alpha\beta}^{(1)}(s) [\hat{A}_\alpha^\dagger(t), [\hat{\rho}_S(t), \hat{A}_\beta(t)]] + iD_{\alpha\beta}(s) [\hat{A}_\alpha^\dagger(t), \{\hat{\rho}_S(t), \hat{A}_\beta(t)\}] \right. \\ &\quad \left. - sD_{\alpha\beta}^{(1)}(s) [\hat{A}_\alpha^\dagger(t), [\hat{\rho}_S(t), \dot{\hat{A}}_\beta(t)]] - isD_{\alpha\beta}(s) [\hat{A}_\alpha^\dagger(t), \{\hat{\rho}_S(t), \dot{\hat{A}}_\beta(t)\}] \right]. \end{aligned} \quad (187)$$

This gives us four integrals over s to perform.

4.9 Simplifications for a harmonic environment

To do this it's helpful to write the correlation functions in the following way. We suppose the environment is in thermal equilibrium: in that case the correlation functions obey the conditions

$$J_{\alpha\beta}(-\omega) = e^{-\beta\hbar\omega} [J_{\alpha^\dagger\beta^\dagger}(\omega)]^*. \quad (188)$$

So, we lose no generality by writing

$$\begin{aligned} J_{\alpha\beta}(\omega) &= [n(|\omega|) + 1] j_{\alpha\beta}(|\omega|) \quad (\omega > 0) \\ &= n(|\omega|) [j_{\alpha^\dagger\beta^\dagger}(|\omega|)]^* \quad (\omega < 0), \end{aligned} \quad (189)$$

where $n(\omega)$ is the Bose occupation number defined in equation (126). This is because $n(\omega)$ is real and satisfies

$$n(\omega) = e^{-\beta\hbar\omega} [n(\omega) + 1]. \quad (190)$$

The advantage of doing this is that in certain circumstances (notably when the environment is harmonic) the function $j(|\omega|)$ is temperature-independent, and all the temperature dependence is contained in the $n(|\omega|)$ factor. We have already seen an example of this in §4.7, where $j(\omega) = 4\omega^3/3\hbar c^3$, but in fact it is generally true whenever the environment is harmonic and the coupling to the system is by some combination of the coordinates x_q of the different modes q :

$$\hat{B}_\alpha = \sum_q g_{\alpha q} \hat{x}_q \quad \Rightarrow \quad j_{\alpha\beta}(\omega) = \sum_q \frac{g_{\alpha q}^* g_{\beta q}}{2M_q \omega_q} \delta(\omega - \omega_q). \quad (191)$$

Note that this also means that *at a particular temperature* and within these approximations, one can always find a linearly-coupled harmonic environment that mimics the effect of the actual environment via equations (189) and (191).

Thus the dissipation kernel becomes

$$\begin{aligned} D_{\alpha\beta}(\tau) &= i[C_{\alpha\beta}(\tau) - C_{\beta^\dagger\alpha^\dagger}(-\tau)] \\ &= i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (1 - e^{-\beta\hbar\omega}) J_{\alpha\beta}(\omega) e^{-i\omega\tau} = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \operatorname{sgn}(\omega) j_{\alpha\beta}(\omega) e^{-i\omega\tau} \\ &= 2 \int_0^\infty \frac{d\omega}{2\pi} [\Re(j_{\alpha\beta}) \sin(\omega\tau) - \Im(j_{\alpha\beta}) \cos(\omega\tau)]. \end{aligned} \quad (192)$$

Similarly, the noise kernel is

$$\begin{aligned} D_{\alpha\beta}^{(1)}(\tau) &= [C_{\alpha\beta}(\tau) + C_{\beta^\dagger\alpha^\dagger}(-\tau)] \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (1 + e^{-\beta\hbar\omega}) J_{\alpha\beta}(\omega) e^{-i\omega\tau} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \operatorname{sgn}(\omega) \coth\left(\frac{\beta\hbar\omega}{2}\right) j_{\alpha\beta}(\omega) e^{-i\omega\tau} \\ &= 2 \int_0^\infty \frac{d\omega}{2\pi} \coth\left(\frac{\beta\hbar\omega}{2}\right) [\Re(j_{\alpha\beta}) \cos(\omega\tau) - \Im(j_{\alpha\beta}) \sin(\omega\tau)]. \end{aligned} \quad (193)$$

Note how, if j is temperature-independent, all the temperature-dependence is contained in the noise kernel $D^{(1)}$ —hence the name.