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SCHREYER HONORS COLLEGE

DEPARTMENT OF PHYSICS

LOW DIMENSIONAL QUANTUM MECHANICAL SYSTEMS
AND THEIR OPEN SYSTEM APPROXIMATIONS

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SEASON 2019

A thesis submitted in partial fulfillment
of the requirements for baccalaureate degrees
in Physics and Mathematics
with honors in Physics

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Abstract

In much of physics the description is focused on idealized, isolated systems. The real world is much more complicated; the real world is composed of messily interacting systems. And besides, to make a measurement on a system one must couple it to something external. As such a study of how systems in contact with an environment is vital to a realistic description of natural phenomena. In this thesis we explore techniques for treating so called open systems in quantum mechanics, specifically systems with low numbers of degrees of freedom. To do this we first review the necessary quantum mechanics of closed systems. We then develop the basic theory of open quantum systems, and apply it to a few simple model systems.

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Part I

Preliminaries

Chapter 1

What is Quantum Mechanics?

Quantum mechanics is a physical theory describing the small and slow. It encompasses a significant move away from classical mechanics both mathematically and conceptually. QM treats the small because its deviations from classical physics are typically only apparent for well isolated systems. As the number of interactions increases within a quantum system the deviations tend cancel out, leaving essentially a thermal ensemble which behaves classically. This is a fairly subtle point, in that it is easy to think of these deviations as parameterized by Planck's constant

$$h = 2\pi\hbar \sim 7 \times 10^{-34} J_s$$

which is manifestly small compared to the classical world, but even for fairly large systems like buckyballs [2] quantum effects are manifest when sufficiently isolated.

QM treats the slow in sense that it is a non-relativistic description of nature, and so any velocities present should be small compared to the speed of light

$$c \sim 3 \times 10^8 \frac{m}{s}$$

The non-relativistic nature of QM will become apparent in the section on dynamics, but it is a result of the theory's dependence on a Newtonian time parameter. There is a model of QM known as quantum field theory which is relativistically invariant, but it is outside the scope of this thesis. For a more complete treatment of non-relativistic QM see [1].

1.1 Definitions and Conventions

The most drastic difference between QM and classical physics is perhaps the description of a system itself. While in classical physics a system is described by a point in phase-space (at least for a system of point particles, which is the classical analogue we are content to describe), in quantum mechanics a system is described by a direction in a complex Hilbert space of generically infinite dimensionality. Additionally, while in classical physics observable properties of the system (such as its energy, angular momentum, or even position) are described by functions on the phase-space (and generically the trajectory of a particle), in QM observables are described by operators on the Hilbert space.

1.1.1 Basics

More precisely, a QM system is given by a complex (separable¹) Hilbert space \mathcal{H} , where the states are given by directions in the Hilbert space. That is, two elements of the Hilbert space represent the same state if they differ by a complex scalar. Then the observables on the system \mathcal{O} are represented by self-adjoint operators on \mathcal{H} .

We will employ the *Bra Ket* notation of P.M. Dirac. In this notation a vector in \mathcal{H} is written $|\psi\rangle$ (a *ket*) and its canonical dual is written $\langle\psi|$ (a *bra*). Operators on \mathcal{H} are written with capital letters as usual. In this notation the inner-product is written $\langle\psi|\phi\rangle$. *Physical States* in \mathcal{H} are exactly the vectors with unit norm.

A measurement of the observable, A , will result in an eigenvalue of A , and the state will be projected onto the eigenspace of that eigenvalue. The probability of a measurement coming back with any given eigenvalue is given by the absolute value squared of the inner-product of the projection with the original state, i.e.

$$P(\alpha)_\psi = |\langle\psi|\Phi_\alpha|\psi\rangle|^2 \quad (1.1)$$

Here Φ_α is the projection onto the eigenspace of A associated with α .

We will assume all self-adjoint operators are orthogonally-diagonalizable². The expectation value of an operator A on a physical state $|\psi\rangle$ is given by $\langle A \rangle_\psi = \langle\psi|A|\psi\rangle$. The commutator of two operators A and B , is written $[A, B]$. The adjoint of an operator A is written A^\dagger , and is assumed to always exist³.

1.1.2 Mixed States

As in classical physics, and especially statistical physics, in QM we want to be able to describe mixed states. A *mixed state* is simply a state described by a statistical mixture of states (notably

¹We always assume \mathcal{H} is separable to ensure the existence of a countable, orthonormal basis.

²Since we will only be concerned with bounded subspaces of an observable's spectrum, this is true for all practical purposes

³Ibid

different from a quantum mechanical superposition of states). To do this in the quantum setting we need to introduce a new object, the *density operator*. The density operator is a unit-trace, positive semi-definite, self-adjoint operator on \mathcal{H} , it describes QM states in statistical mixtures. A pure, physical state $|\psi\rangle$ is described by the operator $\rho = |\psi\rangle\langle\psi|$, and we can see that $\langle A \rangle_\rho = \text{Tr}[A\rho] = \langle\psi| A |\psi\rangle$. A state given by a mixture of $|\psi_i\rangle$ in proportions p_i is described by the density operator $\sum_i p_i |\psi_i\rangle\langle\psi_i|$.

We can measure the degree of mixture of a state by using the *von Neumann entropy*

$$S[\rho] = -\text{Tr}[\rho \ln[\rho]] \quad (1.2)$$

One can see that over a diagonalizing basis $\{|\alpha\rangle\}$ with eigenvalues $\{\lambda_\alpha\}$ the von Neumann entropy gives the Shannon entropy of the distribution $\{\lambda_\alpha\}$. This is a foundational connection between quantum mechanics and information theory.

1.1.3 Composite Systems

Often we will have two or more QM systems which we wish to combine into a single, larger, system. We combine two QM systems \mathcal{H}_1 and \mathcal{H}_2 into the QM system $\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$ via the tensor product. Simple tensors in this space can be written in several ways. We could write $|\psi\rangle \in \mathcal{H}_1$ together with $|\phi\rangle \in \mathcal{H}_2$ as $|\psi\rangle \otimes |\phi\rangle$, $|\psi\rangle_1 |\phi\rangle_2$, or $|\psi, \phi\rangle$. We will use the latter, and when there is no risk of confusion we write $|\psi\phi\rangle$.

A general state in the composite system will not be a simple tensor, and in this case there is generally no unique decomposition. We call such composite states *entangled*, and they are a feature of quantum mechanics with no classical analogue.

One is often interested in only part of a composite system, as we will be in our discussion of open systems. To recover a state in a subsystem (called a *reduced system*) we employ the *partial trace*, written, for example, Tr_2 when “tracing out” the second system. The partial trace over system 2 of a generic composite state $|\psi\rangle$ is the one given by

$$\rho_1 = \text{Tr}_2 |\psi\rangle\langle\psi| = \sum_{\alpha, \beta, \gamma} |\alpha\rangle\langle\alpha, \gamma|\psi\rangle\langle\psi|\beta, \gamma\rangle\langle\alpha| \quad (1.3)$$

where α and β parametrize an orthonormal basis of system 1, and γ parametrizes an orthonormal basis of system 2. Note that even given a pure, composite state the resulting state of the reduced system is generically mixed. This gives a natural measure of entanglement. The *entanglement entropy* of a composite system’s state ρ is given by

$$\tilde{S}_{12}[\rho] = S[\text{Tr}_2[\rho]] + S[\text{Tr}_1[\rho]] - S[\rho] \quad (1.4)$$

1.1.4 Wavefunctions

To describe a system in physical-space, like a particle in a box, we need to know what our Hilbert space is. For systems of a physical-space \mathbb{E} (such as \mathbb{R}^3) we take \mathcal{H} to be $L_2(\mathbb{E})$. That is, the

set of all square-integrable, complex-valued functions of \mathbb{E} . An element of this \mathcal{H} is called a *wavefunction*. When physical-space is given by a real vector space we take the position operator X to be \vec{x} . In this case we also have the momentum operator P given by $-i\hbar\nabla$. This is defined so that $\vec{v} \cdot P$ is the generator of translations in the \vec{v} direction. We can see that in this case $[X^j, P_k] = i\hbar\delta_k^j$ [1].

One can also describe systems in momentum-space, the Fourier dual of physical-space. In this case the momentum-space wavefunction $\hat{\psi}(p)$ is given by the Fourier Transform of the physical-space wavefunction $\psi(x)$. That is

$$\hat{\psi}(p) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int d^3x e^{-\frac{i}{\hbar}x \cdot p} \psi(x) \quad (1.5)$$

in the case of $\mathbb{E} = \mathbb{R}^3$.

Chapter 2

Closed Systems

In this section we will review how to treat closed systems in QM. A *Closed System* is a physical system with no interaction with an external system. That is, all degrees of freedom of the system are influenced only by parameters within the system. We will see that this leads to a relatively simple formalism for dynamics, albeit for a somewhat unrealistic setting.

2.1 Dynamics

The dynamics of a closed QM system are governed by the Hamiltonian of system. The *Hamiltonian*, H , is an observable pertaining to the total energy of the system, and is analogous to the Hamiltonian function of classical mechanics. The *Schrödinger Equation* gives the relationship between the time evolution of a state $|\psi\rangle$ and this Hamiltonian:

$$H|\psi\rangle = i\hbar \frac{\partial}{\partial t} |\psi\rangle \quad (2.1)$$

In the density operator formalism we get

$$i\hbar \frac{\partial}{\partial t} (|\psi\rangle \langle\psi|) = \left(i\hbar \frac{\partial}{\partial t} |\psi\rangle \right) \langle\psi| + |\psi\rangle \left(i\hbar \frac{\partial}{\partial t} \langle\psi| \right) = (H|\psi\rangle) \langle\psi| - |\psi\rangle (\langle\psi| H) = [H, |\psi\rangle \langle\psi|] \quad (2.2)$$

or for a generic mixed state ρ

$$[H, \rho] = i\hbar \frac{\partial}{\partial t} \rho \quad (2.3)$$

This is the equation of motion for a probability distribution in Hamiltonian mechanics, with an additional $i\hbar$.

Equation 2.1 is seen to admit the formal solution

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar} \int_{t_0}^t H(t) dt} |\psi(t_0)\rangle \quad (2.4)$$

Since H is Hermitian we clearly have $\int_{t_0}^t H(t) dt$ Hermitian as well, so that the *time evolution operator*

$$U_H(t) = e^{-\frac{i}{\hbar} \int_{t_0}^t H(t) dt} \quad (2.5)$$

is a Unitary operator. This gives us that the norm of our state is preserved. More generally we have that a density operator evolves into a density operator, since Equation 2.3 admits the formal solution

$$\rho(t) = U_H(t) \rho(t_0) U_H(t)^\dagger \quad (2.6)$$

For time-independent Hamiltonians, this reduces the problem of describing dynamics to an eigenvalue problem. Equation 2.4 says that for an eigenstate, $|\psi\rangle$, of H with eigenvalue (energy) E_i the evolution equation reads

$$|\psi(t)\rangle = e^{-\frac{i(t-t_0)}{\hbar} E_i} |\psi(t_0)\rangle \quad (2.7)$$

Thus for a generic state $|\psi(t_0)\rangle = \sum_n \alpha_n |E_n\rangle$ we have

$$|\psi(t)\rangle = \sum_n \alpha_n e^{-\frac{i(t-t_0)}{\hbar} E_n} |E_n\rangle \quad (2.8)$$

For a density operator $\rho(t_0) = \sum_i p_i |\psi_i\rangle \langle \psi_i|$ with $|\psi_i\rangle = \sum_n \alpha_{i_n} |E_n\rangle$ we have

$$\rho(t) = \sum_i p_i \sum_{n,m} \alpha_{i_n} \alpha_{i_m}^* e^{-\frac{i(t-t_0)}{\hbar}(E_n-E_m)} |E_n\rangle \langle E_m| \quad (2.9)$$

We will consider the case where H depends on time when we consider perturbation theory. Additionally we shall discuss how to treat Hamiltonians that are too complicated to exactly diagonalize.

2.1.1 Pictures

Before treating examples or developing any further theory, we need to discuss the various ‘pictures’ of QM. In the discussion of dynamics above we assumed that the physical states time evolved, while various operators remained stationary. This is the *Schrödinger picture* of QM, and it is generally the more intuitive picture to work in. This is, however, not the only way we can organize the theory [1].

Note that for an operator A , the time-dependent expectation value over a state $|\psi(t)\rangle$ is given by

$$\langle A \rangle_{\psi}(t) = \langle \psi(t) | A | \psi(t) \rangle = \langle \psi(0) | U_H(t)^\dagger A U_H(t) | \psi(0) \rangle =: \langle \psi | A(t) | \psi \rangle \quad (2.10)$$

In this way we can define a stationary set of physical states (the ones which agree with the Schrödinger picture states at $t = t_0$), and time evolving operators (which agree with the Schrödinger picture operators at $t = t_0$). This is called the *Heisenberg picture*. We can see that

$$\begin{aligned} A(t) &= U_H(t)^\dagger A(0) U_H(t) \\ \frac{d}{dt} A(t) &= \frac{i}{\hbar} [H, A(t)] + \frac{\partial}{\partial t} A(t) \end{aligned} \quad (2.11)$$

Thus for Schrödinger picture time-independent operators, the Heisenberg picture time evolution of an operator is given by a sign reversal of the time evolution of density operators.

There is one more possibility of how to assign time evolution. In the *interaction picture* (due to Dirac) we split our Hamiltonian into two parts

$$H = H_0 + V \quad (2.12)$$

where H_0 is assumed to be stationary. We then treat the ‘interaction’ term V as a new Schrödinger-like Hamiltonian. To be precise, we set the interaction picture operator A (denoted A_I) to be

$$A_I := U_{H_0}(t)^\dagger A U_{H_0}(t) \quad (2.13)$$

and the interaction picture states (denoted $|\psi\rangle_I$) to be

$$|\psi(t)\rangle_I = U_{H_0}(t)^\dagger |\psi\rangle \quad (2.14)$$

Then by invoking Equation 2.1 we see that

$$\begin{aligned}
 i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I &= i\hbar \frac{\partial}{\partial t} \left(U_{H_0}(t)^\dagger |\psi(t)\rangle \right) = \\
 &= \left(-H_0 U_{H_0}(t)^\dagger + U_{H_0}(t)^\dagger (H_0 + V) \right) |\psi(t)\rangle = \\
 &= U_{H_0}(t)^\dagger V U_{H_0}(t) U_{H_0}(t)^\dagger |\psi(t)\rangle \tag{2.15}
 \end{aligned}$$

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = V_I |\psi(t)\rangle_I \tag{2.16}$$

Where we have used $[H_0, U_{H_0}] = 0$ and $UU^\dagger = \mathbb{1}$. This picture is extremely useful for treating time-dependent Hamiltonians.

2.2 Perturbation Theory

Perturbation theory is a formal approximation scheme designed to ‘correct’ the eigenstates and eigenvalues of a solvable Hamiltonian, so that they are the eigenstates and eigenvalues of a *perturbed* Hamiltonian. In other words, we want to take the information we have about a simpler problem and use it as the starting point for solving a harder, but similar, problem. There are two flavors of perturbation theory we will be considering. One deals with time-independent perturbations to a time-independent potential, and the other deals with time-dependent perturbations to a time-independent potential. While the latter is a generalization of the former, its techniques are reasonably different in flavor. We will follow the approach of [1].

2.2.1 The Time-Independent Case

Time-independent perturbation theory deals with the setting where the Hamiltonian of interest is given by

$$H = H_0 + \lambda V \quad (2.17)$$

Here H_0 is assumed to have already been solved, so that its eigenvalues, $\{E_n^0\}$, and eigenstates, $\{|n^0\rangle\}$, are known. In this case λV is the perturbation, and it is assumed to be small in the sense that

$$|V| \ll |E_n^0 - E_m^0| \quad (2.18)$$

The presence of λ is to clarify the order of the perturbation in calculations, and is meant to be a real parameter between 0 and 1.

Non-Degenerate Case

Assuming that the energy levels of H_0 are non-degenerate, we may attempt to solve for the new eigenstates and eigenvalues, $\{|n\rangle\}$ and $\{E_n\}$, satisfying $H|n\rangle = E_n|n\rangle$. Introducing $\Delta_n = E_n - E_n^0$ we have

$$(H_0 + \lambda V)|n\rangle = H|n\rangle = E_n|n\rangle = (E_n^0 + \Delta_n)|n\rangle \quad (2.19)$$

or simply

$$(E_n^0 - H_0)|n\rangle = (\lambda V - \Delta_n)|n\rangle \quad (2.20)$$

Multiplying in $\langle n^0|$ we see that

$$\langle n^0|(\lambda V - \Delta_n)|n\rangle = 0 \quad (2.21)$$

Thus $|n\rangle$ can be recursively defined by

$$|n\rangle = a_n |n^0\rangle + \left(\sum_{k \neq n} \frac{1}{E_n^0 - E_k^0} |k^0\rangle \langle k^0| \right) (\lambda V - \Delta_n) |n\rangle \quad (2.22)$$

Where the sum is the partial inverse of $(E_n^0 - H_0)$, and the $a_n |n^0\rangle$ is the component not contained in the inverse. We may fix a_n by asserting that as $\lambda \rightarrow 0$ we have $|n\rangle \rightarrow |n^0\rangle$, and simply taking $a_n = 1$. Note that this enforces the normalization condition $\langle n^0 | n \rangle = 1$, **not** $\langle n | n \rangle = 1$. This, with Equation 2.21, immediately tells us that

$$\Delta_n = \lambda \langle n^0 | V | n \rangle \quad (2.23)$$

The final trick for non-degenerate perturbation theory is to expand the $\{|n\rangle\}$ and $\{\Delta_n\}$ as an asymptotic series in λ . That is we write

$$\begin{aligned} |n\rangle &= |n^0\rangle + \lambda |n^1\rangle + \dots \\ \Delta_n &= \lambda \Delta_n^{(1)} + \lambda^2 \Delta_n^{(2)} + \dots \end{aligned} \quad (2.24)$$

Note Δ_n starts at order λ because $\Delta_n^{(0)} = E_n^0 - E_n^0 = 0$. We may plug Equations 2.2.1 into Equation 2.23 and match order by order in λ to solve for approximate eigenvalues of H . These read

$$\Delta_n^{(i)} = \langle n^0 | V | n^{i-1} \rangle \quad (2.25)$$

Note that the i th order correction to E_n only relies on the $(i - 1)$ th correction to $|n\rangle$. Finally we may plug Equations 2.2.1 into Equation 2.22 to get

$$\begin{aligned} &|n^0\rangle + \lambda |n^1\rangle + \dots = \\ &= |n^0\rangle + \left(\sum_{k \neq n} \frac{1}{E_n^0 - E_k^0} |k^0\rangle \langle k^0| \right) (\lambda V - \lambda \Delta_n^{(1)} - \lambda^2 \Delta_n^{(2)} - \dots) (|n^0\rangle + \lambda |n^1\rangle + \dots) \end{aligned} \quad (2.26)$$

While this results in complicated expressions, it does show that solving for the corrections boils down to computing matrix elements of V within the original eigenbasis of H_0 .

Degenerate Case

When the energy levels of H_0 are degenerate, but finitely so, we can treat the problem in a very similar way as above. The only essential differences are that we must perform a diagonalization procedure over each degenerate subspace of interest, remove the entire subspace from the sum in Equation 2.22, and incorporate as zeroth order energy shifts the eigenvalue of V associated to the subspace.

2.2.2 The Time-Dependent Case

From Equation 2.5, we see that solving for the time evolution operator when the Hamiltonian is time-dependent is highly non-trivial. To solve this problem we utilize the interaction picture, and perturbatively find the time evolution of the interaction picture states. We know that

$$|\psi(t)\rangle_I = U_I(t, t_0) |\psi(t_0)\rangle_I \quad (2.27)$$

where t_0 is the initial time for the problem, i.e. when we know the state of the system. We can differentiate both sides and compare with Equation 2.16 to see that

$$i\hbar \frac{d}{dt} U_I(t, t_0) = V_I(t) U_I(t, t_0) \quad (2.28)$$

Using the initial condition $U_I(t_0, t_0) = \mathbb{1}$ we can formally solve this as

$$U_I(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t V_I(t') U_I(t', t_0) dt' \quad (2.29)$$

This can be iterated to produce a power series in V_I known as the *Dyson series*

$$U_I(t, t_0) = \mathbb{1} + \left(\frac{-i}{\hbar} \right) \int_{t_0}^t dt' V(t') + \left(\frac{-i}{\hbar} \right)^2 \int_{t_0}^t dt' V(t') \int_{t_0}^{t'} dt'' V(t'') + \dots \quad (2.30)$$

Utilizing the the *time ordering operator* T we can write this formally as

$$U_I(t, t_0) = T \left[e^{-\frac{i}{\hbar} \int_{t_0}^t V_I(t') dt'} \right] \quad (2.31)$$

The time ordering operator moves earlier times to the right of later times, and so T preserves the order of the integrals in Equation 2.30. The difference in integration limits introduces the factorial terms in the series expansion of the exponential in Equation 2.31.

2.3 Examples

2.3.1 Harmonic Oscillator

As a first, prototypical, and ubiquitous example we shall consider the QM treatment of the Harmonic oscillator with Hamiltonian

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 \quad (2.32)$$

While it is possible to treat this problem in position space and solve the resulting PDE, there is a more informative algebraic approach [1]. We start by introducing the operator

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(X + \frac{i}{m\omega} P \right) \quad (2.33)$$

and the *Number* operator

$$N = a^\dagger a \quad (2.34)$$

Using the resulting commutation relations:

$$\begin{aligned} [a, a^\dagger] &= \mathbb{1} \\ [N, a] &= -a \\ [N, a^\dagger] &= a^\dagger \end{aligned} \quad (2.35)$$

we may rewrite H as

$$H = \hbar\omega \left(N + \frac{1}{2} \right) \quad (2.36)$$

Since N is Hermitian, we may write it by $N = \sum_n n |n\rangle \langle n|$, and then

$$H = \sum_n \left(n + \frac{1}{2} \right) \hbar\omega |n\rangle \langle n| \quad (2.37)$$

Thus, to understand the spectrum of H we need only determine the eigenvalues $\{n\}$ of N . To this end note that

$$Na |n\rangle = ([N, a] + aN) |n\rangle = (n-1)a |n\rangle \quad (2.38)$$

and similarly

$$Na^\dagger |n\rangle = ([N, a^\dagger] + a^\dagger N) |n\rangle = (n+1)a^\dagger |n\rangle \quad (2.39)$$

where we have utilized Equation 2.3.1. This means that a and its adjoint walk us between eigenstates of N with eigenvalues varying by integers. We know

$$n = \langle n| N |n\rangle = \langle n| a^\dagger a |n\rangle = \langle n-1| (|c|^2) |n-1\rangle = |c|^2 \quad (2.40)$$

and so without loss of generality we can take $c \in \mathbb{R}^+$ and see that

$$\begin{aligned} a |n\rangle &= \sqrt{n} |n-1\rangle \\ a^\dagger |n\rangle &= \sqrt{n+1} |n+1\rangle \end{aligned} \quad (2.41)$$

where the second result follows analogously to the first.

We are almost ready to determine the values of n . First note that since

$$n = \langle n | N | n \rangle = \left(\langle n | a^\dagger \right) (a | n \rangle) \geq 0 \quad (2.42)$$

(the last term in the chain is the norm of $a | n \rangle$), we have $n \in \mathbb{R}^+$. Finally, consider the sequence

$$|n\rangle, a | n \rangle = \sqrt{n} | n - 1 \rangle, a^2 | n \rangle = \sqrt{n(n-1)} | n - 2 \rangle, \dots \quad (2.43)$$

We have two cases:

Case 1: $n \in \mathbb{N}$

Then we reach $a(a^n | n \rangle) = \sqrt{n!} (a | 0 \rangle) = 0$, and we have no issues.

Case 2: $n \notin \mathbb{N}$

Then we reach $a(a^{\lfloor n \rfloor} | n \rangle) \propto a | n - \lfloor n \rfloor \rangle \propto | n - \lfloor n + 1 \rfloor \rangle$, but this is a contradiction, since $n - \lfloor n + 1 \rfloor < 0$.

Thus the spectrum of N is exactly \mathbb{N} , and the spectrum of H is $\hbar\omega (\frac{1}{2} + \mathbb{N})$. In the process of determining the spectrum of the Hamiltonian we have also constructed operators of interest, the creation and annihilation operators: a^\dagger and a . Such operators, and the algebra they define, are foundational to quantum field theory. We can determine the position and momentum moments of our eigenstates algebraically, by writing X and P in terms of a and a^\dagger . Finally, to determine the position space representation of the eigenstates we can take

$$0 = \langle x | a | 0 \rangle = \sqrt{\frac{m\omega}{2\hbar}} \langle x | \left(X + i \frac{P}{m\omega} \right) | 0 \rangle \propto \left(x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) \psi_0(x) \quad (2.44)$$

so that we have the position wavefunctions

$$\begin{aligned} \psi_0(x) &\propto e^{-\frac{x^2 m\omega}{2\hbar}} \\ \psi_n(x) &\propto (a^\dagger)^n \psi_0 = \left(\frac{m\omega}{2\hbar} \right)^{\frac{n}{2}} \left(x - \frac{\hbar}{m\omega} \frac{d}{dx} \right)^n e^{-\frac{x^2 m\omega}{2\hbar}} \end{aligned} \quad (2.45)$$

where the normalization constants are clear.

2.3.2 Infinite Square Well

The *infinite square well* is simply a potential function 0 in some square region, and infinite outside. In 1-D we have

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & x < 0, x > a \end{cases} \quad (2.46)$$

Enforcing continuity of the wavefunction we get that our eigenstates are given by

$$\psi_\alpha(x) \propto \sin\left(\frac{\sqrt{2E_\alpha m}}{\hbar} x\right)$$

$$\frac{\sqrt{2E_\alpha m}}{\hbar} a = n_\alpha \pi \quad (2.47)$$

Thus $E_n = \frac{(n\pi\hbar)^2}{2ma^2}$ are the spectra of H for $n \in \mathbb{N}$, and the eigenstates are $\psi_n \propto \sin\left(\frac{n\pi x}{a}\right)$. This can be easily generalized to arbitrary dimension n with various side lengths a_1, \dots, a_n by separation of variables: $\psi(x_1, \dots, x_n) = \psi_1(x_1) \dots \psi_n(x_n)$. Then the spectrum looks like

$$E_{\{m_1, \dots, m_n\}} = \frac{(\pi\hbar)^2}{2m} \left[\left(\frac{m_1}{a_1}\right)^2 + \dots + \left(\frac{m_n}{a_n}\right)^2 \right] \quad (2.48)$$

with eigenstates

$$\psi_{\{m_1, \dots, m_n\}}(x_1, \dots, x_n) = \sin\left(\frac{m_1 \pi x_1}{a_1}\right) \times \dots \times \sin\left(\frac{m_n \pi x_n}{a_n}\right) \quad (2.49)$$

2.3.3 Finite Systems

An important class of problems for the later sections is that of finite systems. In this case the system being considered has only a finite number of available states, as opposed to the infinite number in continuous systems like above. The preeminent example of these systems is the qubit (quantum-bit), a system with Hilbert space $\mathcal{H} = \mathbb{C}^2$.

Qubit in an External Field

A simple example of a finite system is that of a qubit in an external field. This can be a model of the spin degree of freedom of an electron interacting with a macroscopic external magnetic field. In this setting we take

$$H = a |1\rangle \langle 1| - a |0\rangle \langle 0| \quad (2.50)$$

so that $|0\rangle$ is the ground state and $|1\rangle$ is the excited state of our system. Of course only the energy gap $2a$ is important, and we could have taken $H \propto |1\rangle\langle 1|$ for simplicity. Instead we take Equation 2.50 for clarity.

In this case it is trivial to see that the eigenstates of H are $|0\rangle$ and $|1\rangle$, and that a given state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ evolves as $|\psi(t)\rangle = \alpha e^{i\frac{at}{\hbar}}|0\rangle + \beta e^{-i\frac{at}{\hbar}}|1\rangle$, and so the expected energy of our state at time t is given by

$$E(t) = \langle \psi(t) | H | \psi(t) \rangle = a (|\beta|^2 - |\alpha|^2) \quad (2.51)$$

which is stationary, as expected. On the other hand the probability of measuring the initial state at time t is given by

$$P(t) = |\langle \psi | \psi(t) \rangle|^2 = |e^{i\frac{at}{\hbar}}\alpha|^2 + |e^{-i\frac{at}{\hbar}}\beta|^2 = |\alpha|^4 + |\beta|^4 + |\alpha|^2|\beta|^2 \cos\left(\frac{2at}{\hbar}\right) \quad (2.52)$$

Here we see the dependence on the energy gap, $2a$, and we see that, for initial states close to equal mixtures of the two eigenstates, we have oscillations to essentially perfectly distinguishable states. If, however, the initial state is close to an eigenstate, then it oscillates to states largely indistinguishable from the initial state.

Qubit Interaction

Building from the above example, we can introduce an interaction between the qubits in our system. For a two-qubit system we have our Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ and our Hamiltonian

$$H = H_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes H_2 + H_{int} \quad (2.53)$$

where we will take

$$\begin{aligned} H_1 = H_2 &= E |1\rangle\langle 1| \\ H_{int} &= \alpha |10\rangle\langle 01| + \alpha^* |01\rangle\langle 10| \end{aligned} \quad (2.54)$$

Here the advantage of the finite dimensionality of the problem becomes apparent, because to describe the dynamics of this composite system it is easiest to directly compute the time evolution operator Equation 2.5. In this case, for $\alpha \in \mathbb{R}$, we get

$$U_H(t) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-\frac{iEt}{\hbar}} \cos\left(\frac{at}{\hbar}\right) & -ie^{-\frac{iEt}{\hbar}} \sin\left(\frac{at}{\hbar}\right) & 0 \\ 0 & -ie^{-\frac{iEt}{\hbar}} \sin\left(\frac{at}{\hbar}\right) & e^{-\frac{iEt}{\hbar}} \cos\left(\frac{at}{\hbar}\right) & 0 \\ 0 & 0 & 0 & e^{-\frac{2iEt}{\hbar}} \end{pmatrix} \quad (2.55)$$

Thus we can see that generically, an initially unentangled pure state will oscillate to an entangled one:

$$\tilde{S}_{12}[\rho(t)] = S[\text{Tr}_2[U_H(t)(|\psi\rangle\langle\psi|)U_H(t)^\dagger]] + S[\text{Tr}_1[U_H(t)(|\psi\rangle\langle\psi|)U_H(t)^\dagger]] \neq 0 \quad (2.56)$$

For the case of $|\psi\rangle = |0\rangle$ and $|\phi\rangle = |1\rangle$ we have Equation 2.56 resulting in the plot in Figure 2.1.

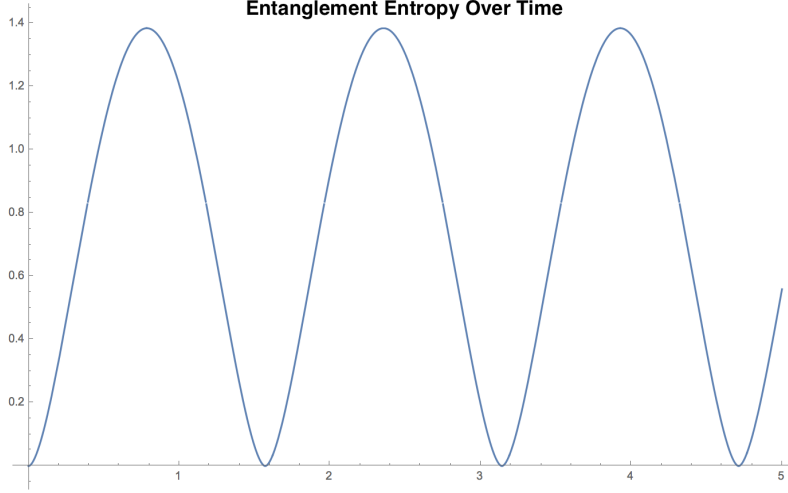


Figure 2.1: For a composite system of two initially pure states we can have an entanglement entropy which oscillates

2.3.4 Slanted Wells

An example of non-degenerate, time-independent, perturbation theory comes from adding a linear potential to an infinite square well. We wish to determine the new spectrum of our well when an additional potential $\tilde{V} = \alpha x$ is introduced to the Hamiltonian of Equation 2.3.2. We know we need $\alpha x \ll \frac{(\pi\hbar)^2}{2ma^2}$ for all x , so $\alpha \ll \frac{(\pi\hbar)^2}{2ma^3}$.

We first compute

$$\Delta_n^{(1)} = \langle n | \tilde{V} | n \rangle = \frac{\alpha a}{2} \quad (2.57)$$

and so we can see

$$\begin{aligned} |n^1\rangle &= \left(\sum_{k \neq n} \frac{1}{E_n^0 - E_k^0} |k^0\rangle \langle k^0| \right) \tilde{V} |n^0\rangle = \\ &= \left(\sum_{k \neq n} \frac{2ma^2}{(\pi\hbar)^2(n^2 - k^2)} \sqrt{\frac{2}{a}} \sin\left(\frac{k\pi x}{a}\right) \right) \int_0^a \frac{2}{a} \sin\left(\frac{k\pi x}{a}\right) \alpha x \sin\left(\frac{n\pi x}{a}\right) dx \end{aligned} \quad (2.58)$$

which simplifies to

$$|n^1\rangle = \sum_{k+n \neq 2l} \frac{-16ma^3 \alpha k n}{(\pi^2 \hbar)^2 (n^2 - k^2)^3} |k^0\rangle \quad (2.59)$$

Therefore, our perturbation mixes states with opposite parity, up to first order. Because of the $(n^2 - k^2)^3$ damping, only nearby states contribute significantly to the new energy eigenstates. The first order correction to the energy is linear in the perturbation, and independent of the energy level. This all makes sense because we introduced an odd function for our perturbation, breaking the symmetry of the well, and we essentially lifted the minimum energy.

The second order correction to the energy is more interesting

$$\begin{aligned} \Delta_n^{(2)} &= \langle n^0 | \tilde{V} | n^1 \rangle = \langle n^0 | \tilde{V} \sum_{k+n \neq 2l} \frac{-16ma^3 \alpha k n}{(\pi^2 \hbar)^2 (n^2 - k^2)^3} | k^0 \rangle = \\ &= \sum_{k+n \neq 2l} \frac{128ma^4 \alpha^2 k^2 n^2}{(\pi^3 \hbar)^2 (n^2 - k^2)^5} \end{aligned} \quad (2.60)$$

Evaluating such a sum is non-trivial, and not particularly enlightening, but we can see that this perturbation does shift the low lying states more than the excited states due to the $\sim 1/n^8$ damping.

These results can be extended to higher order, and compared to expansions of the exact solution (which is in terms of Airy functions), which can be seen in [3].

Part II

Low-Dimensions and Open Systems

Chapter 3

Low-Dimensional Quantum Systems

In this section we examine the general structure of finite-dimensional quantum systems, in particular we study n -qubit systems. Of interest is how these systems behave under energy conserving dynamics, since while n -qubit systems have been well studied within quantum computation their behavior in more restricted settings is still largely open. This difference is examined in how the Lie-algebras of interactions which are energy conserving differ from those which are used in quantum computation.

3.1 n -Qubit Systems

The primary examples of low-dimensional systems we will be considering are n -qubit systems. Each qubit will have a state space given by

$$\mathcal{H}_Q = \mathbb{C}^2 \quad (3.1)$$

and Hamiltonian

$$H_Q = E |1\rangle \langle 1| \quad (3.2)$$

thus the total system will be given by the state space

$$\mathcal{H} = \bigotimes_{i=1}^n \mathcal{H}_Q \quad (3.3)$$

and Hamiltonian

$$H = \sum_{j, J \in \mathcal{J}_j} jE |J\rangle \langle J| \quad (3.4)$$

where

$$\mathcal{J}_j = \left\{ \{s_i\}_{i=1}^n \mid s_i \in \{0, 1\}, \sum_{i=1}^n s_i = j \right\} \quad (3.5)$$

3.1.1 States

Throughout this chapter we will place certain conditions on the states of our system. First and foremost, we assume there is some initial time (taken to be $t_0 = 0$ for simplicity) when our system is in a product state, i.e.

$$\rho(0) = \bigotimes_{i=1}^n \tau_i \quad (3.6)$$

This means that our systems are initially uncorrelated (unentangled) with each other. We will often take the states τ_i to be thermal distributions with some inverse temperature β_i so that they are given by

$$\tau_i = \frac{e^{-H_Q \beta_i}}{\text{Tr}[e^{-H_Q \beta_i}]} = \frac{1}{1 + e^{-E \beta_i}} |0\rangle \langle 0| + \frac{1}{1 + e^{E \beta_i}} |1\rangle \langle 1| \quad (3.7)$$

In the case of qubits, this is equivalent to insisting τ_i be diagonal in the energy eigenbasis. This condition will not always be enforced, since the behavior of coherence terms (off-diagonal entries in the energy eigenbasis) is generally interesting.

3.1.2 Energy-Conserving Dynamics

An interesting class of dynamics to study is the class of energy-conserving dynamics. In this setting we wish to study the behavior of our system under the action of

$$\mathcal{U} = \{U \in \text{U}(2^n) \mid [U, H] = 0\} \quad (3.8)$$

i.e. the unitaries which commute with our systems Hamiltonian.

A Brief Step into Lie-Theory

The function

$$[\bullet, H] : \text{U}(2^n) \rightarrow \text{GL}(2^n)$$

is continuous, and so the preimage of 0 (i.e. \mathcal{U}) is a closed (hence compact) subset of $\text{U}(2^n)$. The product of two elements of \mathcal{U} is clear again an element, as is the inverse, and so \mathcal{U} is a Lie-subalgebra of $\text{U}(2^n)$. Together this means that the Lie-Algebra \mathfrak{u} of \mathcal{U} will be surjectively mapped to it by the exponential operation

$$\begin{aligned} \exp : \mathfrak{u} &\rightarrow \mathcal{U} \\ A &\mapsto e^{iA} \end{aligned}$$

All of this means that we may study the properties of \mathcal{U} in terms of interaction Hamiltonians which commute with H [4].

Interaction Hamiltonians

The set of interaction Hamiltonians \mathfrak{u} can be seen to be all Hamiltonians of the form

$$H_{int} = \sum_{j; J, J' \in \mathcal{J}_j} \alpha_{J, J'} |J\rangle \langle J'| + \alpha_{J, J'}^* |J'\rangle \langle J| \quad (3.9)$$

In the case where we start with thermal qubits, diagonal-type terms ($J = J'$) can be ignored without changing the physics.

Subsets of interaction Hamiltonians that can be interesting are k -qubit interactions, i.e. interactions where energy is exchanged among sets of only k qubits. These consist of both swaps over multiple qubits, e.g.

$$|1001\rangle \langle 0110| + |0110\rangle \langle 1001| \quad (3.10)$$

and swaps controlled by ancillary qubits, e.g.

$$|100\rangle \langle 010| + |010\rangle \langle 100| \quad (3.11)$$

Any k -qubit interaction can be realized as a sum of controlled $k + l$ qubit interactions, and so the sets of k -qubit interactions form a lattice by inclusion. We will denote this by

$$\mathfrak{u}_1 \subset \cdots \subset \mathfrak{u}_{n-1} \subset \mathfrak{u} \quad (3.12)$$

Importantly, this is not respected as an algebra, since the commutator of k -qubit interactions is not necessarily of order no more than k , e.g.

$$i[(|01\rangle\langle 10| + |10\rangle\langle 01|) \otimes \mathbb{1}_2, \mathbb{1}_2 \otimes |00\rangle\langle 00|] = i|010\rangle\langle 100| - i|100\rangle\langle 010| \quad (3.13)$$

where the left hand side is the commutator of two 2-qubit interactions while the right hand side is a controlled swap operation, that is a 3-qubit interaction.

Dimensions

An interesting question is how the dimensionality of these constrained interactions compares to the dimensionality of all interactions. We know $\dim \mathcal{U}(2^n) = 4^n$ as a real Lie-group, but what about \mathcal{U} and the k -qubit interactions?

We can easily see that a complex dimension of \mathfrak{u} is given by choosing $J, J' \in \mathcal{J}_j$ for some j , that is we can find $\text{Bin}(\text{Bin}(n, j), 2)$ pairs J, J' generating interactions for which we can have some complex scalar multiple. The $\text{Bin}(n, j)$ counts the size of \mathcal{J}_j exactly because the set requires choosing j of the n slots to be 1s. There are an additional $\text{Bin}(n, j)$ terms ($J = J'$) generating interactions for which we can have some real scalar multiple. this means we have

$$\dim \mathfrak{u} = \sum_j (2 (\text{Bin}(\text{Bin}(n, j), 2)) + \text{Bin}(n, j)) = \sum_j (\text{Bin}(n, j))^2 = \text{Bin}(2n, n) \quad (3.14)$$

as a real Lie-algebra. Note that

$$\lim_{n \rightarrow \infty} \frac{\dim \mathfrak{u}}{\dim \mathcal{U}(2^n)} = 0 \quad (3.15)$$

so that even the class of all energy-conserving interactions captures essentially none of the possible dynamics.

Since the k -qubit interactions do not create a closed algebra it is difficult to say what their dimension is. In fact, if we apply various k -qubit interactions $\{H_j\}$ in succession (that is we act on our state by $e^{iH_j t_j} e^{iH_{j-1} t_{j-1}} \dots e^{iH_0 t_0}$) we may be acting in effect by some l -qubit interaction, $l > k$. To know precisely what is accessible by k -qubit interactions one must compute the closure of the algebra generated by the interactions.

3.1.3 Comparison with Quantum-Computation

In the world of quantum-computation the energy-conservation requirement is generally lifted, but one can introduce a constraint that only 1 and 2-qubit interactions may be used (in particular 2-qubit exclusive or) [5]. In this case there is actually no reduction to the space of allowed transformations. That is, the closure of the algebra of 1 and 2-qubit interactions is the entire set of hermitian matrices. Clearly in the energy conserving setting there is no hope to access all possible transformations (since energy-conservation is respected by the commutator), but this result suggests that the closure of k -qubit interactions may be large in the set of all energy-conserving interactions (potentially the entire space).

Chapter 4

Open System Dynamics

In this section we will work on a bipartite system $\hat{\mathcal{H}} = \mathcal{H}_1 \otimes \mathcal{H}_2$ with Hamiltonian

$$\hat{H} = H_S \otimes \mathbb{1} + \mathbb{1} \otimes H_E + \hat{H}_{int} \quad (4.1)$$

We will take these two subsystems to be the *system* and the *environment*, where the *system* is composed of all the degrees of freedom of interest, and the *environment* is everything else. The goal is to find a way to trace out the environment degrees of freedom and still capture the relevant dynamics of the system. That is, we want to be able to write down an equation like Equation 2.3 for our system, which does not require knowledge of the trajectory of the environment.

An important detail in this formalism, is that we always assume there is some time $t = t_0$ such that $\hat{\rho}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0)$, i.e. there exists some time at which the two systems are uncorrelated/unentangled. In practice this could mean that the system is prepared in isolation, and then at time t_0 it is allowed to interact with the environment. If this assumption were dropped, then we would be unable to effectively decouple the system and environment degrees of freedom, and it would be unclear how to proceed.

4.1 Main Techniques

Here we shall follow the approach of [6]. We start from the evolution equation for the composite system

$$\hat{\rho}(t) = U(t)(\rho_0 \otimes \gamma)U^\dagger(t) \quad (4.2)$$

and recover a dynamical map on the system

$$V(t) : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}) \quad (4.3)$$

defined by

$$\rho(t) = V(t)\{\rho_0\} = \text{Tr}_B[\hat{\rho}(t)] \quad (4.4)$$

By employing the spectral decomposition of the environment

$$\gamma = \sum_l \lambda_l |\varphi_l\rangle \langle \varphi_l| \quad (4.5)$$

we can see that

$$\begin{aligned} \rho(t) &= \text{Tr}_B[U(t) \left(\rho_0 \otimes \sum_l \lambda_l |\varphi_l\rangle \langle \varphi_l| \right) U^\dagger(t)] = \sum_{k,l} \langle \varphi_k | U(t) | \varphi_l \rangle \sqrt{\lambda_l} \rho_0 \sqrt{\lambda_l} \langle \varphi_l | U^\dagger(t) | \varphi_k \rangle \\ \rho(t) &= \sum_{k,l} W_{kl}(t) \rho_0 W_{kl}^\dagger(t) \end{aligned} \quad (4.6)$$

where we have defined

$$W_{kl}(t) = \sqrt{\lambda_l} \langle \varphi_k | U(t) | \varphi_l \rangle \quad (4.7)$$

These $W_{kl}(t)$ have the important property

$$\sum_{k,l} W_{kl}^\dagger(t) W_{kl}(t) = \sum_{k,l} \lambda_k \langle \varphi_k | U(t) | \varphi_l \rangle \langle \varphi_l | U^\dagger(t) | \varphi_k \rangle = \sum_k \lambda_k \langle \varphi_k | \mathbb{1} | \varphi_k \rangle = \text{Tr}_B[\mathbb{1}] = \mathbb{1}_S \quad (4.8)$$

independent of time, and so

$$\text{Tr}[\rho(t)] = 1 \quad (4.9)$$

It is clear from Equation 4.1 that $\rho(t)$ is Hermitian. In fact $V(t)$ is also a completely positive map (this is much more involved to show), and so $\rho(t)$ is a valid density operator for all t , i.e. mixing two systems together does not irreparably combine them.

An important note is that

$$\begin{aligned} V(t_2)V(t_1)\rho(0) &= \sum_{ijkl} W_{ij}(t_2)W_{kl}(t_1)\rho(0)W_{kl}^\dagger(t_1)W_{ij}^\dagger(t_2) = \sum_{ij} W_{ij}(t_2) \text{Tr}_E[\hat{\rho}(t_1)]W_{ij}^\dagger(t_2) \\ V(t_2)V(t_1)\rho(0) &= \text{Tr}_E[U(t_2) (\text{Tr}_E[\hat{\rho}(t_1)] \otimes \gamma) U^\dagger(t_2)] \end{aligned} \quad (4.10)$$

The application of $V(t_2)$, therefore, yields the time evolution of a new product state for an additional time t_2 , not the further evolution of the original product state for time t_2 . That is, in general $V(t_2)V(t_1) \neq V(t_2 + t_1)$.

4.1.1 Markovian Master Equation

Throughout this section we will set $\hbar = 1$. In [6] they take Equation 4.1 and massage it into the form of a Lindblad master equation

$$\frac{d}{dt}\rho(t) = -i[H, \rho(t)] + \sum_{ij}^{N^2-1} a_{ij} \left(F_i \rho(t) F_j^\dagger - 1/2 \{ F_j^\dagger F_i, \rho(t) \} \right) \quad (4.11)$$

where the F_i form an orthonormal basis of the Liouville space for a Hilbert space of dimension N with respect to the inner product

$$(A, B) = \text{Tr} [A^\dagger B] \quad (4.12)$$

with $F_{N^2} \propto \mathbb{1}$, and the matrix a_{ij} positive and Hermitian.

The derivation [6] employs is problematic though. The issue lies in how the coefficients a_{ij} are defined. First they define the time-dependent coefficients $c_{ij}(t)$ by

$$c_{ij}(t) = \sum_{kl} (F_i, W_{kl}(t)) (F_j, W_{kl}(t))^* \quad (4.13)$$

which allows them to write

$$\rho(t) = \sum_{ij} c_{ij}(t) F_i \rho_0 F_j^\dagger \quad (4.14)$$

In order to write this as a dynamical map, [6] wants to generate this by the action of a superoperator at $t = 0$. In doing so, they essentially take the derivative of the c_{ij} evaluated at $t = 0$. Specifically they define

$$\begin{aligned} a_{N^2 N^2} &= \lim_{\epsilon \rightarrow 0} \frac{c_{N^2 N^2} - N}{\epsilon} \\ a_{i N^2} &= \lim_{\epsilon \rightarrow 0} \frac{c_{i N^2}}{\epsilon}, \forall i < N^2 \\ a_{ij} &= \lim_{\epsilon \rightarrow 0} \frac{c_{ij}}{\epsilon}, \forall i, j < N^2 \end{aligned} \quad (4.15)$$

We can see though, that there is generally a problem. Working out the a_{ij} more explicitly

$$a_{N^2 N^2} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left(\frac{1}{N} \sum_{\alpha\beta kl} \lambda_\beta \langle k\beta | U^\dagger(\epsilon) | k\alpha \rangle \langle l\alpha | U(\epsilon) | l\beta \rangle - N \right) \quad (4.16)$$

Assuming that we can expand $U(t)$ as a Taylor series in time

$$U(t) = \mathbb{1} + tA + t^2 B + \dots \quad (4.17)$$

and noting that, because $U^\dagger U = \mathbb{1}$, we have $A + A^\dagger = 0$. Thus the parenthetical of Equation 4.16 reads as

$$\frac{1}{N} \sum_{\alpha\beta lk} \lambda_\beta \langle k\beta | k\alpha \rangle \langle l\alpha | l\beta \rangle - N + \epsilon \sum_{\alpha\beta lk} \lambda_\beta \left(\langle k\beta | A^\dagger | k\alpha \rangle \langle l\alpha | l\beta \rangle + \langle k\beta | k\alpha \rangle \langle l\alpha | A | l\beta \rangle \right) + \mathcal{O}(\epsilon^2) \quad (4.18)$$

The first sum clearly yields N^2 while the second yields 0. This means that the first non-zero term will be the $\mathcal{O}(\epsilon^2)$ term. In the limit $\epsilon \rightarrow 0$ all of these higher order terms vanish. Therefore, if we can Taylor expand $U(t)$ about $t = 0$, $a_{N^2 N^2} = 0$.

A similar result holds for the a_{ij} , $i, j < N^2$ terms, relying on the traceless nature of the F_i , $i < N^2$. In the end this means that the only non-zero terms in the Equation 4.11 will be the Hamiltonian term, which is controlled by the a_{iN^2} . This means that the derivation given in [6] yields only Hamiltonian like dynamics, and cannot capture anything dissipative. To get around this we will use the formalism in [7]. While it does not produce a true Lindblad equation, it captures the dissipative dynamics.

4.2 Deriving an approximate Equation of Motion

4.2.1 Setup and Result

In the following we will use the formalism as in [7] to derive an equation of motion (EOM) for an open system to second order in perturbation theory. The result will look like a Lindblad master equation, although certain entries will be time-dependent and so the resulting EOM may not be Markovian. Again we set $\hbar = 1$.

We start with a composite system given by $\mathcal{H}_S \otimes \mathcal{H}_E$, where the S system is the open system we care about, and the E system is its environment. We take the total Hamiltonian to be

$$H = H_S \otimes \mathbb{1} + \mathbb{1} \otimes H_E + \lambda V(t) = H_0 + \lambda V(t) \quad (4.19)$$

where λ is a dimensionless scale factor we will use to keep track of the order of our perturbation. Note that H_S and H_E are time-independent. Denote the interaction picture interaction as

$$V_I(t) := e^{iH_0 t} V(t) e^{-iH_0 t} \quad (4.20)$$

and then write the time evolution operator for the whole system as

$$U(t, t_0) = e^{-iH_0(t-t_0)} T \left[e^{-i\lambda \int_{t_0}^t V_I(s) ds} \right] \quad (4.21)$$

where T is the time ordering operator. Let the initial state of our system be given by $\hat{\rho} = \rho_S \otimes \tau_E$, where ρ_S is an arbitrary density operator over \mathcal{H}_S and τ_E is a density operator over \mathcal{H}_E which is diagonal in the H_E basis. We will take

$$\tau_E = \sum_{\bar{u}} q_{\bar{u}} |\bar{u}\rangle \langle \bar{u}| =: \sum_{\bar{u}} |\bar{u}_\tau\rangle \langle \bar{u}_\tau| \quad (4.22)$$

with $H_E |\bar{u}\rangle = E_{\bar{u}} |\bar{u}\rangle$. In the following we treat only elements like $|\bar{u}_\tau\rangle \langle \bar{u}_\tau|$, which is permissible because the results will extend to mixed states via linearity. By moving to non-normalized states we will see how the weightings in the density operator $\{q_{\bar{u}}\}$ are accounted for.

We are interested in solving for

$$\rho(t) := \rho_S(t) = \text{Tr}_E[U(t, t_0) \hat{\rho}(t_0) U^\dagger(t, t_0)] \quad (4.23)$$

which is approximated by the EOM

$$\dot{\rho}(t) = -i[H_{eff}(t), \rho(t)] + \{A(t), \rho(t)\} + \gamma_t[\rho(t)] \quad (4.24)$$

where we have

$$H_{eff} := H_S + \sum_{\bar{u}} \left(q_{\bar{u}} \langle \bar{u}| V(t) |\bar{u}\rangle - \frac{i}{2} \sum_u \left(L_{\bar{u}u}^\dagger(t) L_{\bar{u}u}^2(t) - h.c. \right) \right) \quad (4.25)$$

$$A(t) := \sum_{\bar{u}} -\frac{1}{2} \sum_u \left(L_{\bar{u}u}^{1\dagger}(t) L_{\bar{u}u}^2(t) + h.c. \right) \quad (4.26)$$

$$\gamma_t[\rho(t)] := \sum_{\bar{u}} \sum_u \left(L_{\bar{u}u}^1(t) \rho(t) L_{\bar{u}u}^{2\dagger}(t) + h.c. \right) \quad (4.27)$$

$$L_{\bar{u}u}^1(t) := \langle u | V(t) | \bar{u}_\tau \rangle = \sqrt{q_{\bar{u}}} \langle u | V(t) | \bar{u} \rangle \quad (4.28)$$

$$L_{\bar{u}u}^2(t) := \langle u | \int_{t_0}^t V_I(s-t) ds | \bar{u}_\tau \rangle = \sqrt{q_{\bar{u}}} \langle u | \int_{t_0}^t V_I(s-t) ds | \bar{u} \rangle \quad (4.29)$$

with *h.c.* the hermitian conjugate of the proceeding term.

4.2.2 Derivation

To derive this we will write

$$\rho(t) = \rho^0(t) + \lambda \rho^1(t) + \lambda^2 \rho^2(t) + \dots \quad (4.30)$$

and solve for the derivative of each term by matching powers of λ with Equation 4.23 for

$$U(t) = e^{-iH_0(t-t_0)} \left(\mathbb{1} - i\lambda \int_{t_0}^t V_I(s) ds - \lambda^2 \int_{t_0}^t V_I(s) ds \int_{t_0}^s V_I(r) dr + \dots \right) \quad (4.31)$$

From here we will set $t_0 = 0$ for simplicity. First we see

$$\rho_{\bar{u}}^0(t) = \sum_u \langle u | (e^{-iH_0 t} | \bar{u}_\tau \rangle \rho(0) \langle \bar{u}_\tau | e^{iH_0 t}) | u \rangle = q_{\bar{u}} e^{-iH_0 t} \rho(0) e^{iH_0 t} \quad (4.32)$$

$$\rho_{\bar{u}}^1(t) = \sum_u \langle u | \left(i e^{-iH_0 t} | \bar{u}_\tau \rangle \rho(0) \langle \bar{u}_\tau | \left(\int_0^t V_I(s) ds \right) e^{iH_0 t} + h.c. \right) | u \rangle \quad (4.33)$$

$$\rho_{\bar{u}}^1(t) = i q_{\bar{u}} e^{-iH_0 t} \rho(0) \langle \bar{u} | \left(\int_0^t V_I(s) ds \right) | \bar{u} \rangle e^{iH_0 t} + h.c. \quad (4.34)$$

$$\begin{aligned} \rho_{\bar{u}}^2(t) = & \sum_u \langle u | - e^{-iH_0 t} \left(\int_0^t V_I(s) ds \int_0^s V_I(r) dr \right) | \bar{u}_\tau \rangle \rho(0) \langle \bar{u}_\tau | e^{iH_0 t} + h.c. + \\ & + e^{-iH_0 t} \left(\int_0^t V(s) ds \right) | \bar{u}_\tau \rangle \rho(0) \langle \bar{u}_\tau | \left(\int_0^t V(s) ds \right) e^{iH_0 t} | u \rangle \end{aligned} \quad (4.35)$$

$$\begin{aligned} \rho_{\bar{u}}^2(t) = & e^{-iH_0 t} \langle \bar{u}_\tau | \left(\int_0^t V_I(s) ds \int_0^s V_I(r) dr \right) | \bar{u}_\tau \rangle \rho(0) e^{iH_0 t} + h.c. + \\ & + \sum_u e^{-iH_0 t} \langle u | \left(\int_0^t V(s) ds \right) | \bar{u}_\tau \rangle \rho(0) \langle \bar{u}_\tau | \left(\int_0^t V(s) ds \right) | u \rangle e^{iH_0 t} \end{aligned} \quad (4.36)$$

By inserting the $\mathbb{1} = e^{iH_0 t} e^{-iH_0 t}$ identity and recognizing $e^{-iH_S t} \rho(0) e^{iH_S t} = \rho^0(t)$ we can write Equations 4.34 & 4.2.2 as

$$\rho_{\bar{u}}^1 = iq_{\bar{u}} \rho^0(t) \langle \bar{u} | \int_0^t V_I(s-t) ds | \bar{u} \rangle + h.c. \quad (4.37)$$

$$\begin{aligned} \rho_{\bar{u}}^2 &= \langle \bar{u}_\tau | \int_0^t V_I(s-t) ds \int_0^r V_I(r-t) dr | \bar{u}_\tau \rangle \rho^0(t) + h.c. + \\ &+ \sum_u \langle u | \int_0^t V_I(s-t) ds | \bar{u}_\tau \rangle \rho^0(t) \langle \bar{u}_\tau | \int_0^t V_I(s-t) ds | u \rangle \end{aligned} \quad (4.38)$$

From here we can start taking derivatives for each order and we see

$$\dot{\rho}^0(t) = -i[H_S, \rho^0(t)] \quad (4.39)$$

$$\dot{\rho}_{\bar{u}}^1(t) = -i[H_S, \rho_{\bar{u}}^1(t)] - i[q_{\bar{u}} \langle \bar{u} | V(t) | \bar{u} \rangle, \rho^0(t)] \quad (4.40)$$

$$\begin{aligned} \dot{\rho}_{\bar{u}}^2(t) &= -i[H_S, \rho_{\bar{u}}^2(t)] + \left(\langle \bar{u}_\tau | V(t) \int_0^t V_I(s-t) ds | \bar{u}_\tau \rangle \rho^0(t) + h.c. \right) + \\ &+ \sum_u \left(\langle u | V(t) | \bar{u}_\tau \rangle \rho^0(t) \langle \bar{u}_\tau | \int_0^t V_I(s-t) ds | u \rangle + h.c. \right) \end{aligned} \quad (4.41)$$

now by inserting $\mathbb{1} = \sum_u |u\rangle \langle u|$ into the middle of the second term of Equation 4.2.2 and utilizing the notation of Equations 4.28 & 4.29 we may write

$$\dot{\rho}_{\bar{u}}^2(t) = -i[H_S, \rho_{\bar{u}}^2(t)] + \sum_u \left(-L_{\bar{u}u}^{1\dagger} L_{\bar{u}u}^2 \rho^0(t) + L_{\bar{u}u}^1 \rho^0(t) L_{\bar{u}u}^{2\dagger} + h.c. \right) \quad (4.42)$$

Finally we will decompose

$$L_{\bar{u}u}^{1\dagger} L_{\bar{u}u}^2 = \frac{1}{2} \left[\left(L_{\bar{u}u}^{1\dagger} L_{\bar{u}u}^2 + L_{\bar{u}u}^{2\dagger} L_{\bar{u}u}^1 \right) + \left(L_{\bar{u}u}^{1\dagger} L_{\bar{u}u}^2 - L_{\bar{u}u}^{2\dagger} L_{\bar{u}u}^1 \right) \right] \quad (4.43)$$

and this will finally leave us with Equation 4.24.

4.3 Examples for One-Qubit Systems

We take our composite system to be $\mathcal{H}_Q \otimes \mathcal{H}_E$, that is a single qubit coupled to an environment, with Hamiltonians $H_Q = E |1\rangle \langle 1|$ for the qubit, and H_E for the environment (where we assume we can solve for the eigenstates of H_E). We then add an interaction term $V(t)$ yielding the total Hamiltonian $H = H_Q \otimes \mathbb{1} + \mathbb{1} \otimes H_E + V(t)$.

We further assume that there is a time, taken to be $t = 0$ for simplicity, when the composite system state is given by

$$\sigma = \rho_Q \otimes \tau_E \quad (4.44)$$

where we additionally assume τ_E is diagonal in the H_E basis but ρ_Q is a generic density operator over \mathcal{H}_Q

$$\rho_Q = \begin{pmatrix} 1-p & a+ib \\ a-ib & p \end{pmatrix} \quad (4.45)$$

Finally, we assume $V(t)$ to be globally energy conserving (i.e. $[H_Q \otimes \mathbb{1} + \mathbb{1} \otimes H_E, V(t)] = 0$). In doing so we see immediately that $V_I(t) = V(t)$.

4.3.1 n -Qubit Environment

As a first example, we take our environment to be composed of n qubits, with

$$H_E = \sum_{i=1}^n \mathbb{1}^{i-1} \otimes H_Q \otimes \mathbb{1}^{n-i} \quad (4.46)$$

and a model pairwise interaction

$$V_{ij} = g_{ij}(|01\rangle \langle 10| + |10\rangle \langle 01|) \quad (4.47)$$

Where $\{ij\}$ indicates that the interaction is between qubits i and j of the composite system. The total interaction is then given by a sum of V_{ij} over all pairs of qubits

$$V = \sum_{i < j} V_{ij} \quad (4.48)$$

We see that the action of each V_{ij} is to switch qubit i with qubit j with a rate governed by g_{ij} . Our assumption that V can be treated perturbatively is that the maximal eigenvalue of V be much smaller than E , so that evolution due to the interaction is slow compared to the internal evolution, but the maximal eigenvalue of V grows quadratically in the size of the bath.

One-Qubit Environment

If we carry out the explicit calculations for a one-qubit environment in the state

$$\tau_E = (1-q) |0\rangle \langle 0| + q |1\rangle \langle 1| \quad (4.49)$$

our EOM is

$$\dot{\rho}(t) = \begin{pmatrix} 2g^2(p(t) - q)t & (a(t) + ib(t))(iE - g^2t) \\ (a(t) - ib(t))(-iE - g^2t) & -2g^2(p(t) - q)t \end{pmatrix} \quad (4.50)$$

Thus, for an arbitrary initial state of the system, the population of the excited state decays as

$$p(t) = (p_0 - q)e^{-g^2t^2} + q \quad (4.51)$$

that is we have an exponential relaxation to the population of the environment state.

The coherence terms ($a \pm ib$) are more complicated, but we can see that H_Q causes the phase to oscillate with frequency E , while the interaction causes it to exponentially damp with rate g^2 .

Two-Qubit Environment

If we carry this calculation out for both environment qubits in different states

$$\tau_1 = (1 - q_1) |0\rangle \langle 0| + q_1 |1\rangle \langle 1|$$

$$\tau_2 = (1 - q_2) |0\rangle \langle 0| + q_2 |1\rangle \langle 1|$$

with $g_{01} := g_1$, $g_{02} := g_2$ and arbitrary g_{12} , we find

$$p(t) = \left(p_0 - \frac{g_1^2 q_1 + g_2^2 q_2}{g_1^2 + g_2^2} \right) e^{-(g_1^2 + g_2^2)t^2} + \frac{g_1^2 q_1 + g_2^2 q_2}{g_1^2 + g_2^2} \quad (4.52)$$

That is we have an exponential relaxation to a weighted combination of the environment states, with a rate equal to the sum of the two individual rates. Importantly, the system evolution has no dependence on g_{12} .

The coherence term here behaves as it did with the one-qubit environment, only the damping rate is the $g_1^2 + g_2^2$ like for the population.

Generalizing

From the previous work, we see that, given an n -qubit environment, the behavior of the population of the excited state of the system will be to exponentially relax to the state

$$p = \frac{\sum_i g_i^2 q_i}{\sum_i g_i^2} \quad (4.53)$$

with effective rate

$$g'^2 = \sum_i g_i^2 \quad (4.54)$$

and the coherence will be exponentially damped with the same rate. Upon introducing the $g_i \ll \frac{E}{n^2}$ condition, we see that the effective rate goes like $\frac{1}{n^3}$. This means that as the bath grows, this approximation is increasingly unable to describe the dynamics. This failure can be understood as arising from the increasing complexity of the interaction.

4.3.2 n -Level Environment

The goal of this example is to understand how the presence of degeneracies in the n -qubit environment contribute to the behavior of the system. To do so we take an n -level system for the environment, with Hamiltonian

$$H_E = \sum_{l=0}^{n-1} lE |l\rangle \langle l|$$

and an interaction

$$V = \sum_{l=1}^{n-1} g_l (|0, l\rangle \langle 1, l-1| + |1, l-1\rangle \langle 0, l|) \quad (4.55)$$

To treat V perturbatively we again require its maximal eigenvalue be much less than E , but now that is equivalent to $g_l \ll E$ for all l .

3-Level Environment

Taking explicitly the case for $n = 3$ and setting the environment's initial state to

$$\tau_E = (1 - (q_1 + q_2)) |0\rangle \langle 0| + q_1 |1\rangle \langle 1| + q_2 |2\rangle \langle 2|$$

we find the population of the excited state of our qubit is given by

$$p(t) = (p_0 - q') e^{-g'^2 t^2} + q' \quad (4.56)$$

where we have defined

$$g'^2 = g_1^2 (1 - q_2) + g_2^2 (q_1 + q_2)$$

$$q' = \frac{g_1^2 q_1 + g_2^2 q_2}{g'^2} \quad (4.57)$$

The coherences again behave as they did for n -qubit environments, with the rate given by g'^2 .

Generalizing

We can see from here that for any n -level system with populations $\{q_l\}_{l=0}^{n-1}$ such that $\sum_l q_l = 1$ and couplings $\{g_l\}_{l=1}^{n-1}$ we will have effective rate

$$g'^2 = \sum_{l=1}^{n-1} g_l^2 (q_l + q_{l-1}) \quad (4.58)$$

and effective population

$$q' = \frac{\sum_{l=1}^{n-1} g_l^2 q_l}{g'^2} \quad (4.59)$$

In units where $k_B = 1$ and $E = 1$, working with an environment given by thermal a state with inverse temperature β , and with all coupling terms g equal. We see

$$g'^2 = g^2 \frac{1}{\sum_{l=0}^{n-1} e^{-l\beta}} \sum_{l=1}^{n-1} (e^{-l\beta} + e^{-(l-1)\beta}) = g^2 \left(1 + \cosh(\beta) - \coth\left(\frac{\beta n}{2}\right) \sinh(\beta) \right)$$

$$q' = \frac{1}{1 + e^\beta} \quad (4.60)$$

That is, the system relaxes to a thermal state with inverse temperature β with a rate converging to

$$\lim_{n \rightarrow \infty} g'^2 = g^2 (1 + e^{\pm\beta}) \quad (4.61)$$

where the \pm is chosen such that $\pm\beta \leq 0$. This demonstrates that regardless of the number of levels, the n -level system never achieves a rate greater than that of a two-qubit environment. At the same time though, the complexity of this interaction does not grow with the size of the environment, and so it can always be effectively treated in this approximation.

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Education

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Research Experience

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- Build simulations of complicated quantum dynamics such as decoherence phenomenon
- Construct thermodynamic measures on non-equilibrium systems
- Classify behavior under various allowed dynamics such as multi-partite interactions

STAR Collaboration at Brookhaven National Lab

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- Designed, constructed, and installed novel addition to RHIC at BNL to improve detector sensitivity
 - Measured and modeled radiation damage within FMS detector parts to improve simulations
 - Improved extant simulations of collider physics run time by streamlining algorithms
-

Awards and Honors

- Evan Pugh Junior (Spring 2017)
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Visits

- August 2017 I was a visitor at Perimeter Institute with Dr. Shandera
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Presentations

- Rauch, S. (2018, Sep.) A Survey of Open Quantum Systems, Eberly College of Science Poster Exhibition, University Park
 - Rauch, S. (2017, Oct.) An Analysis of Small Quantum Systems out of Equilibrium, Eberly College of Science Fall Poster Exhibition, University Park
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Extracurriculars

- Open Music, a contemporary and experimental music ensemble
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