Entropy Growth in Quantum Mechanics

by

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[This page should maybe be removed.] The following individuals certify that they have read, and recommend to the Faculty of Science for acceptance, the thesis entitled:

Entropy Growth in Quantum Mechanics

submitted by **Duncan MacIntyre** in partial fulfillment of the requirements for the degree of **Combined Honours** in **Physics and Mathematics**

Examining Committee:

Supervisor: Gordon Semenoff

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Abstract

Write the abstract last! Maximum 350 words.

Lay Summary

[Required, Maximum 150 words]

This is a simple summary of your thesis, written so that members of the public will get some idea about what you have done.

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I would like to thank Gordon Semenoff for being a superb supervisor. I have learned much from him.

The general approach taken in this thesis was his suggestion and subsequent work benefitted much from his guidance and advice.

Chapter 1

Introduction

These sections were taken from the thesis proposal and need to be updated.

1.1 Premise

Non-relativistic scattering has long been studied in quantum mechanics. More recently, people began to study the quantum entropy of mixed states (for example, Reference [**?**]). I continue this work by analyzing a concrete example: the scattering of one particle off another. My findings could give us insight into entropy change during weak interactions in general.

I will consider the situation where two distinguishable particles scatter and then we make measurements on the first particle while the second particle exits the system and is lost. This loss of information should increase entropy for the first particle. I will assume that the scattering is very weak (i.e., most particles continue in their initial states without interacting) so that I can use perturbation theory.

I will first investigate hard-shell scattering (i.e., with the potential $V(r) \propto \delta(r)$ where r is the distance between the particles) because it has the simplest computations. Hard-shell scattering is also a good approximation for some physical systems, e.g., if one nucleon is scattered off another at a low speed. I might then consider how my results for hard-shell scattering generalize to other potentials.

I investigate scattering rather than other interactions because scattering experiments are common. It is nevertheless conceivable that results obtained from my particular example might give insight into the entropy of weak interactions in general.

1.2 Theory

In quantum mechanics, one first learns about "pure states" of the form $|\Psi\rangle$. I will consider "mixed states," that is, statistical combinations of pure states. We might have a situation where there is a probability of P_i that we are in the pure state $|\Psi_i\rangle$. (In this case, all of the P_i should add to 1.) Instead of describing this mixed state with a ket, we describe it with the "density operator"

$$\hat{\rho} = \sum_{i=1}^{N} P_i \left|\Psi_i\right\rangle .$$

This is indeed a valid Hermitian operator in quantum mechanics. By looking at how this operator changes over time, we can see how the possible pure states $|\psi_i\rangle$ change and also how the probabilities P_i that we're in each state change.

We can now define the von Neumann entropy to be

$$S = -\sum_{i=1}^{N} P_i \log P_i.$$

This entropy is zero for pure states ($N = 1$) and non-zero for mixed states $N > 1$). In this way, entropy measures the amount of mixedness.

Von Neumann entropy is the quantum mechanical version of the usual Gibbs energy from statistical mechanics. One would naively expect that results like the Second Law of Thermodynamics would hold for von Neumann entropy.

I will use first-order perturbation theory to calculate the change in von Neumann entropy for scattered particles. In this approach, we take λ to be a number proportional to the interaction strength and write

$$\hat{\rho} = \hat{\rho}_0 + \lambda\hat{\rho}_1 + \mathcal{O}\left(\lambda^2\right).$$

We can then compute $\hat{\rho}_1$ and take $\hat{\rho} \approx \hat{\rho}_0 + \lambda\hat{\rho}_1$ for small enough λ.

I will do my analysis in non-relativistic quantum mechanics. I would guess that some of my results could be extended to relativistic field theories by following similar derivations.

Chapter 2

What is Entropy?

2.0.1 Time evolution of a pure state

Suppose we have a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}(t)$$

where $\hat{H}_0$ is a well-understood Hamiltonian that does not depend on time and $\lambda \hat{V}(t)$ is "small". For example, $\hat{H}_0$ might be the free particle Hamiltonian $\hat{H}_0 = \frac{m}{2}\nabla^2$. Our equation of motion is the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi, t\rangle = \left(\hat{H}_0 + \lambda \hat{V}(t)\right) |\Psi, t\rangle$$

where $|\Psi, t\rangle$ is the usual Schrödinger-picture state at time t.

Let $\hat{U}(t_0, t) = e^{-i\hat{H}_0(t-t_0)/\hbar}$. Then $\hat{U}(t_0, t)$ is the operator that evolves a state from time t_0 to time t according to $\hat{H}_0$. We define the interaction-picture state to be

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

so $|\Psi, t\rangle = \hat{U}(t_0, t) |\Psi_I, t\rangle$. Plugging this in to the Schrödinger equation,

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \hat{U}(t_0, t) |\Psi_I, t\rangle &= \left(\hat{H}_0 + \lambda \hat{V}(t)\right) \hat{U}(t_0, t) |\Psi, t\rangle \\
i\hbar \left[\frac{\partial}{\partial t} e^{-i\hat{H}_0(t-t_0)/\hbar}\right] |\Psi_I, t\rangle + i\hbar e^{-i\hat{H}_0(t-t_0)/\hbar} \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \hat{H}_0 e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle + \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
\cancel{-i^2 \hat{H}_0 e^{i\hat{H}_0(t-t_0)/\hbar}} |\Psi_I, t\rangle + i\hbar e^{-i\hat{H}_0(t-t_0)/\hbar} \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \cancel{\hat{H}_0 e^{-i\hat{H}_0(t-t_0)/\hbar}} |\Psi_I, t\rangle + \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
i\hbar \frac{\partial}{\partial t} |\Psi_I, t\rangle &= e^{i\hat{H}_0(t-t_0)/\hbar} \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
i\hbar \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \lambda \hat{H}_I(t) |\Psi_I, t\rangle
\end{aligned}$$

where we define the interaction Hamiltonian to be

$$\hat{H}_I(t) = \hat{U}(t_0, t)^\dagger \hat{V}(t) \hat{U}(t_0, t) = e^{i\hat{H}_0(t-t_0)/\hbar} \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar}.$$

This sets up the interaction picture. We have rephrased our problem so that we can continue with quantum mechanics normally without having to worry about the time evolution due to $\hat{H}_0$.

We now integrate both sides of our expression.

$$\begin{aligned}
\int_{t_0}^{t} \frac{\partial}{\partial t'} |\Psi_I, t'\rangle &= -\frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') |\Psi_I, t'\rangle \, dt' \\
|\Psi_I, t\rangle - |\Psi_I, t_0\rangle &= -\frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') |\Psi_I, t'\rangle \, dt' \\
|\Psi_I, t\rangle &= |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') |\Psi_I, t'\rangle \, dt' \qquad (2.1)
\end{aligned}$$

This is called the integral form of the Schrödinger equation.

We can now iteratively calculate perturbative approximations where we assume $\hat{H}_I(t)$ is small. The zero order approximation is simply

$$|\Psi_I, t\rangle = |\Psi_I, t_0\rangle + \mathcal{O}(\lambda).$$

Plugging this in for the state inside the integral in (6.1), we get the first order approximation

$$|\Psi_I, t\rangle = |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t')\,|\Psi_I, t_0\rangle\; dt' + \mathcal{O}(\lambda^2). \tag{2.2}$$

Plugging this in to (6.1) again we get the second order approximation

$$\begin{aligned}
|\Psi_I, t\rangle &= |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left[|\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t'} \hat{H}_I(t'')\,|\Psi_I, t_0\rangle\; dt'' \right] dt' + \mathcal{O}(\lambda^3) \\
&= |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t')\,|\Psi_I, t_0\rangle\; dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t'} \hat{H}_I(t')\hat{H}_I(t'')\,|\Psi_I, t_0\rangle\; dt''\, dt' + \mathcal{O}(\lambda^3).
\end{aligned} \tag{2.3}$$

In general, we can keep going to achieve higher order approximations. For us, however, the second order approximation (6.3) is enough.

2.0.2 Time evolution of the density operator

We now consider mixed states. We will need to describe the system by the density operator $\hat{\rho}(t)$. Let's derive the time evolution of $\hat{\rho}(t)$ in second order perturbation theory based on (6.3).

Suppose at time t_0 we have a statistical ensemble of interaction-picture states $|\psi_{In}, t_0\rangle$ each with probability P_n. Then

$$\hat{\rho}(t_0) = \sum_n P_n\,|\Psi_{In}, t_0\rangle\,\langle\Psi_{In}, t_0|\,.$$

At time t states will have evolved according to (6.3), so

$$\hat{\rho}(t) = \sum_n P_n\,|\Psi_{In}, t\rangle\,\langle\Psi_{In}, t|\,.$$

From (6.3) we have

$$\begin{aligned}
|\Psi_{In}, t\rangle &= |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t')\,|\Psi_I, t_0\rangle\; dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t'} \hat{H}_I(t')\hat{H}_I(t'')\,|\Psi_I, t_0\rangle\; dt''\, dt' + \mathcal{O}(\lambda^3) \\
\langle\Psi_{In}, t| &= \langle\Psi_I, t_0| - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \langle\Psi_I, t_0|\,\hat{H}_I(t')\, dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t'} \langle\Psi_I, t_0|\,\hat{H}_I(t'')\hat{H}_I(t')\, dt''\, dt' + \mathcal{O}(\lambda^3)
\end{aligned}$$

so

$$\begin{aligned}
|\Psi_{In}, t\rangle\,\langle\Psi_{In}, t| \;=\; & |\Psi_{In}, t_0\rangle\,\langle\Psi_{In}, t_0| \;-\; \frac{i}{\hbar}\lambda \int_{t_0}^{t} \Big(\hat{H}(t')\,|\Psi_{In}, t_0\rangle\,\langle\Psi_{In}, t_0| - |\Psi_{In}, t_0\rangle\,\langle\Psi_{In}, t_0|\,\hat{H}_I(t') \Big)\, dt' \\
& - \;\frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t'} \Big(\hat{H}_I(t')\hat{H}_I(t'')\,|\Psi_{In}, t_0\rangle\,\langle\Psi_{In}, t_0| + \;|\Psi_{In}, t_0\rangle\,\langle\Psi_{In}, t_0|\,\hat{H}_I(t'')\hat{H}_I(t') \Big)\, dt''\, dt' \\
& + \;\frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t} \hat{H}_I(t')\,|\Psi_{In}, t_0\rangle\,\langle\Psi_{In}, t_0|\,\hat{H}_I(t'')\, dt''\, dt' \;+\; \mathcal{O}(\lambda^3).
\end{aligned}$$

Then

$$
\begin{aligned}
\hat{\rho}(t) \;&=\; \hat{\rho}\,(t_0) \;-\; \frac{i}{\hbar}\lambda \int_{t_0}^{t} \Big[\hat{H}(t'),\; \hat{\rho}(t_0)\Big]\; dt' \\
&-\; \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t'} \Big(\hat{H}_I(t')\hat{H}_I(t'')\;\hat{\rho}(t_0) + \hat{\rho}(t_0)\;\hat{H}_I(t'')\hat{H}_I(t')\Big)\; dt''\, dt' \\
&+\; \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t} \hat{H}_I(t')\hat{\rho}(t_0)\hat{H}_I(t'')\, dt''\, dt' \;+\; \mathcal{O}\big(\lambda^3\big).
\end{aligned} \tag{2.4}
$$

Chapter 3

Theoretical Tools

3.1 Time-dependent perturbation theory in the interaction picture

3.1.1 Time evolution of a pure state

Suppose we have a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}(t)$$

where $\hat{H}_0$ is a well-understood Hamiltonian that does not depend on time and $\lambda \hat{V}(t)$ is "small". For example, $\hat{H}_0$ might be the free particle Hamiltonian $\hat{H}_0 = \frac{m}{2}\nabla^2$. Our equation of motion is the Schrödinger equation

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Let $\hat{U}(t_0, t) = e^{-i\hat{H}_0(t-t_0)/\hbar}$. Then $\hat{U}(t_0, t)$ is the operator that evolves a state from time t_0 to time t according to $\hat{H}_0$. We define the interaction-picture state to be

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

so $|\Psi, t\rangle = \hat{U}(t_0, t) |\Psi_I, t\rangle$. Plugging this in to the Schrödinger equation,

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \hat{U}(t_0, t) |\Psi_I, t\rangle &= \left(\hat{H}_0 + \lambda \hat{V}(t)\right) \hat{U}(t_0, t) |\Psi, t\rangle \\
i\hbar \left[\frac{\partial}{\partial t} e^{-i\hat{H}_0(t-t_0)/\hbar}\right] |\Psi_I, t\rangle + i\hbar e^{-i\hat{H}_0(t-t_0)/\hbar} \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \hat{H}_0 e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle + \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
\cancel{-i^2 \hat{H}_0 e^{i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle} + i\hbar e^{-i\hat{H}_0(t-t_0)/\hbar} \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \cancel{\hat{H}_0 e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle} + \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
i\hbar \frac{\partial}{\partial t} |\Psi_I, t\rangle &= e^{i\hat{H}_0(t-t_0)/\hbar} \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
i\hbar \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \lambda \hat{H}_I(t) |\Psi_I, t\rangle
\end{aligned}$$

where we define the interaction Hamiltonian to be

$$\hat{H}_I(t) = \hat{U}(t_0, t)^\dagger \hat{V}(t) \hat{U}(t_0, t) = e^{i\hat{H}_0(t-t_0)/\hbar} \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar}.$$

This sets up the interaction picture. We have rephrased our problem so that we can continue with quantum mechanics normally without having to worry about the time evolution due to $\hat{H}_0$.

We now integrate both sides of our expression.

$$\begin{aligned}\int_{t_0}^{t} \frac{\partial}{\partial t'} \left|\Psi_I, t'\right\rangle &= -\frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left|\Psi_I, t'\right\rangle\, dt' \\ \left|\Psi_I, t\right\rangle - \left|\Psi_I, t_0\right\rangle &= -\frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left|\Psi_I, t'\right\rangle\, dt' \\ \left|\Psi_I, t\right\rangle &= \left|\Psi_I, t_0\right\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left|\Psi_I, t'\right\rangle\, dt' \end{aligned} \tag{3.1}$$

This is called the integral form of the Schrödinger equation.

We can now iteratively calculate perturbative approximations where we assume $\hat{H}_I(t)$ is small. The zero order approximation is simply

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Plugging this in for the state inside the integral in (6.1), we get the first order approximation

$$\left|\Psi_I, t\right\rangle = \left|\Psi_I, t_0\right\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left|\Psi_I, t_0\right\rangle\, dt' + \mathcal{O}\big(\lambda^2\big). \tag{3.2}$$

Plugging this in to (6.1) again we get the second order approximation

$$\begin{aligned}\left|\Psi_I, t\right\rangle &= \left|\Psi_I, t_0\right\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left[\left|\Psi_I, t_0\right\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t'} \hat{H}_I(t'') \left|\Psi_I, t_0\right\rangle\, dt''\right] dt' + \mathcal{O}\big(\lambda^3\big) \\ &= \left|\Psi_I, t_0\right\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left|\Psi_I, t_0\right\rangle\, dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t'} \hat{H}_I(t')\hat{H}_I(t'') \left|\Psi_I, t_0\right\rangle\, dt''\, dt' + \mathcal{O}\big(\lambda^3\big). \end{aligned} \tag{3.3}$$

In general, we can keep going to achieve higher order approximations. For us, however, the second order approximation (6.3) is enough.

3.1.2 Time evolution of the density operator

We now consider mixed states. We will need to describe the system by the density operator $\hat{\rho}(t)$. Let's derive the time evolution of $\hat{\rho}(t)$ in second order perturbation theory based on (6.3).

Suppose at time t_0 we have a statistical ensemble of interaction-picture states $\left|\psi_{In}, t_0\right\rangle$ each with probability P_n. Then

$$\hat{\rho}(t_0) = \sum_n P_n \left|\Psi_{In}, t_0\right\rangle \left\langle\Psi_{In}, t_0\right|.$$

At time t states will have evolved according to (6.3), so

$$\hat{\rho}(t) = \sum_n P_n \left|\Psi_{In}, t\right\rangle \left\langle\Psi_{In}, t\right|.$$

From (6.3) we have

$$\begin{aligned}\left|\Psi_{In}, t\right\rangle &= \left|\Psi_I, t_0\right\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left|\Psi_I, t_0\right\rangle\, dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t'} \hat{H}_I(t')\hat{H}_I(t'') \left|\Psi_I, t_0\right\rangle\, dt''\, dt' + \mathcal{O}\big(\lambda^3\big) \\ \left\langle\Psi_{In}, t\right| &= \left\langle\Psi_I, t_0\right| - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \left\langle\Psi_I, t_0\right| \hat{H}_I(t')\, dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t}\int_{t_0}^{t'} \left\langle\Psi_I, t_0\right| \hat{H}_I(t'')\hat{H}_I(t')\, dt''\, dt' + \mathcal{O}\big(\lambda^3\big)\end{aligned}$$

so

$$\begin{aligned}
|\Psi_{In},t\rangle\langle\Psi_{In},t| &= |\Psi_{In},t_0\rangle\langle\Psi_{In},t_0| - \frac{i}{\hbar}\lambda\int_{t_0}^{t}\Big(\hat{H}(t')\,|\Psi_{In},t_0\rangle\langle\Psi_{In},t_0| - |\Psi_{In},t_0\rangle\langle\Psi_{In},t_0|\,\hat{H}_I(t')\Big)\,dt' \\
&- \frac{\lambda^2}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t'}\Big(\hat{H}_I(t')\hat{H}_I(t'')\,|\Psi_{In},t_0\rangle\langle\Psi_{In},t_0| + |\Psi_{In},t_0\rangle\langle\Psi_{In},t_0|\,\hat{H}_I(t'')\hat{H}_I(t')\Big)\,dt''\,dt' \\
&+ \frac{\lambda^2}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t}\hat{H}_I(t')\,|\Psi_{In},t_0\rangle\langle\Psi_{In},t_0|\,\hat{H}_I(t'')\,dt''\,dt' + \mathcal{O}\big(\lambda^3\big).
\end{aligned}$$

Then

$$\begin{aligned}
\hat{\rho}(t) &= \hat{\rho}(t_0) - \frac{i}{\hbar}\lambda\int_{t_0}^{t}\Big[\hat{H}(t'),\ \hat{\rho}(t_0)\Big]\,dt' \\
&- \frac{\lambda^2}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t'}\Big(\hat{H}_I(t')\hat{H}_I(t'')\,\hat{\rho}(t_0) + \hat{\rho}(t_0)\,\hat{H}_I(t'')\hat{H}_I(t')\Big)\,dt''\,dt' \\
&+ \frac{\lambda^2}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t}\hat{H}_I(t')\hat{\rho}(t_0)\hat{H}_I(t'')\,dt''\,dt' + \mathcal{O}\big(\lambda^3\big).
\end{aligned} \tag{3.4}$$

3.2 Eigenvalue corrections from perturbation theory

The goal of this section is to compute the second-order perturbative corrections to the eigenvalues of an operator. We use the approach known as time-independent perturbation theory.

Suppose $\hat{\rho}$ is an operator with eigenstates $|\Psi_n\rangle$ and eigenvalues σ_n. Suppose we have the asymptotic expansions

$$\begin{aligned}
\hat{\rho} &= \hat{\rho}_0 + \lambda\hat{\rho}_1 + \lambda^2\hat{\rho}_2 + \mathcal{O}\big(\lambda^3\big) \\
|\Psi_n\rangle &= \left|\Psi_n^{(0)}\right\rangle + \lambda\left|\Psi_n^{(1)}\right\rangle + \lambda^2\left|\Psi_n^{(2)}\right\rangle + \mathcal{O}\big(\lambda^3\big) \\
\sigma_n &= \sigma_n^{(0)} + \lambda\sigma_n^{(1)} + \lambda^2\sigma_n^{(2)} + \mathcal{O}\big(\lambda^3\big)
\end{aligned}$$

where $\left\{\left|\Psi_n^{(0)}\right\rangle\right\}$ is an orthonormal basis for the Hilbert space.

We have $\hat{\rho}\,|\Psi_n\rangle = \sigma_n\,|\Psi_n\rangle$. In the zeroth order of λ this gives $\hat{\rho}_0\left|\Psi_n^{(0)}\right\rangle = \sigma_n^{(0)}\left|\Psi_n^{(0)}\right\rangle$, that is, $\left|\Psi_n^{(0)}\right\rangle$ is an eigenstate of $\hat{\rho}_0$ with eigenvalue $\sigma_n^{(0)}$.

Now, we have

$$\begin{aligned}
\sigma_n\,|\Psi_n\rangle &= \hat{\rho}\,|\Psi_n\rangle \\
\Big(\sigma_n^{(0)} - \sigma_m^{(0)} + \lambda\sigma_n^{(1)} + \lambda^2\sigma_n^{(2)} + \mathcal{O}\big(\lambda^3\big)\Big)\left\langle\Psi_m^{(0)}|\Psi_n\right\rangle &= \left\langle\Psi_m^{(0)}\right|\lambda\hat{\rho}_1 + \lambda^2\hat{\rho}_2 + \mathcal{O}\big(\lambda^3\big)\,|\Psi_n\rangle \\
\left\langle\Psi_m^{(0)}|\Psi_n\right\rangle &= \frac{\left\langle\Psi_m^{(0)}\right|\lambda\hat{\rho}_1 + \lambda^2\hat{\rho}_2 + \mathcal{O}\big(\lambda^3\big)\,|\Psi_n\rangle}{\sigma_n^{(0)} - \sigma_m^{(0)} + \lambda\sigma_n^{(1)} + \lambda^2\sigma_n^{(2)} + \mathcal{O}(\lambda^3)}.
\end{aligned}$$

We will next proceed to get rid of the denominator by using the Taylor expansion $\frac{1}{1+x} = 1 - x + \mathcal{O}\big(x^2\big)$.

Let D_n be the indices degenerate with n. That is, let $D_n = \{m : \sigma_m^{(0)} = \sigma_n^{(0)}\}$. Consider the case where $m \in D_n$. Let δ be a small real number. In the limit as $\delta \to 0$,

$$\begin{aligned}
\left\langle \Psi_m^{(0)} | \Psi_n \right\rangle &= \frac{\left\langle \Psi_m^{(0)} \right| \lambda\hat{\rho}_1 + \lambda^2\hat{\rho}_2 + \mathcal{O}\big(\lambda^3\big) \left|\Psi_n\right\rangle}{\lambda\sigma_n^{(1)} + \lambda^2\sigma_n^{(2)} + \mathcal{O}(\lambda^3) + \lambda\delta} \\
&= \frac{\left\langle \Psi_m^{(0)} \right| \lambda\hat{\rho}_1 + \lambda^2\hat{\rho}_2 + \mathcal{O}\big(\lambda^3\big) \left|\Psi_n\right\rangle}{\lambda\left(\sigma_n^{(1)} + \delta\right)\left(1 + \lambda\frac{\sigma_n^{(2)}}{\sigma_n^{(1)}+\delta} + \mathcal{O}(\lambda^2)\right)} \\
&= \frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 + \lambda\hat{\rho}_2 + \mathcal{O}\big(\lambda^2\big) \left|\Psi_n\right\rangle}{\sigma_n^{(1)} + \delta}\left(1 - \lambda\frac{\sigma_n^{(2)}}{\sigma_n^{(1)} + \delta} + \mathcal{O}\big(\lambda^2\big)\right) \\
&= \frac{\left\langle \Psi_m^{(0)} \right| \left(\hat{\rho}_1 + \lambda\hat{\rho}_2 + \mathcal{O}\big(\lambda^2\big)\right)\left(\left|\Psi_n^{(0)}\right\rangle + \lambda\left|\Psi_n^{(1)}\right\rangle + \mathcal{O}\big(\lambda^2\big)\right)}{\sigma_n^{(1)} + \delta}\left(1 - \lambda\frac{\sigma_n^{(2)}}{\sigma_n^{(1)} + \delta} + \mathcal{O}\big(\lambda^2\big)\right) \\
&= \frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(1)} + \delta} + \lambda\left[\frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(1)} + \delta} + \frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_2 \left|\Psi_n^{(1)}\right\rangle}{\sigma_n^{(1)} + \delta} - \frac{\sigma_n^{(2)}\left\langle \Psi_m^{(0)} \right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle}{\left(\sigma_n^{(1)} + \delta\right)^2}\right] + \mathcal{O}\big(\lambda^2\big)
\end{aligned}$$

(The δ ensured that we did not divide by zero if $\sigma_n^{(1)} = 0$.) Now consider the case where $m \notin D_n$. Then

$$\begin{aligned}
\left\langle \Psi_m^{(0)} | \Psi_n \right\rangle &= \frac{\left\langle \Psi_m^{(0)} \right| \lambda\hat{\rho}_1 + \mathcal{O}\big(\lambda^2\big) \left|\Psi_n\right\rangle}{\left(\sigma_n^{(0)} - \sigma_m^{(0)}\right)(1 + \mathcal{O}(\lambda))} \\
&= \frac{\left\langle \Psi_m^{(0)} \right| \lambda\hat{\rho}_1 + \mathcal{O}\big(\lambda^2\big) \left|\Psi_n\right\rangle}{\sigma_n^{(0)} - \sigma_m^{(0)}}(1 + \mathcal{O}(\lambda)) \\
&= \lambda\frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left|\Psi_n\right\rangle}{\sigma_n^{(0)} - \sigma_m^{(0)}} + \mathcal{O}\big(\lambda^2\big).
\end{aligned}$$

Putting this all together,

$$\begin{aligned}
\left|\Psi_n\right\rangle &= \sum_{m\in D_n}\left|\Psi_m^{(0)}\right\rangle\left\langle \Psi_m^{(0)} | \Psi_n \right\rangle + \sum_{m\notin D_n}\left|\Psi_m^{(0)}\right\rangle\left\langle \Psi_m^{(0)} | \Psi_n \right\rangle \qquad (3.5)\\
&= \sum_{m\in D_n}\left|\Psi_m^{(0)}\right\rangle \lim_{\delta\to 0}\frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(1)} + \delta} \\
&\quad + \lambda\left(\sum_{m\in D_n}\left|\Psi_m^{(0)}\right\rangle \lim_{\delta\to 0}\left[\frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(1)} + \delta} + \frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left|\Psi_n^{(1)}\right\rangle}{\sigma_n^{(1)} + \delta} - \frac{\sigma_n^{(2)}\left\langle \Psi_m^{(0)} \right| \hat{\rho}_0 \left|\Psi_n^{(0)}\right\rangle}{\left(\sigma_n^{(1)} + \delta\right)^2}\right]\right. \\
&\qquad \left. + \sum_{m\notin D_n}\left|\Psi_m^{(0)}\right\rangle\frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left|\Psi_n\right\rangle}{\sigma_n^{(0)} - \sigma_m^{(0)}}\right) \\
&\quad + \mathcal{O}\big(\lambda^2\big)
\end{aligned}$$

In the zeroth order of λ, equation (3.5) gives

$$\left|\Psi_n^{(0)}\right\rangle = \sum_{m\in D_n} \left|\Psi_m^{(0)}\right\rangle \lim_{\delta\to 0} \frac{\left\langle \Psi_m^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(1)} + \delta}.$$

Multiplying by $\left\langle \Psi_n^{(0)}\right|$ we get

$$\boxed{\sigma_n^{(1)} = \left\langle \Psi_n^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle.} \tag{3.6}$$

If we instead multiply by $\left\langle \Psi_k^{(0)}\right|$ where $k \in D_n$ but $k \neq n$ we get

$$\boxed{0 = \left\langle \Psi_k^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle, \qquad k \in D_n, \qquad m \neq n.} \tag{3.7}$$

In other words, the matrix given by $\left\langle \Psi_k^{(0)}\right| \hat{\rho}_1 \left|\Psi_j^{(0)}\right\rangle$ is diagonal on $k, j \in D_n$, for any n.

In the first order of λ, equation (3.5) says

$$\left|\Psi_n^{(1)}\right\rangle = \sum_{m\in D_n} \left|\Psi_m^{(0)}\right\rangle \lim_{\delta\to 0} \left[\frac{\left\langle \Psi_m^{(0)}\right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(1)} + \delta} + \frac{\left\langle \Psi_m^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(1)}\right\rangle}{\sigma_n^{(1)} + \delta} - \frac{\sigma_n^{(2)} \left\langle \Psi_m^{(0)}\right| \hat{\rho}_0 \left|\Psi_n^{(0)}\right\rangle}{\left(\sigma_n^{(1)} + \delta\right)^2} \right] + \sum_{m\notin D_n} \left|\Psi_m^{(0)}\right\rangle \frac{\left\langle \Psi_m^{(0)}\right| \hat{\rho}_1 \left|\Psi_n\right\rangle}{\sigma_n^{(0)} - \sigma_m^{(0)}}$$

Multiplying by $\left\langle \Psi_k^{(0)}\right|$ where $k \notin D_n$ gives

$$\left\langle \Psi_k^{(0)} | \Psi_n^{(1)}\right\rangle = \frac{\left\langle \Psi_k^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(0)} - \sigma_k^{(0)}}.$$

If we instead multiply by $\left\langle \Psi_n^{(0)}\right|$ we get

$$0 = \left\langle \Psi_n^{(0)} | \Psi_n^{(1)}\right\rangle = \lim_{\delta\to 0} \left[\frac{\left\langle \Psi_n^{(0)}\right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(1)} + \delta} + \frac{\left\langle \Psi_n^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(1)}\right\rangle}{\sigma_n^{(1)} + \delta} - \frac{\sigma_n^{(2)} \left(\sigma_n^{(1)} + \delta\right)}{\left(\sigma_n^{(1)} + \delta\right)^2} \right]$$

so

$$\begin{aligned}
\sigma_n^{(2)} &= \left\langle \Psi_n^{(0)}\right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle + \left\langle \Psi_n^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(1)}\right\rangle - \left\langle \Psi_n^{(0)} | \Psi_n^{(1)}\right\rangle \sigma_n^{(1)} \\
&= \left\langle \Psi_n^{(0)}\right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle + \sum_{m\in D_n} \left\langle \Psi_n^{(0)}\right| \hat{\rho}_1 \left|\Psi_m^{(0)}\right\rangle \left\langle \Psi_m^{(0)} | \Psi_n^{(1)}\right\rangle + \sum_{m\notin D_n} \left\langle \Psi_n^{(0)}\right| \hat{\rho}_1 \left|\Psi_m^{(0)}\right\rangle \left\langle \Psi_m^{(0)} | \Psi_n^{(1)}\right\rangle - \left\langle \Psi_n^{(0)} | \Psi_n^{(1)}\right\rangle \sigma_n^{(1)} \\
&= \left\langle \Psi_n^{(0)}\right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle + \sigma_n^{(1)} \left\langle \Psi_n^{(0)} | \Psi_n^{(1)}\right\rangle + \sum_{m\notin D_n} \left\langle \Psi_n^{(0)}\right| \hat{\rho}_1 \left|\Psi_m^{(0)}\right\rangle \frac{\left\langle \Psi_m^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle}{\sigma_n^{(0)} - \sigma_m^{(0)}} - \left\langle \Psi_n^{(0)} | \Psi_n^{(1)}\right\rangle \sigma_n^{(1)}
\end{aligned}$$

hence

$$\boxed{\sigma_n^{(2)} = \left\langle \Psi_n^{(0)}\right| \hat{\rho}_2 \left|\Psi_n^{(0)}\right\rangle + \sum_{m\notin D_n} \frac{\left|\left\langle \Psi_m^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle\right|^2}{\sigma_n^{(0)} - \sigma_m^{(0)}}.} \tag{3.8}$$

Chapter 4

Growth of Von Neumann Entropy due to a Perturbation

Suppose we have a Hilbert space of the form $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. The $\mathcal{H}_A$-reduced density operator of a density operator $\hat{\rho}$ is defined to be

$$\overline{\hat{\rho}} = \sum_m \left(\cdot \otimes \langle \beta_m |\right) \hat{\rho} \left(\cdot \otimes | \beta_m \rangle\right)$$

where $\{|\beta_m\rangle\}$ is any orthonormal basis for $\mathcal{H}_B$. (One can verify that all choices of basis give the same $\overline{\hat{\rho}}$.) We can consider $\overline{\hat{\rho}}$ to act on the Hilbert space $\mathcal{H}_A$.

Define the $\mathcal{H}_A$-subsystem entropy to be $S = -\operatorname{Tr} \overline{\hat{\rho}} \log \overline{\hat{\rho}}$. If $\overline{\hat{\rho}}$ is diagonalized like

$$\overline{\hat{\rho}} = \sum_n \overline{\sigma_n} \, |\alpha_n\rangle \langle \alpha_n| \,, \tag{4.1}$$

where $\{|\alpha_n\rangle\}$ is an orthonormal basis of $\mathcal{H}_A$, then

$$S = -\sum_n \overline{\sigma_n} \log \overline{\sigma_n}. \tag{4.2}$$

Now, looking at equation (6.4), we see that at some fixed time t we can form asymptotic expansions

$$\begin{aligned}
\overline{\hat{\rho}}(t) &= \overline{\hat{\rho}}_0 + \lambda \overline{\hat{\rho}}_1 + \lambda^2 \overline{\hat{\rho}}_2 + \mathcal{O}(\lambda^3) \\
|\alpha_n\rangle &= \left|\alpha_n^{(0)}\right\rangle + \lambda \left|\alpha_n^{(1)}\right\rangle + \lambda^2 \left|\alpha_n^{(2)}\right\rangle + \mathcal{O}(\lambda^3) \\
\overline{\sigma_n} &= \overline{\sigma_n^{(0)}} + \lambda \overline{\sigma_n^{(1)}} + \lambda^2 \overline{\sigma_n^{(2)}} + \mathcal{O}(\lambda^3)
\end{aligned}$$

by taking

$$\hat{\rho}_0 = \hat{\rho}\,(t_0)$$

$$\overline{\hat{\rho}}_0 = \overline{\hat{\rho}}\,(t_0) = \sum_m \left(\cdot \otimes \langle \beta_m |\right) \hat{\rho}_0 \left(\cdot \otimes | \beta_m \rangle\right)$$

$$\overline{\hat{\rho}}_1 = -\frac{i}{\hbar} \int_{t_0}^{t} \sum_m \left(\cdot \otimes \langle \beta_m |\right) \left[\hat{H}_I(t'),\ \hat{\rho}_0\right] \left(\cdot \otimes | \beta_m \rangle\right) \, dt' \tag{4.3}$$

$$\begin{aligned}
\overline{\hat{\rho}}_2 = &-\frac{1}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t'} \sum_m \left(\cdot \otimes \langle \beta_m |\right) \left(\hat{H}_I(t')\hat{H}_I(t'')\,\hat{\rho}_0 + \hat{\rho}_0\,\hat{H}_I(t'')\hat{H}_I(t')\right) \left(\cdot \otimes | \beta_m \rangle\right) \, dt''\, dt' \\
&+ \frac{1}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t} \sum_m \left(\cdot \otimes \langle \beta_m |\right) \hat{H}_I(t')\,\hat{\rho}_0\,\hat{H}_I(t'') \left(\cdot \otimes | \beta_m \rangle\right) \, dt''\, dt'.
\end{aligned} \tag{4.4}$$

From (4.1) we see that

$$\overline{\hat{\rho}}_0 = \sum_n \overline{\sigma_n^{(0)}} \left|\alpha_n^{(0)}\right\rangle \left\langle\alpha_n^{(0)}\right|. \tag{4.5}$$

Therefore we can take $\left\{\left|\alpha_n^{(0)}\right\rangle\right\}$ to be an orthonormal basis for $\mathcal{H}_A$ and we must have $\sum_n \overline{\sigma_n^{(0)}} = 1$.

It will be useful to work in the basis $\left\{\left|\alpha_n^{(0)}\right\rangle \otimes |\beta_m\rangle\right\}$ of $\mathcal{H}$. To simplify notation, let

$$|n\ m\rangle = \left|\alpha_n^{(0)}\right\rangle \otimes |\beta_m\rangle\,.$$

Also let

$$I = \left\{n : \overline{\sigma_n^{(0)}} \neq 0\right\}.$$

We now compute the subsystem entropy at time t. Let us examine the terms in (4.2). If $\sigma_n^{(0)} \neq 0$ (i.e. $n \in I$) then

$$\begin{aligned}
\overline{\sigma_n} \log \overline{\sigma_n} &= \left(\overline{\sigma_n^{(0)}} + \lambda\overline{\sigma_n^{(1)}} + \lambda^2\overline{\sigma_n^{(2)}} + \mathcal{O}(\lambda^3)\right) \log\left(\overline{\sigma_n^{(0)}}\left(1 + \frac{\lambda\overline{\sigma_n^{(1)}}}{\overline{\sigma_n^{(0)}}} + \frac{\lambda^2\overline{\sigma_n^{(2)}}}{\overline{\sigma_n^{(0)}}} + \mathcal{O}(\lambda^3)\right)\right) \\
&= \left(\overline{\sigma_n^{(0)}} + \lambda\overline{\sigma_n^{(1)}} + \lambda^2\overline{\sigma_n^{(2)}}\right)\left(\log\overline{\sigma_n^{(0)}} + \frac{\lambda\overline{\sigma_n^{(1)}}}{\overline{\sigma_n^{(0)}}} + \frac{\lambda^2\overline{\sigma_n^{(2)}}}{\overline{\sigma_n^{(0)}}}\right) + \mathcal{O}(\lambda^3) \\
&= \overline{\sigma_n^{(0)}}\log\overline{\sigma_n^{(0)}} + \lambda\,\overline{\sigma_n^{(1)}} + \lambda\,\overline{\sigma_n^{(1)}}\log\overline{\sigma_n^{(0)}} + \lambda^2\overline{\sigma_n^{(2)}} + \lambda^2\overline{\sigma_n^{(2)}}\log\overline{\sigma_n^{(0)}} + \lambda^2\,\frac{\overline{\sigma_n^{(1)}}^2}{\overline{\sigma_n^{(0)}}} + \mathcal{O}(\lambda^3).
\end{aligned}$$

On the other hand, if $\sigma_n^{(0)} \neq 0$ (i.e. $n \in I$) but $\overline{\sigma_n} \neq 0$, then $\overline{\sigma_n^{(1)}} = 0$ since we have $\langle n\ m|\left[\hat{H}_I(t'),\ \hat{\rho}_0\right]|n\ m\rangle$ for all m. Now, for each of these n, we can let k_n be the lowest positive integer such that $\overline{\sigma_n^{(k_n)}} \neq 0$. Then $k_n \geq 2$ and

$$\begin{aligned}
\overline{\sigma_n}\log\overline{\sigma_n} &= \left(\lambda^{k_n}\overline{\sigma_n^{(k_n)}} + \mathcal{O}\left(\lambda^{k_n+1}\right)\right)\log\left(\lambda^{k_n}\overline{\sigma_n^{(k_n)}}\left(1+\mathcal{O}(\lambda)\right)\right) \\
&= \lambda^{k_n}\overline{\sigma_n^{(k_n)}}\log\left(\lambda^{k_n}\overline{\sigma_n^{(k_n)}}\right) + \mathcal{O}\left(\lambda^{k_n+1}\right) \\
&= \lambda^2\overline{\sigma_n^{(2)}}\log\left(\lambda^2\overline{\sigma_n^{(2)}}\right) + \mathcal{O}\left(\lambda^3\log\lambda^3\right) \\
&= \left(\lambda^2\log\lambda^2\right)\overline{\sigma_n^{(2)}} + \lambda^2\overline{\sigma_n^{(2)}}\log\overline{\sigma_n^{(2)}} + \mathcal{O}\left(\lambda^3\log\lambda^3\right)
\end{aligned}$$

Putting this all into (4.2),

$$\begin{aligned}
S = &-\sum_{n\in I}\overline{\sigma_n^{(0)}}\log\overline{\sigma_n^{(0)}} - \lambda\sum_{n\in I}\overline{\sigma_n^{(1)}} - \lambda\sum_{n\in I}\overline{\sigma_n^{(1)}}\log\overline{\sigma_n^{(0)}} + \left(\lambda^2\log\frac{1}{\lambda^2}\right)\sum_{n\notin I}\overline{\sigma_n^{(2)}} \\
&- \lambda^2\sum_{n\in I}\overline{\sigma_n^{(2)}} - \lambda^2\sum_{n\in I}\overline{\sigma_n^{(2)}}\log\overline{\sigma_n^{(0)}} - \lambda^2\sum_{n\in I}\frac{\overline{\sigma_n^{(1)}}^2}{\overline{\sigma_n^{(0)}}} - \sum_{n\notin I}\lambda^2\overline{\sigma_n^{(2)}}\log\overline{\sigma_n^{(2)}} + \mathcal{O}\left(\lambda^3\log\lambda^3\right).
\end{aligned}$$

The first term, $-\sum_{n\in I}\overline{\sigma_n^{(0)}}\log\overline{\sigma_n^{(0)}}$, would be the entropy if $\lambda = 0$, that is, with no perturbation. Also, since $\sum_n\overline{\sigma_n} = 1$ we must have $\sum_{n\in I}\overline{\sigma_n^{(1)}} = 0$. *[Explanation needed.]* Thus the change in entropy due to the perturbation is

$$\boxed{\begin{aligned}\Delta S = &-\lambda \sum_{n\in I} \overline{\sigma_n^{(1)}} \log \overline{\sigma_n^{(0)}} + \left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n\notin I} \overline{\sigma_n^{(2)}} \\ &+ \lambda^2 \left(-\sum_{n\in I} \overline{\sigma_n^{(2)}} - \sum_{n\in I} \overline{\sigma_n^{(2)}} \log \overline{\sigma_n^{(0)}} - \sum_{n\in I} \frac{\overline{\sigma_n^{(1)}}^2}{\overline{\sigma_n^{(0)}}} - \sum_{n\notin I} \overline{\sigma_n^{(2)}} \log \overline{\sigma_n^{(2)}} \right) \\ &+ \mathcal{O}\big(\lambda^3 \log \lambda^3\big).\end{aligned}} \tag{4.6}$$

Recall our Hamiltonian $\hat{H} = \hat{H}_0 + \lambda \hat{V}$. If $\hat{H}_0 = \hat{H}_0^A + \hat{H}_0^B$, where $\hat{H}_0^A$ acts only on $\mathcal{H}_A$ and $\hat{H}_0^B$ acts only on $\mathcal{H}_B$, then $\hat{H}_0$ does not cause mixing between the two subsystems. In this case ΔS is the change in entropy from time t_0 to time t.

On the other hand, if $\hat{H}_0$ is not of this form, $\hat{H}_0$ might cause mixing between subsystems. Then there could be some zeroth-order change in entropy due to $\hat{H}_0$. In this case ΔS is not the *total* change in entropy from time t_0 to time t but rather the change in entropy from time t_0 to time t due to the perturbation $\lambda \hat{V}$.

(4.6) is a rather complicated expression. Let us consider some cases where it becomes simpler.

4.1 Case where the Hilbert space is already fully occupied

Suppose that all n with $\overline{\sigma_n} \neq 0$ have $\overline{\sigma_n^{(0)}} \neq 0$. Then, at time t_0, the system already occupies the accessible part of the Hilbert space $\mathcal{H}_A$. It does not evolve into new states in our perturbative timeframe. (States with $\overline{\sigma_n} = 0$ are occupied at neither t_0 nor t and might as well have just been excluded from the Hilbert space. They will not matter for our entropy calculations.) The sum over $n \notin I$ does not contribute to entropy, so (4.6) is replaced with

$$\Delta S = -\lambda \sum_{n\in I} \overline{\sigma_n^{(1)}} \log \overline{\sigma_n^{(0)}} - \lambda^2 \sum_{n\in I} \overline{\sigma_n^{(2)}} \log \overline{\sigma_n^{(0)}} - \lambda^2 \sum_{n\in I} \frac{\overline{\sigma_n^{(1)}}^2}{\overline{\sigma_n^{(0)}}} + \mathcal{O}\big(\lambda^3\big). \tag{4.7}$$

Here we used that $\sum_n \overline{\sigma_n^{(2)}} = 0$ and we replaced the error term with the stronger statement we had for only $n \in I$.

4.2 Case where first-order corrections vanish

Suppose that some n have $\overline{\sigma_n^{(0)}} = 0$ and $\overline{\sigma_n} \neq 0$. Suppose also that all $\sigma_n^{(1)} = 0$. Then (4.6) becomes

$$\Delta S = \left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n\notin I} \overline{\sigma_n^{(2)}} + \mathcal{O}\big(\lambda^2\big). \tag{4.8}$$

If $n \notin I$, then $\overline{\sigma_n^{(0)}} = 0$ but $\overline{\sigma_n} \geq 0$, so the leading perturbative correction to $\overline{\sigma_n}$ must be non-negative. In particular, $\overline{\sigma_n^{(2)}} \geq 0$ for all $n \notin I$. Therefore the entire sum (4.8) is non-negative.

This shows that the **subsystem entropy cannot decrease if the first-order corrections vanish, the second-order corrections don't vanish, and also $\overline{\rho}$ has null eigenvalues for states that we can transition to**. In this case, the entropy will increase or remain constant over time (until the system evolves so that all eigenvalues are non-zero). As we will see in a later example, the converse is not true. If $\overline{\hat{\rho}}$ has only non-zero eigenvalues, entropy may decrease, increase, or remain constant.

Now, since $\sum_n \overline{\sigma_n^{(2)}} = 0$ we can rewrite (4.8) as

$$\Delta S = -\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n \in I} \overline{\sigma_n^{(2)}} + \mathcal{O}(\lambda^2). \tag{4.9}$$

Substituting in (3.8),

$$\Delta S = -\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \left(\sum_{n \in I} \left\langle \alpha_n^{(0)} \middle| \overline{\hat{\rho}_2} \middle| \alpha_n^{(0)} \right\rangle + \sum_{n \in I} \sum_{n' \notin D_n} \frac{\left| \left\langle \alpha_{n'}^{(0)} \middle| \overline{\hat{\rho}_1} \middle| \alpha_n^{(0)} \right\rangle \right|^2}{\overline{\sigma_n^{(0)}} - \overline{\sigma_{n'}^{(0)}}} \right) + \mathcal{O}(\lambda^2).$$

Now, in the second term with the double sum, for every term $\frac{\left| \left\langle \alpha_{n'}^{(0)} \middle| \overline{\hat{\rho}_1} \middle| \alpha_n^{(0)} \right\rangle \right|^2}{\overline{\sigma_n^{(0)}} - \overline{\sigma_{n'}^{(0)}}}$ with $n' \in I$ there is an equal but oppositely signed term $\frac{\left| \left\langle \alpha_{n'}^{(0)} \middle| \overline{\hat{\rho}_1} \middle| \alpha_n^{(0)} \right\rangle \right|^2}{\overline{\sigma_{n'}^{(0)}} - \overline{\sigma_n^{(0)}}}$ in the sum. The portion of the sum over $n' \in I$ evaluates to zero. We end up with

$$\Delta S = -\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \left(\sum_{n \in I} \left\langle \alpha_n^{(0)} \middle| \overline{\hat{\rho}_2} \middle| \alpha_n^{(0)} \right\rangle + \sum_{n \in I} \sum_{n' \notin I} \frac{\left| \left\langle \alpha_n^{(0)} \middle| \overline{\hat{\rho}_1} \middle| \alpha_{n'}^{(0)} \right\rangle \right|^2}{\overline{\sigma_n^{(0)}}} \right) + \mathcal{O}(\lambda^2). \tag{4.10}$$

Putting in (4.3) and (4.4),

$$\begin{aligned} \Delta S = \frac{1}{\hbar^2} \left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n \in I} \Bigg(& \\ & \sum_m \int_{t_0}^{t} \int_{t_0}^{t'} \langle n\ m| \left(\hat{H}_I(t') \hat{H}_I(t'')\ \hat{\rho}_0 + \hat{\rho}_0\ \hat{H}_I(t'') \hat{H}_I(t') \right) |n\ m\rangle \ dt''\ dt' \\ & - \sum_m \int_{t_0}^{t} \int_{t_0}^{t} \langle n\ m|\ \hat{H}_I(t')\ \hat{\rho}_0\ \hat{H}_I(t'')\ |n\ m\rangle \ dt''\ dt' \\ & - \sum_{n' \notin I} \frac{1}{\overline{\sigma_n^{(0)}}} \left| \sum_m \int_{t_0}^{t} \langle n\ m| \left[\hat{H}_I(t'),\ \hat{\rho}_0 \right] |n'\ m\rangle \ dt' \right|^2 \Bigg) + \mathcal{O}(\lambda^2). \end{aligned} \tag{4.11}$$

4.2.1 Case of separable initial state

We will now consider the special case where, at the time t_0, the density operator takes the form

$$\hat{\rho}_0 = \hat{\rho}\,(t_0) = \sum_{n,m} \sigma_{n,m}^{(0)} \left(\left| \alpha_n^{(0)} \right\rangle \otimes |\beta_m\rangle \right) \left(\left\langle \alpha_n^{(0)} \right| \otimes \langle \beta_m| \right) \tag{4.12}$$

where $\left\{ \left| \alpha_n^{(0)} \right\rangle \right\}$ is *any* orthonormal basis for $\mathcal{H}_A$ and $\{|\beta_m\rangle\}$ is *any* orthonormal basis for $\mathcal{H}_B$. We call such states "separable states".

(4.12) implies that the reduced density operator at time t_0 is

$$\overline{\hat{\rho}}_0 = \overline{\hat{\rho}}\left(t_0\right) = \sum_n \overline{\sigma_n^{(0)}} \left|\alpha_n^{(0)}\right\rangle \left\langle\alpha_n^{(0)}\right|$$

where

$$\overline{\sigma_n^{(0)}} = \sum_m \sigma_{n,m}^{(0)}.$$

Now, if we fix a time t, there should be some basis $\{|\alpha_n\rangle\}$ of $\mathcal{H}_A$ and some quantities $\overline{\sigma_n}$ such that

$$\overline{\hat{\rho}}(t) = \sum_n \overline{\sigma_n} \left|\alpha_n\right\rangle \left\langle\alpha_n\right|.$$

The eigenstate/eigenvalue decomposition of an operator is unique up to relabeling. Therefore, comparing our equations to (4.1) and (4.5), we see that our above analysis must hold with the notation unchanged. Indeed, now

$$\hat{\rho}_0 = \sum_{n,m} \sigma_{n,m}^{(0)} \left|n\ m\right\rangle \left\langle n\ m\right|. \tag{4.13}$$

We have

$$\begin{aligned} \langle n\ m|\ \hat{H}_I(t')\ \hat{\rho}_0 \left|n\ m\right\rangle &= \sigma_{n,m}^{(0)} \left\langle n\ m\right| \hat{H}_I(t') \left|n\ m\right\rangle \\ &= \left\langle n\ m\right| \hat{\rho}_0\ \hat{H}_I(t') \left|n\ m\right\rangle \end{aligned}$$

so the first-order eigenvalue correction vanishes. *[Explanation needed.]* We will assume that the second-order eigenvalue correction $\overline{\sigma_n^{(2)}}$ does not vanish and turn to (4.11).

The first two terms in (4.11) are

$$\sum_{n\in I}\sum_{m}\int_{t_0}^{t}\int_{t_0}^{t'}\langle n\ m|\left(\hat{H}_I(t')\hat{H}_I(t'')\ \hat{\rho}_0+\hat{\rho}_0\ \hat{H}_I(t'')\hat{H}_I(t')\right)|n\ m\rangle\ dt''\ dt'$$
$$-\sum_{n\in I}\sum_{m}\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\ \hat{\rho}_0\ \hat{H}_I(t'')\,|n\ m\rangle\ dt''\ dt'$$
$$=\sum_{n\in I}\sum_{m}\sigma^{(0)}_{n,m}\int_{t_0}^{t}\int_{t_0}^{t'}\langle n\ m|\left\{\hat{H}_I(t'),\ \hat{H}_I(t'')\right\}|n\ m\rangle\ dt''\ dt'$$
$$-\sum_{m}\sum_{n^\star}\sum_{m^\star}\sigma^{(0)}_{n^\star,m^\star}\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\,|n^\star\ m^\star\rangle\,\langle n^\star\ m^\star|\ \hat{H}_I(t'')\,|n\ m\rangle\ dt''\ dt'$$
$$=\sum_{n\in I}\sum_{m}\sigma^{(0)}_{n,m}\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\hat{H}_I(t'')\,|n\ m\rangle\ dt''\ dt'$$
$$-\sum_{n\in I}\sum_{m}\sum_{n^\star}\sum_{m^\star}\sigma^{(0)}_{n^\star,m^\star}\int_{t_0}^{t}\int_{t_0}^{t}\langle n^\star\ m^\star|\ \hat{H}_I(t'')\,|n\ m\rangle\,\langle n\ m|\ \hat{H}_I(t')\,|n^\star\ m^\star\rangle\ dt''\ dt'$$
$$=\sum_{n\in I}\sum_{m}\sigma^{(0)}_{n,m}\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\hat{H}_I(t'')\,|n\ m\rangle\ dt''\ dt'$$
$$-\sum_{n^\star}\sum_{m^\star}\sigma^{(0)}_{n^\star,m^\star}\int_{t_0}^{t}\int_{t_0}^{t}\langle n^\star\ m^\star|\ \hat{H}_I(t'')\left[\left(\sum_{n\in I}\left|\alpha^{(0)}_n\right\rangle\left\langle\alpha^{(0)}_n\right|\right)\otimes\cdot\right]\hat{H}_I(t')\,|n^\star\ m^\star\rangle\ dt''\ dt'$$
$$=\sum_{n\in I}\sum_{m}\sigma^{(0)}_{n,m}\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\hat{H}_I(t'')\,|n\ m\rangle\ dt''\ dt'$$
$$-\sum_{n}\sum_{m}\sigma^{(0)}_{n,m}\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t'')\left[\left(1-\sum_{n'\notin I}\left|\alpha^{(0)}_{n'}\right\rangle\left\langle\alpha^{(0)}_{n'}\right|\right)\otimes\cdot\right]\hat{H}_I(t')\,|n\ m\rangle\ dt''\ dt'$$
$$=\sum_{n\in I}\sum_{m}\sigma^{(0)}_{n,m}\left[\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\hat{H}_I(t'')\,|n\ m\rangle\ dt''\ dt'-\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\hat{H}_I(t'')\,|n\ m\rangle\ dt''\ dt'\right]$$
$$+\sum_{n}\sum_{m}\sigma^{(0)}_{n,m}\sum_{n'\notin I}\sum_{m'}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t'')\left|n'\ m'\right\rangle\ dt''\int_{t_0}^{t}\left\langle n'\ m'\right|\hat{H}_I(t')\,|n\ m\rangle\ dt'$$
$$=\sum_{n\in I}\sum_{n'\notin I}\sum_{m}\sigma^{(0)}_{n,m}\sum_{m'}\left|\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\left|n'\ m'\right\rangle\ dt'\right|^2.$$

Meanwhile, the third term in (4.11) is

$$-\sum_{n\in I}\sum_{n'\notin I}\frac{1}{\sigma^{(0)}_n}\left|\sum_{m}\int_{t_0}^{t}\langle n\ m|\left[\hat{H}_I(t'),\ \hat{\rho}_0\right]\left|n'\ m\right\rangle\ dt'\right|^2$$
$$=-\sum_{n\in I}\sum_{n'\notin I}\frac{1}{\sigma^{(0)}_n}\left|\sum_{m}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\left|n'\ m\right\rangle\ \left(\sigma^{(0)}_{n,m}-\cancel{\sigma^{(0)}_{n',m}}\right)\ dt'\right|^2\Bigg)+\mathcal{O}(\lambda^2)$$
$$=-\sum_{n\in I}\sum_{n'\notin I}\frac{1}{\sum_{\tilde{m}}\sigma^{(0)}_{n,\tilde{m}}}\left|\sum_{m}\sigma^{(0)}_{n,m}\int_{t_0}^{t}\langle n\ m|\ \hat{H}_I(t')\left|n'\ m\right\rangle\ dt'\right|^2.$$

Putting this all back into (4.11), we obtain the rather interesting result that

$$\boxed{\begin{aligned}\Delta S = \frac{1}{\hbar^2}\left(\lambda^2 \log\frac{1}{\lambda^2}\right)\sum_{n\in I}\sum_{n'\notin I}\Bigg(&\sum_m \sigma^{(0)}_{n,m}\sum_{m'}\left|\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m'\rangle\ dt'\right|^2 \\ &-\frac{1}{\sum_{\tilde{m}}\sigma^{(0)}_{n,\tilde{m}}}\left|\sum_m \sigma^{(0)}_{n,m}\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m\rangle\ dt'\right|^2\Bigg) + \mathcal{O}(\lambda^2).\end{aligned}} \tag{4.14}$$

Assuming that these terms do not vanish, we see that the entropy grows proportionally to $(t-t_0)^2$.

We also observe that this expression vanishes if $\mathcal{H}_B$ has only a single possible state. This situation is equivalent to taking the entropy of the whole system rather than the subsystem entropy. We have thus shown that the entropy of the whole system is conserved (at the order of $\lambda^2 \log\frac{1}{\lambda^2}$, for separable states).

Upper and lower bounds for entropy growth

We can apply the triangle inequality to (4.14) to obtain an illuminating lower bound on ΔS for separable initial states. We have

$$\begin{aligned}\frac{1}{\sum_m \sigma^{(0)}_{n,m}}\left|\sum_m \sigma^{(0)}_{n,m}\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m\rangle\ dt'\right|^2 &\leq \frac{1}{\sum_{\tilde{m}}\sigma^{(0)}_{n,\tilde{m}}}\sum_m\left|\sigma^{(0)}_{n,m}\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m\rangle\ dt'\right|^2 \\ &= \sum_m \frac{\sigma^{(0)}_{n,m}}{\sum_{\tilde{m}}\sigma^{(0)}_{n,\tilde{m}}}\,\sigma^{(0)}_{n,m}\left|\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m\rangle\ dt'\right|^2 \\ &\leq \sum_m \sigma^{(0)}_{n,m}\left|\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m\rangle\ dt'\right|^2.\end{aligned}$$

Applying this to (4.14), we see at order $\lambda^2 \log\frac{1}{\lambda^2}$ that

$$\Delta S \geq \frac{1}{\hbar^2}\left(\lambda^2 \log\frac{1}{\lambda^2}\right)\sum_{n\in I}\sum_{n'\notin I}\sum_m \sigma^{(0)}_{n,m}\sum_{m'\neq m}\left|\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m'\rangle\ dt'\right|^2.$$

This result confirms that the change in entropy for a separable state is non-negative.

We can also obtain an upper bound for (4.14) by keeping only the first term. Then, at order $\lambda^2 \log\frac{1}{\lambda^2}$,

$$\begin{aligned}&\frac{1}{\hbar^2}\left(\lambda^2 \log\frac{1}{\lambda^2}\right)\sum_{n\in I}\sum_{n'\notin I}\sum_m \sigma^{(0)}_{n,m}\sum_{m'\neq m}\left|\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m'\rangle\ dt'\right|^2 \\ &\leq\ \Delta S\ \leq\ \frac{1}{\hbar^2}\left(\lambda^2 \log\frac{1}{\lambda^2}\right)\sum_{n\in I}\sum_{n'\notin I}\sum_m \sigma^{(0)}_{n,m}\sum_{m'}\left|\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,|n'\ m'\rangle\ dt'\right|^2.\end{aligned} \tag{4.15}$$

Interestingly, the only difference between the upper bound and the lower bound is whether we include the terms where $m' = m$ in the sum.

4.2.2 Case of pure, separable initial state

If the initial state is pure and separable, let $|n\ m\rangle$ be the initial state so that $\hat{\rho}_0 = |n\ m\rangle \langle n\ m|$. Then (4.14) simplifies to

$$\Delta S = \frac{1}{\hbar^2}\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n' \neq n} \sum_{m' \neq m} \left| \int_{t_0}^{t} \langle n\ m| \hat{H}_I(t') \left|n'\ m'\right\rangle dt' \right|^2 + \mathcal{O}\big(\lambda^2\big). \tag{4.16}$$

We observe a crucial exclusion principle: in our expression for entropy, we only have transition amplitudes where the state changes in both subsystems, never transition amplitudes for a change in only one subsystem. Furthermore, since this expression is symmetric with respect to n and m, the change in subsystem entropy for $\mathcal{H}_A$ is the same as the change in subsystem entropy for $\mathcal{H}_B$.

Chapter 5

Examples

5.1 A Toy Example: Two Qubits

In this section we will study a simple bipartite system and calculate the growth in subsystem entropy due to a weak interaction. Consider the Hilbert space $\{|0\rangle, |1\rangle\} \otimes \{|0\rangle, |1\rangle\}$ describing two qubits. To simplify notation, write $|ab\rangle$ to mean $|a\rangle \otimes |b\rangle$.

Suppose the qubits interact according to the Hamiltonian

$$\hat{H} = \hat{S}_z^A \otimes \hat{S}_z^B + \lambda \hat{S}_x^A \otimes \hat{S}_x^B.$$

One can calculate that this Hamiltonian has eigenstates and eigenvalues

$$\begin{aligned}
|E_0\rangle &= \frac{1}{\sqrt{2}} \left(|10\rangle - |01\rangle \right) & E_0 &= \frac{\hbar}{2} \left(-1 - \lambda \right) \\
|E_1\rangle &= \frac{1}{\sqrt{2}} \left(|10\rangle + |01\rangle \right) & E_1 &= \frac{\hbar}{2} \left(-1 + \lambda \right) \\
|E_2\rangle &= \frac{1}{\sqrt{2}} \left(|11\rangle - |00\rangle \right) & E_2 &= \frac{\hbar}{2} \left(1 - \lambda \right) \\
|E_3\rangle &= \frac{1}{\sqrt{2}} \left(|11\rangle + |00\rangle \right) & E_3 &= \frac{\hbar}{2} \left(1 + \lambda \right).
\end{aligned}$$

Let's start by calculating the exact change in entropy; then we can calculate the perturbative result and compare.

Suppose at $t = 0$ we start in the initial state $|11\rangle = \frac{1}{\sqrt{2}} \left(|E_2\rangle + |E_3\rangle \right)$. At time t, the state is then

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}} \left(e^{-itE_2/\hbar} |E_2\rangle + e^{-itE_3/\hbar} |E_3\rangle \right)$$

and the density operator is

$$\hat{\rho} = \frac{1}{2} |E_2\rangle \langle E_2| + \frac{1}{2} |E_3\rangle \langle E_3| + \frac{1}{2} e^{it(E_3 - E_2)/\hbar} |E_2\rangle \langle E_3| + \frac{1}{2} e^{-it(E_3 - E_2)/\hbar} |E_3\rangle \langle E_2|.$$

Then the reduced density operator for the first qubit is

$$\begin{aligned}
\overline{\hat{\rho}} &= \cdot \otimes \langle 0| \hat{\rho} \cdot \otimes |0\rangle + \cdot \otimes \langle 1| \hat{\rho} \cdot \otimes |1\rangle \\
&= \frac{1}{2} \left(1 + \cos \left[(E_3 - E_2) \frac{t}{\hbar} \right] \right) |1\rangle \langle 1| + \frac{1}{2} \left(1 - \cos \left[(E_3 - E_2) \frac{t}{\hbar} \right] \right) |0\rangle \langle 0|.
\end{aligned}$$

Recognizing that $\frac{E_3 - E_2}{\hbar} = \lambda$, we see that the Von Neumann subsystem entropy is

$$S = \frac{1}{2} \left(1 + \cos \lambda t \right) \log \left(1 + \cos \frac{\lambda t}{2} \right) + \frac{1}{2} \left(1 - \cos \lambda t \right) \log \left(1 - \cos \frac{\lambda t}{2} \right).$$

Approximating $\cos x \approx 1 - x^2$, this becomes

$$\begin{aligned} S &\approx \frac{1}{2}\left(2-\lambda^2 t^2\right)\log\left(2-\lambda^2 t^2/4\right) + \frac{1}{2}\lambda^2 t^2 \log\left(\lambda^2 t^2\right) \\ &\approx \log 2 - \frac{1}{2}\lambda^2 t^2 \log\left(\frac{1}{\lambda^2 t^2}\right). \end{aligned}$$

We observe that the leading order term for the change in entropy is of order $\lambda^2 t^2 \log \frac{1}{\lambda^2 t^2}$. Interestingly, the entropy decreases with time. This makes sense given that we started in a maximally entangled state (i.e. a Bell state). *[Actually, I'm not sure that this is a good explanation of the decreasing entropy...]*

We did the derivation above by solving the Schrödinger equation exactly. Let's now apply our perturbative calculation and see that we get the same result. The Schrödinger picture Hamiltonian is $\hat{H} = \hat{H}_0 + \lambda \hat{V}$ where

$$\begin{aligned} \hat{H}_0 &= \frac{\hbar}{2}\left(-\left|E_0\right\rangle\left\langle E_0\right| - \left|E_1\right\rangle\left\langle E_1\right| + \left|E_2\right\rangle\left\langle E_2\right| + \left|E_3\right\rangle\left\langle E_3\right|\right) \\ \hat{V} &= \frac{\hbar}{2}\left(-\left|E_0\right\rangle\left\langle E_0\right| + \left|E_1\right\rangle\left\langle E_1\right| - \left|E_2\right\rangle\left\langle E_2\right| + \left|E_3\right\rangle\left\langle E_3\right|\right). \end{aligned}$$

Because $[\hat{H}_0, \hat{V}] = 0$ we have $[\hat{U}(0,t), \hat{V}] = 0$. Thus the interaction picture Hamiltonian is just

$$\hat{H}_I = \hat{V} = \frac{\hbar}{2}\left(-\left|E_0\right\rangle\left\langle E_0\right| + \left|E_1\right\rangle\left\langle E_1\right| - \left|E_2\right\rangle\left\langle E_2\right| + \left|E_3\right\rangle\left\langle E_3\right|\right).$$

We must now diagonalize the initial density operator in a basis that easily separates into bases for the two subspaces. Indeed, we get

$$\begin{aligned} \hat{\rho} &= \frac{1}{2}\left|E_2\right\rangle\left\langle E_2\right| + \frac{1}{2}\left|E_3\right\rangle\left\langle E_3\right| + \frac{1}{2}e^{it\lambda}\left|E_2\right\rangle\left\langle E_3\right| + \frac{1}{2}e^{-it\lambda}\left|E_3\right\rangle\left\langle E_2\right| \\ &= \left(\frac{1}{\sqrt{2}}e^{it\lambda}|E_2\rangle + \frac{1}{\sqrt{2}}\left|E_3\right\rangle\right)\left(\frac{1}{\sqrt{2}}e^{-it\lambda}\langle E_2| + \frac{1}{\sqrt{2}}\left\langle E_3\right|\right) \\ &= \left(\frac{1}{2}\left(1-e^{it\lambda}\right)|00\rangle + \frac{1}{2}\left(1+e^{it\lambda}\right)|11\rangle\right)\left(\frac{1}{2}\left(1+e^{-it\lambda}\right)\langle 00| + \frac{1}{2}\left(1+e^{-it\lambda}\right)\langle 11|\right) \end{aligned}$$

[This is not a separable state, so we cannot use the perturbation formula. Should maybe change the example to a separable state.]

5.2 Scattering

[The following should be vastly edited to fit better with the above framework. It should be much shorter. A comparison should be made with the perturbative method.]

5.2.1 The first-order approximation for pure states in scattering

We will continue for scattering between two particles. We will assume that the particles are distinguishable so that we don't need to restrict ourselves to symmetric or antisymmetric states. We will also assume that the particles interact in a way that only depends on the distance between them. That is, in the position basis, we can write

$$\langle x_1, x_2|\,\hat{V}(t)\,|\psi\rangle = \int_{x_1,x_2} d^3x_1\, d^3x_2\; V(x_1 - x_2)\,\langle x_1, x_2|\psi\rangle\,. \tag{5.1}$$

(Note that this is not time dependent.) Take $\hat{H}_0$ to be the free particle Hamiltonian.

It will be easiest to work in the momentum basis. We will do our calculations for momentum eigenstates—that is, plane waves. Write momentum eigenstates as $|k_1, k_2\rangle$. In the position basis these have wavefunctions

$$\langle x_1, x_2 | k_1, k_2\rangle = \frac{1}{(2\pi)^3}\, e^{ik_1\cdot x_1 + ik_2\cdot x_2}. \tag{5.2}$$

Here x_1 and x_2 are the (3-vector) positions of the first and second particles and k_1 and k_2 are the (3-vector) momenta of the first and second particle. Also, we note that $|k_1, k_2\rangle$ has energy $\frac{1}{2m_1}{k_1}^2 + \frac{1}{2m_2}{k_2}^2$ and so

$$\hat{U}(t_0, t)\,|k_1, k_2\rangle = e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}{k_1}^2 + \frac{1}{2m_2}{k_2}^2\right)}\,|k_1, k_2\rangle\,. \tag{5.3}$$

Let $\widetilde{V}(p)$ be the Fourier transform of $V(x_1 - x_2)$ so that

$$V(x_1 - x_2) = \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^3}\widetilde{V}(p)e^{ip\cdot(x_1 - x_2)}. \tag{5.4}$$

We now consider (6.2) and take the limits $t_0 \to -\infty$ and $t \to \infty$ because, in scattering, we measure states long before and long after the scattering occurs. Then, dropping the higher-order terms,

$$|\Psi_I, \infty\rangle = |\Psi_I, -\infty\rangle - \frac{i}{\hbar}\int_{-\infty}^{\infty} \hat{H}_I(t)\,|\Psi_I, -\infty\rangle\; dt.$$

Take the initial state to be $|\Psi_I, -\infty\rangle = |k_1, k_2\rangle$. Multiplying by the bra $\langle k_1', k_2'|$,

$$\begin{aligned}\left\langle k_1', k_2' | \Psi_I, \infty\right\rangle &= \left\langle k_1', k_2' | k_1, k_2\right\rangle - \frac{i}{\hbar}\int_{-\infty}^{\infty} \left\langle k_1', k_2'\right| \hat{H}_I(t)\,|k_1, k_2\rangle\; dt \\ &= \delta^3(k_1' - k_1)\delta^3(k_2' - k_2) - \frac{i}{\hbar}\int_{-\infty}^{\infty} \left\langle k_1', k_2'\right| \hat{H}_I(t)\,|k_1, k_2\rangle\; dt. \end{aligned} \tag{5.5}$$

This motivates us to compute the matrix element $\langle k_1', k_2'|\, \hat{H}_I(t)\,|k_1, k_2\rangle$. We can start by using (5.3):

$$\begin{aligned}\left\langle k_1', k_2'\right| \hat{H}_I(t)\,|k_1, k_2\rangle &= \left\langle k_1', k_2'\right| \hat{U}(t_0, t)^\dagger \hat{V}(t)\hat{U}(t_0, t)\,|k_1, k_2\rangle \\ &= \left\langle k_1', k_2'\right| e^{\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}{k_1'}^2 + \frac{1}{2m_2}{k_2'}^2\right)}\hat{V}(t)e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}{k_1}^2 + \frac{1}{2m_2}{k_2}^2\right)}\,|k_1, k_2\rangle \\ &= e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}{k_1'}^2 + \frac{1}{2m_2}{k_2'}^2 - \frac{1}{2m_1}{k_1}^2 - \frac{1}{2m_2}{k_2}^2\right)}\left\langle k_1', k_2'\right| \hat{V}(t)\,|k_1, k_2\rangle\,. \end{aligned}$$

We see that

$$\begin{aligned}
\langle k_1', k_2' | \hat{V}(t) | k_1, k_2 \rangle &= \langle k_1', k_2' | \left\{ \int_{x_1,x_2} d^3x_1 d^3x_2 \;\; |x_1, x_2\rangle \langle x_1, x_2| \right\} \hat{V}(t) | k_1, k_2 \rangle \\
&= \int_{x_1,x_2} d^3x_1 d^3x_2 \;\; \langle k_1', k_2' | x_1, x_2 \rangle \langle x_1, x_2 | \hat{V}(t) | k_1, k_2 \rangle \\
&= \int_{x_1,x_2} \frac{d^3x_1 d^3x_2}{(2\pi)^6} \; e^{-ik_1'\cdot x_1 - ik_2'\cdot x_2} V(x_1 - x_2) e^{ik_1\cdot x_1 + ik_2 \cdot x_2} && \text{(by (5.1) and (5.2))} \\
&= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \int_{x_1,x_2} d^3x_1 d^3x_2 \;\; e^{-ik_1'\cdot x_1 - ik_2'\cdot x_2} \, \widetilde{V}(p) \, e^{ip\cdot(x_1 - x_2)} e^{ik_1\cdot x_1 + ik_2\cdot x_2} && \text{(by (5.4))} \\
&= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \widetilde{V}(p) \int_{x_1,x_2} d^3x_1 d^3x_2 \;\; e^{i(k_1 - k_1' + p)\cdot x_1} e^{i(k_2 - k_2' - p)\cdot x_2} \\
&= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \widetilde{V}(p) \, (2\pi)^6 \, \delta^3(k_1 - k_1' + p) \, \delta^3(k_2 - k_2' - p) \\
&= \frac{1}{(2\pi)^3} \; \widetilde{V}(k_1' - k_1) \; \delta^3(k_1' - k_1 - k_2' + k_2).
\end{aligned}$$

so

$$\langle k_1', k_2' | \hat{H}_I(t) | k_1, k_2 \rangle = e^{-\frac{i}{\hbar}(t - t_0)\left(\frac{1}{2m_1}{k_1'}^2 + \frac{1}{2m_2}{k_2'}^2 - \frac{1}{2m_1}{k_1}^2 - \frac{1}{2m_2}{k_2}^2\right)} \frac{1}{(2\pi)^3} \; \widetilde{V}(k_1' - k_1) \; \delta^3(k_1' - k_1 - k_2' + k_2)$$

If we integrate over all time, we get a delta function:

$$\int_{-\infty}^{\infty} dt \; \langle k_1', k_2' | \hat{H}_I(t) | k_1, k_2 \rangle = \frac{\hbar}{(2\pi)^2} \; \widetilde{V}(k_1' - k_1) \, \delta\left(\tfrac{1}{2m_1}{k_1'}^2 + \tfrac{1}{2m_2}{k_2'}^2 - \tfrac{1}{2m_1}{k_1}^2 - \tfrac{1}{2m_2}{k_2}^2 \right) \delta^3(k_1' - k_1 - k_2' + k_2). \tag{5.6}$$

Putting this into (5.5),

$$\begin{aligned}
\langle k_1', k_2' | \Psi_I, \infty \rangle = \;& \delta^3(k_1' - k_1) \; \delta^3(k_2' - k_2) \\
& - \frac{i}{(2\pi)^2} \; \widetilde{V}(k_1' - k_1) \; \delta^3(k_1' - k_1 - k_2' + k_2) \; \delta\left(\frac{{k_1'}^2}{2m_1} + \frac{{k_2'}^2}{2m_2} - \frac{{k_1}^2}{2m_1} - \frac{{k_2}^2}{2m_2} \right).
\end{aligned} \tag{5.7}$$

Interestingly, we see that the delta functions cause energy and momentum to be conserved.

5.2.2 Reduced density operator

We are interested in the situation where the second particle exits the system and becomes lost. We therefore consider the reduced density operator

$$\begin{aligned}
\hat{\rho}_{\text{reduced}}(t) &= \int d^3k_2 \, \langle k_2 | \, \hat{\rho}(t) \, | k_2 \rangle \\
&= \hat{\rho}_{\text{reduced}}(t_0) - \frac{i}{\hbar} \int_{t_0}^{t} dt' \int_{-\infty}^{\infty} d^3k_2 \, \langle k_2 | \left[\hat{H}_I(t'), \; \hat{\rho}(t_0) \right] | k_2 \rangle + \mathcal{O}\left(\hat{H}_I(t)^2 \right).
\end{aligned}$$

In the momentum basis the matrix elements are

$$\langle k_1' | \, \hat{\rho}_{\text{reduced}}(t) \, | k_1 \rangle = \langle k_1' | \, \hat{\rho}_{\text{reduced}}(t_0) \, | k_1 \rangle - \frac{i}{\hbar} \int_{t_0}^{t} dt' \int_{-\infty}^{\infty} d^3k_2 \, \langle k_1', k_2 | \left[\hat{H}_I(t'), \; \hat{\rho}(t_0) \right] | k_1, k_2 \rangle + \mathcal{O}\left(\hat{H}_I(t)^2 \right).$$

As before, we drop the higher order terms and take $t \to \infty$ and $t_0 \to -\infty$. Then

$$
\begin{aligned}
\left\langle {k_1}' \right| \hat{\rho}_{\text{reduced}}(\infty) \left| k_1 \right\rangle &= \left\langle k_1' \right| \hat{\rho}_{\text{reduced}}(-\infty) \left| k_1 \right\rangle - \frac{i}{\hbar} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} d^3 k_2 \left\langle k_1', k_2 \right| \left[\hat{H}_I(t),\ \hat{\rho}(-\infty) \right] \left| k_1, k_2 \right\rangle \\
&= \left\langle k_1' \right| \hat{\rho}_{\text{reduced}}(-\infty) \left| k_1 \right\rangle \\
&\quad - \frac{i}{\hbar} \int_{-\infty}^{\infty} d^3k_2\, d^3\widetilde{k}_1\, d^3\widetilde{k}_2 \left\{ \int_{-\infty}^{\infty} dt \left\langle k_1', k_2 \right| \hat{H}_I(t) \left| \widetilde{k}_1, \widetilde{k}_2 \right\rangle \right\} \left\langle \widetilde{k}_1, \widetilde{k}_2 \right| \hat{\rho}(-\infty) \left| k_1, k_2 \right\rangle \\
&\quad + \frac{i}{\hbar} \int_{-\infty}^{\infty} d^3k_2\, d^3\widetilde{k}_1\, d^3\widetilde{k}_2 \left\langle k_1', k_2 \right| \hat{\rho}(-\infty) \left| \widetilde{k}_1, \widetilde{k}_2 \right\rangle \left\{ \int_{-\infty}^{\infty} dt \left\langle \widetilde{k}_1, \widetilde{k}_2 \right| \hat{H}_I(t) \left| k_1, k_2 \right\rangle \right\}.
\end{aligned}
$$

Plugging in our result (5.6),

$$
\begin{aligned}
\left\langle {k_1}' \right| \hat{\rho}_{\text{reduced}}(\infty) \left| k_1 \right\rangle &= \left\langle k_1' \right| \hat{\rho}_{\text{reduced}}(-\infty) \left| k_1 \right\rangle \\
&\quad - i \int_{-\infty}^{\infty} d^3k_2\, d^3\widetilde{k}_1\, d^3\widetilde{k}_2 \ \left(\frac{1}{(2\pi)^2}\ \widetilde{V}\left(k_1' - \widetilde{k}_1\right)\ \delta\left(\tfrac{{k_1'}^2}{2m_1} + \tfrac{{k_2}^2}{2m_2} - \tfrac{\widetilde{k}_1^2}{2m_1} - \tfrac{\widetilde{k}_2^2}{2m_2} \right) \right. \\
&\qquad\qquad \left. \delta^3(k_1' - \widetilde{k}_1 - k_2 + \widetilde{k}_2)\ \ \left\langle \widetilde{k}_1, \widetilde{k}_2 \right| \hat{\rho}(-\infty) \left| k_1, k_2 \right\rangle \right) \\
&\quad + i \int_{-\infty}^{\infty} d^3k_2\, d^3\widetilde{k}_1\, d^3\widetilde{k}_2 \ \left(\frac{1}{(2\pi)^2}\ \widetilde{V}\left(\widetilde{k}_1 - k_1\right)\ \delta\left(\tfrac{\widetilde{k}_1^2}{2m_1} + \tfrac{\widetilde{k}_2^2}{2m_2} - \tfrac{{k_1}^2}{2m_1} - \tfrac{{k_2}^2}{2m_2} \right) \right. \\
&\qquad\qquad \left. \delta^3(\widetilde{k}_1 - k_1 - \widetilde{k}_2 + k_2)\ \ \left\langle k_1', k_2 \right| \hat{\rho}(-\infty) \left| \widetilde{k}_1, \widetilde{k}_2 \right\rangle \right).
\end{aligned}
$$

Finally, we use the delta functions to get rid of the $\widetilde{k}_1$ integrals. This gives us

$$
\begin{aligned}
\left\langle {k_1}' \right| \hat{\rho}_{\text{reduced}}(\infty) \left| k_1 \right\rangle &= \left\langle k_1' \right| \hat{\rho}_{\text{reduced}}(-\infty) \left| k_1 \right\rangle \\
&\quad - i \int_{-\infty}^{\infty} d^3k_2\, d^3\widetilde{k}_2\ \ \frac{1}{(2\pi)^2}\ \widetilde{V}\left(k_2 - \widetilde{k}_2\right)\ \left\langle k_1' + \widetilde{k}_2 - k_2,\ \widetilde{k}_2 \right| \hat{\rho}(-\infty) \left| k_1, k_2 \right\rangle\ D(k_1', k_2, \widetilde{k}_2) \\
&\quad + i \int_{-\infty}^{\infty} d^3k_2\, d^3\widetilde{k}_2\ \ \frac{1}{(2\pi)^2}\ \widetilde{V}\left(\widetilde{k}_2 - k_2\right)\ \left\langle k_1', k_2 \right| \hat{\rho}(-\infty) \left| k_1 + \widetilde{k}_2 - k_2,\ \widetilde{k}_2 \right\rangle\ D(k_1, k_2, \widetilde{k}_2).
\end{aligned}
$$

where

$$
D(k_1, k_2, \widetilde{k}_2) = \delta\left(\tfrac{1}{2}\ {k_2}^2 \left(\tfrac{1}{m_1} - \tfrac{1}{m_2} \right) + \tfrac{1}{2}\ \widetilde{k}_2^2 \left(\tfrac{1}{m_1} + \tfrac{1}{m_2} \right) - \tfrac{1}{2m_1} \left(-k_1 \cdot \widetilde{k}_2 + k_1 \cdot k_2 + \widetilde{k}_2 \cdot k_2 \right) \right).
$$

Then, assuming $\widetilde{V}$ is an even function,

$$
\begin{aligned}
\left\langle {k_1}' \right| \hat{\rho}_{\text{reduced}}(\infty) \left| k_1 \right\rangle = \Bigg(& \left\langle k_1' \right| \hat{\rho}_{\text{reduced}}(-\infty) \left| k_1 \right\rangle\ + \\
& \int_{-\infty}^{\infty} \frac{d^3k_2\, d^3\widetilde{k}_2}{(2\pi)^2}\ \widetilde{V}\left(k_2 - \widetilde{k}_2\right)\ \left(P\left(k_1, k_1' k_2, \widetilde{k}_2\right) D\left(k_1, k_2, \widetilde{k}_2\right) + P^*\left(k_1', k_1, k_2, \widetilde{k}_2\right) D\left(k_1', k_2, \widetilde{k}_2\right) \right) \Bigg)
\end{aligned}
\tag{5.8}
$$

where

$$
P(k_1, k_1', k_2, \widetilde{k}_2) = i \left\langle k_1', k_2 \right| \hat{\rho}(-\infty) \left| k_1 + \widetilde{k}_2 - k_2,\ \widetilde{k}_2 \right\rangle.
$$

Chapter 6

Conclusion

6.0.1 Time evolution of a pure state

Suppose we have a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}(t)$$

where $\hat{H}_0$ is a well-understood Hamiltonian that does not depend on time and $\lambda \hat{V}(t)$ is "small". For example, $\hat{H}_0$ might be the free particle Hamiltonian $\hat{H}_0 = \frac{m}{2}\nabla^2$. Our equation of motion is the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi, t\rangle = \left(\hat{H}_0 + \lambda \hat{V}(t)\right) |\Psi, t\rangle$$

where $|\Psi, t\rangle$ is the usual Schrödinger-picture state at time t.

Let $\hat{U}(t_0, t) = e^{-i\hat{H}_0(t-t_0)/\hbar}$. Then $\hat{U}(t_0, t)$ is the operator that evolves a state from time t_0 to time t according to $\hat{H}_0$. We define the interaction-picture state to be

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

so $|\Psi, t\rangle = \hat{U}(t_0, t) |\Psi_I, t\rangle$. Plugging this in to the Schrödinger equation,

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \hat{U}(t_0, t) |\Psi_I, t\rangle &= \left(\hat{H}_0 + \lambda \hat{V}(t)\right) \hat{U}(t_0, t) |\Psi, t\rangle \\
i\hbar \left[\frac{\partial}{\partial t} e^{-i\hat{H}_0(t-t_0)/\hbar}\right] |\Psi_I, t\rangle + i\hbar e^{-i\hat{H}_0(t-t_0)/\hbar} \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \hat{H}_0 e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle + \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
\cancel{-i^2 \hat{H}_0 e^{i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle} + i\hbar e^{-i\hat{H}_0(t-t_0)/\hbar} \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \cancel{\hat{H}_0 e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle} + \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
i\hbar \frac{\partial}{\partial t} |\Psi_I, t\rangle &= e^{i\hat{H}_0(t-t_0)/\hbar} \lambda \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar} |\Psi_I, t\rangle \\
i\hbar \frac{\partial}{\partial t} |\Psi_I, t\rangle &= \lambda \hat{H}_I(t) |\Psi_I, t\rangle
\end{aligned}$$

where we define the interaction Hamiltonian to be

$$\hat{H}_I(t) = \hat{U}(t_0, t)^\dagger \hat{V}(t) \hat{U}(t_0, t) = e^{i\hat{H}_0(t-t_0)/\hbar} \hat{V}(t) e^{-i\hat{H}_0(t-t_0)/\hbar}.$$

This sets up the interaction picture. We have rephrased our problem so that we can continue with quantum mechanics normally without having to worry about the time evolution due to $\hat{H}_0$.

We now integrate both sides of our expression.

$$\begin{aligned}
\int_{t_0}^{t} \frac{\partial}{\partial t'} |\Psi_I, t'\rangle &= -\frac{i}{\hbar} \lambda \int_{t_0}^{t} \hat{H}_I(t') |\Psi_I, t'\rangle \, dt' \\
|\Psi_I, t\rangle - |\Psi_I, t_0\rangle &= -\frac{i}{\hbar} \lambda \int_{t_0}^{t} \hat{H}_I(t') |\Psi_I, t'\rangle \, dt' \\
|\Psi_I, t\rangle &= |\Psi_I, t_0\rangle - \frac{i}{\hbar} \lambda \int_{t_0}^{t} \hat{H}_I(t') |\Psi_I, t'\rangle \, dt' \qquad (6.1)
\end{aligned}$$

This is called the integral form of the Schrödinger equation.

We can now iteratively calculate perturbative approximations where we assume $\hat{H}_I(t)$ is small. The zero order approximation is simply

$$|\Psi_I, t\rangle = |\Psi_I, t_0\rangle + \mathcal{O}(\lambda).$$

Plugging this in for the state inside the integral in (6.1), we get the first order approximation

$$|\Psi_I, t\rangle = |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \, |\Psi_I, t_0\rangle \; dt' + \mathcal{O}\big(\lambda^2\big). \tag{6.2}$$

Plugging this in to (6.1) again we get the second order approximation

$$\begin{aligned} |\Psi_I, t\rangle &= |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \left[|\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t'} \hat{H}_I(t'') \, |\Psi_I, t_0\rangle \; dt'' \right] dt' + \mathcal{O}\big(\lambda^3\big) \\ &= |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \, |\Psi_I, t_0\rangle \; dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t'} \hat{H}_I(t')\hat{H}_I(t'') \, |\Psi_I, t_0\rangle \; dt'' \, dt' + \mathcal{O}\big(\lambda^3\big). \end{aligned} \tag{6.3}$$

In general, we can keep going to achieve higher order approximations. For us, however, the second order approximation (6.3) is enough.

6.0.2 Time evolution of the density operator

We now consider mixed states. We will need to describe the system by the density operator $\hat{\rho}(t)$. Let's derive the time evolution of $\hat{\rho}(t)$ in second order perturbation theory based on (6.3).

Suppose at time t_0 we have a statistical ensemble of interaction-picture states $|\psi_{In}, t_0\rangle$ each with probability P_n. Then

$$\hat{\rho}(t_0) = \sum_n P_n \, |\Psi_{In}, t_0\rangle \, \langle \Psi_{In}, t_0| \, .$$

At time t states will have evolved according to (6.3), so

$$\hat{\rho}(t) = \sum_n P_n \, |\Psi_{In}, t\rangle \, \langle \Psi_{In}, t| \, .$$

From (6.3) we have

$$|\Psi_{In}, t\rangle = |\Psi_I, t_0\rangle - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \hat{H}_I(t') \, |\Psi_I, t_0\rangle \; dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t'} \hat{H}_I(t')\hat{H}_I(t'') \, |\Psi_I, t_0\rangle \; dt'' \, dt' + \mathcal{O}\big(\lambda^3\big)$$

$$\langle \Psi_{In}, t| = \langle \Psi_I, t_0| - \frac{i}{\hbar}\lambda \int_{t_0}^{t} \langle \Psi_I, t_0| \, \hat{H}_I(t') \, dt' - \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t'} \langle \Psi_I, t_0| \, \hat{H}_I(t'')\hat{H}_I(t') \, dt'' \, dt' + \mathcal{O}\big(\lambda^3\big)$$

so

$$\begin{aligned} |\Psi_{In}, t\rangle \, \langle \Psi_{In}, t| \;=\; & |\Psi_{In}, t_0\rangle \, \langle \Psi_{In}, t_0| \;-\; \frac{i}{\hbar}\lambda \int_{t_0}^{t} \Big(\hat{H}(t') \, |\Psi_{In}, t_0\rangle \, \langle \Psi_{In}, t_0| - |\Psi_{In}, t_0\rangle \, \langle \Psi_{In}, t_0| \, \hat{H}_I(t') \Big) \; dt' \\ & - \; \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t'} \Big(\hat{H}_I(t')\hat{H}_I(t'') \, |\Psi_{In}, t_0\rangle \, \langle \Psi_{In}, t_0| + \; |\Psi_{In}, t_0\rangle \, \langle \Psi_{In}, t_0| \, \hat{H}_I(t'')\hat{H}_I(t') \Big) \; dt'' \, dt' \\ & + \; \frac{\lambda^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t} \hat{H}_I(t') \, |\Psi_{In}, t_0\rangle \, \langle \Psi_{In}, t_0| \, \hat{H}_I(t'') \, dt'' \, dt' \;+\; \mathcal{O}\big(\lambda^3\big). \end{aligned}$$

Then

$$\begin{aligned}\hat{\rho}(t) \;&=\; \hat{\rho}\,(t_0) \;-\; \frac{i}{\hbar}\lambda \int_{t_0}^{t} \Big[\hat{H}(t'),\; \hat{\rho}(t_0)\Big]\; dt' \\ &-\; \frac{\lambda^2}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t'} \Big(\hat{H}_I(t')\hat{H}_I(t'')\;\hat{\rho}(t_0) + \hat{\rho}(t_0)\;\hat{H}_I(t'')\hat{H}_I(t')\Big)\; dt''\,dt' \\ &+\; \frac{\lambda^2}{\hbar^2}\int_{t_0}^{t}\int_{t_0}^{t} \hat{H}_I(t')\hat{\rho}(t_0)\hat{H}_I(t'')\,dt''\,dt' \;\;+\;\; \mathcal{O}\big(\lambda^3\big).\end{aligned} \tag{6.4}$$