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**

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Abstract

Write the abstract last! Maximum 350 words.

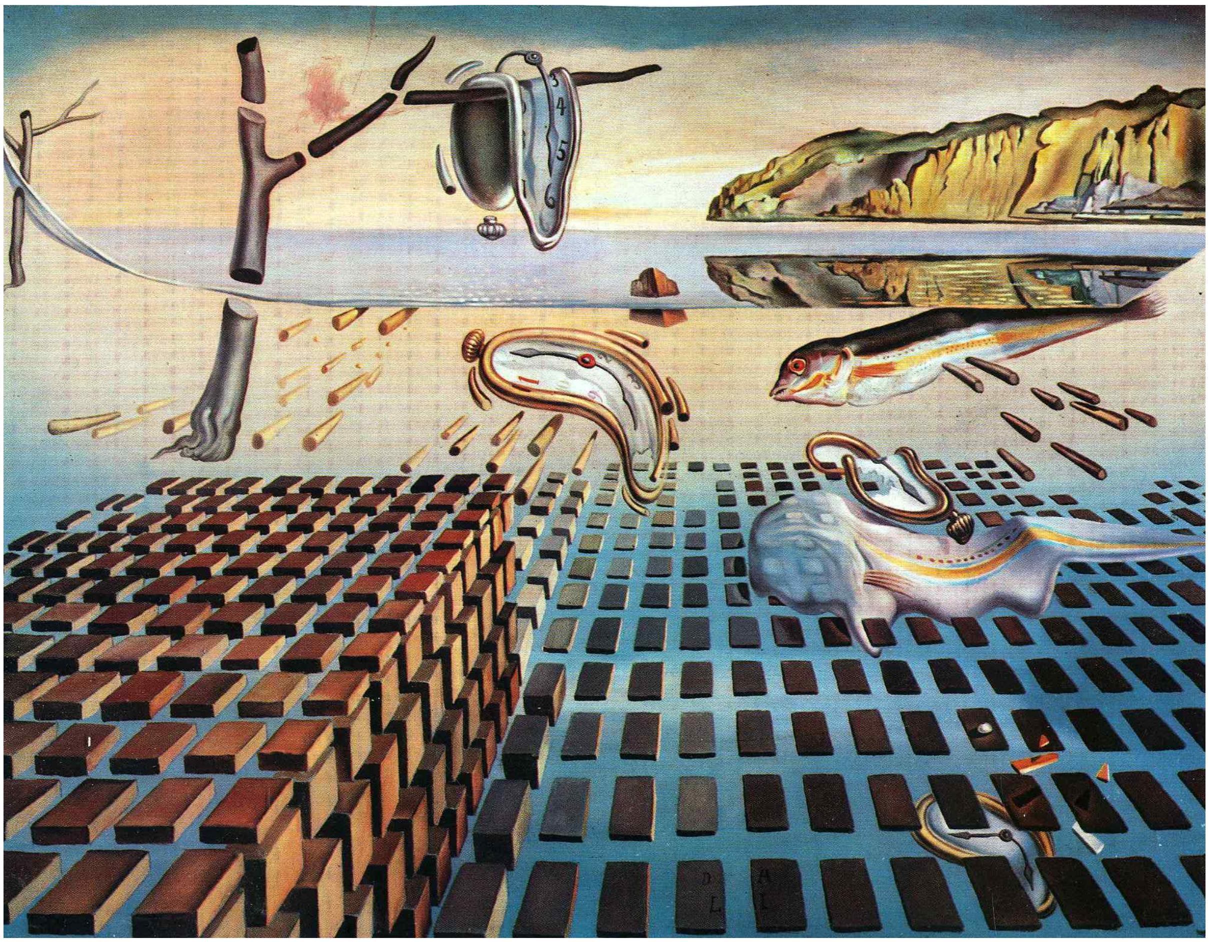


Figure 1: "The Disintegration of the Persistence of Memory" by Salvador Dali (1952-54)
Image from WikiArt

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.

Table of Contents

List of Figures

Acknowledgements

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

In quantum mechanics, physical laws are written down as Hamiltonians, that is, expressions describing total energy. I will use a set of techniques called perturbation theory to study Hamiltonians of the form $\hat{H} = \hat{H}_0 + \lambda V$ where $\hat{H}_0$ is a Hamiltonian that is well understood and λ is very small. I will ask: how much does the entropy change due to λV?

I start in Chapter 2 by explaining what entropy is. In Chapter 3, I develop the perturbation theory tools that I will need later on. In Chapter 4, I apply these tools to derive general formulae for the change in entropy due to the perturbation λV. In Chapter 5, I will discuss a few examples of entropy evolution. Finally, in Chapter 6, I summarize the results and speculate about future research directions.

The physicist reading this thesis may want to jump straight to Chapter 4 because that is where the important results are to be found. The philosopher or casual reader may be more interested in Chapters 2 and 6.

Chapter 2

What is Entropy?

2.1 Missing Information

A shuffled deck of cards. A gas of who-knows-what. A messy room. When we say that these are high-entropy systems, we really mean that we lack the information needed to have a complete description. If a room is messy, how can one find a certain book? We do not know where it is. We know what the room looks *like* but we cannot say much about the details. Conversely, in a tidy room, the book can easily be found because we are able, in our mind, to completely describe the room. A tidy room is a low-entropy system.

Unlike some other areas of study, entropy is a field that the physicist can approach with a myriad of tools. The first is painting. Consider "The Disintegration of the Persistence of Memory" by Salvador Dali (Figure 1). Time is warped. Geometric structures turn about as if they are unsure which laws to follow. A discombobulated fish—is it alive or dead? or both simultaneously?—drowns in the ocean. The ocean drowns the land. Objects are reflected unnaturally, incompletely. The painting begs to be understood, but understanding is lacking. The closer you look, the more you realize that something is missing. It is as if we have lost a framework of knowledge. We have bits and pieces of memory but not the structure to understand all.

This is precisely what entropy is in physics. To say there is lots of entropy is to say much more information would be needed to understand every detail of reality. An increase in entropy really is a disintegration of the persistence of memory.

Having exhausted her patience for painting, the hasty physicist will now want equations. The first one defines the Gibbs entropy

$$S = -\sum P_i \log P_i$$

for a situation with N possibilities, each with probability P_i. If $N = 1$, we say that the system is in a "pure state." If $N > 1$, we say that the system is in a "mixed state."

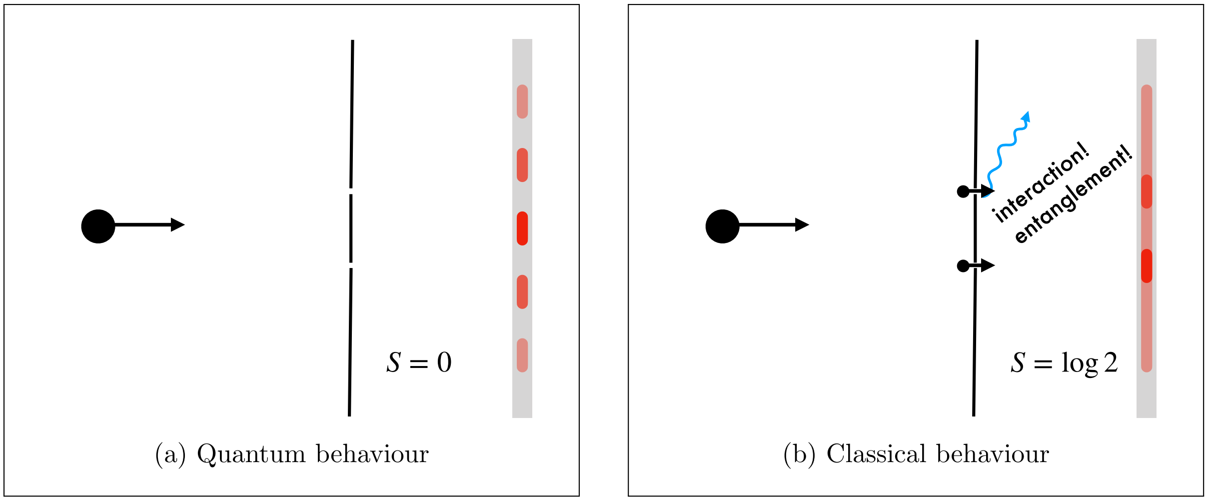
In quantum mechanics, we can keep the exact same definition and merely clarify that by a *possibility* we mean a *possible wavefunction*. Then we have Von Neumann entropy. It turns out that Von Neumann entropy is the only reasonably definition of entropy in quantum mechanics that properly corresponds to Gibbs entropy. [CITATION NEEDED]

Because we consider systems with multiple possible wavefunctions, we describe states with density operators, defined as

$$\hat{\rho} = \sum_i P_i \left|\Psi_i\right\rangle \left\langle\Psi_i\right|$$

where $\{\left|\Psi_i\right\rangle\}$ are the possible wavefunctions and each has probability P_i of being the true wavefunction. By studying how the eigenvalues and eigenstates of the density operator change over time, we understand how the probabilities and states change over time.

We can now write the Von Neumann entropy as a trace. Indeed, $S = \mathrm{Tr}\left(\hat{\rho} \log \hat{\rho}\right)$.



(a) Quantum behaviour

(b) Classical behaviour

Figure 2.1: The double slit experiment.

2.2 The Subsystem Entropy

If we have a bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$ and a basis $\{|\beta_m\rangle\}$ for $\mathcal{H}_B$, we can the reduced density operator

$$\bar{\hat{\rho}} = \sum_m \langle \beta_m | \, \hat{\rho} \, | \beta_m \rangle$$

that acts in the space $\mathcal{H}_A$. Then we can define the $\mathcal{H}_B$ subsystem entropy to be $\operatorname{Tr}\left(\bar{\hat{\rho}}\right)$.

We can think of $\bar{\hat{\rho}}$ to be a version of $\hat{\rho}$ that is "averaged out" at the resolution of $\mathcal{H}_A$. If we consider $\hat{\rho}$ to be a random variable, measurable on the sigma algebra $\mathcal{H}_A \otimes \mathcal{H}_B$, and we understand $\mathcal{H}_A$ to be sub-sigma-algebra inside the larger space, then we can identify $\bar{\hat{\rho}}$ with the conditional expectation $\mathbb{E}\,\hat{\rho}|\mathcal{H}_A$. In this sense, the subsystem entropy describes how much information is lost when we average out (take the conditional expectation).

2.3 Example: Double Slit Experiment

But how does entropy arise, and why is it useful? Let us consider the example of the double slit experiment. A particle is launched towards two slits, passes through the slits, lands on a detector, and has its position measured. Quantum mechanics predicts (and experimentalists verify) that the particle's wavefunction will pass through *both* slits simultaneously. The wavefunction through the upper slit will interfere with the wavefunction through the lower slit, creating a beautiful fringe pattern in the distribution of positions (Figure 2.1a).

But what happens if we try to measure which slit the particle goes through, for example, by shooting photons at the location in the top slit? Then, we observe the fringe pattern predicted by classical mechanics, where the particle goes through only one slit (Figure 2.1b). Let's examine this process. To start, there is just the particle and the photons.

$$|\text{particle}\rangle\,|\text{photons}\rangle$$

If the particle doesn't interact with the photons, it proceeds through the slits as before and does not become entangled with the photons.

$$\frac{1}{\sqrt{2}}\left(|\text{through upper slit}\rangle + |\text{through lower slit}\rangle\right)|\text{photons}\rangle$$

Because $\langle \text{through upper slit} | \text{through lower slit} \rangle \neq 0$, we will have quantum interference and observe the result in Figure 2.1a. We calculate that the subsystem entropy for the particle is 0. On the other hand, if the part of the wavefunction in the upper slit becomes entangled with the photons, our state becomes

$$\frac{1}{\sqrt{2}} \left(|\text{through upper slit}\rangle \, |\text{photons} \sim\rangle + |\text{through lower slit}\rangle \, |\text{photons}\rangle \right)$$

where $|\text{photons} \sim\rangle$ is the state of the photons after the interaction. If $\langle \text{photons} \sim | \text{photons} \rangle = 0$, then we will no longer have quantum interference. We will observe the result in Figure 2.1b. We now calculate that the subsystem entropy for the particle is $\log 2$. This process of losing quantum behaviour is called decoherence. Notice that the decoherence happened when the particle became entangled with the outside world.

In reality, some part of the wavefunction will interact while some will not. We will have some mix of the quantum and classical fringes. The entropy seems to quantify the amount of decoherence; it will be between 0 and $\log 2$.

Finally, we note that the key property here was that $\langle \text{photons} \sim | \text{photons} \rangle = 0$. If instead $\langle \text{photons} \sim | \text{photons} \rangle \neq 0$, we would still have quantum interference and entropy would increase even though decoherence might not occur. We must add this assumption, then, if we are to use entropy to quantify decoherence.

2.4 Decoherence is Measurement by the Universe

Next I hope to dispel some of the magical aura (a.k.a. confusion) that surrounds how we should talk about decoherence as a concept. It is really quite simple: decoherence is measurement by the universe.

Physicists typically describe measurement as "collapsing the wavefunction," but what does this really mean? Suppose we start in a superposition of two possible outcomes.

$$\frac{1}{\sqrt{2}} \left(|\uparrow\rangle + |\downarrow\rangle \right) |\text{observer}\rangle$$

After the measurement, the observer has become entangled with the outcome.

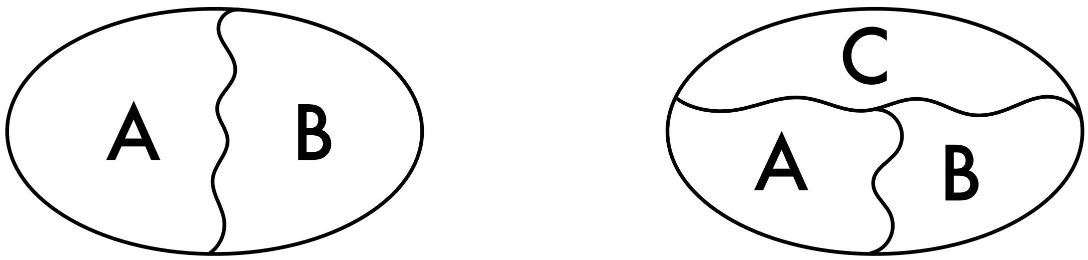
$$\frac{1}{\sqrt{2}} \left(|\uparrow\rangle \, |\text{observed } \uparrow\rangle + |\downarrow\rangle \, |\text{observed } \downarrow\rangle \right)$$

Because $\langle \text{observed } \uparrow | \text{observed } \downarrow \rangle = 0$, there is no more quantum interference between $|\uparrow\rangle$ and $|\downarrow\rangle$. To the observer, it looks as if the system has switched to either $|\uparrow\rangle$ or $|\downarrow\rangle$ (depending on what outcome was measured).

Notice that this is exactly the same process as the decoherence that we saw in Section SECTION! It is exactly appropriate, therefore, to describe decoherence as "the universe measuring the wavefunction".

2.5 Entropy is Entanglement with the Universe

We should note that whenever we talk about Von Neumann entropy, we are really talking about the Von Neumann entropy of a *subsystem*. It doesn't make sense to talk about the Von Neumann entropy of the *whole universe* because there is just one possible wavefunction—the



(a) Conceptualized (b) Reality

Figure 2.2: A bipartite system.

real one! We can only consider systems like the one in Figure 2.2a. The subsystem entropy quantifies the amount of entanglement over the boundary between A and B.

"That's fine," another hasty physicist says, "But what if you start in a classical superposition? You could start with more than one possible wavefunction for the whole universe simply because you don't know which is correct." Saying this, the hasty physicist has made a mistake. He has forgotten that he is in the universe.

The hasty physicist himself is already entangled with the system he wants to measure. Recall our messy room. The room's owner has done things that cause a book to be here, a teapot to be there, and a pencil to be somewhere else, but he forgets what exactly he has done. Nevertheless his own state is entangled with the room's state. If he had a perfect memory, the room would not seem messy, for he would know where everything is—but he has forgotten the nature of the entanglement. This fact does not alter that the entanglement exists.

The hasty physicist who says the A+B system can start in a classical superposition is really saying that there is a third part, C, that we ignore because it is impossibly complicated (Figure 2.2b). When we say that A+B is in a classical superposition, we really mean that A+B is entangled with C, but we already take the reduced density operator for the A+B system because we don't know how to begin thinking about C. This does not alter that there is a single true global wavefunction for the universe. The hasty physicist has simplified life by averaging out the part of the universe he doesn't understand. Having done so, when he computes the entropy of A, the hasty physicist is actually quantifying the entanglement of A with B *as well as* the entanglement of A with C.

"That's fine," the hasty physicist says, "but now you're talking philosophy, not physics." This interpretation, though, allows us to intuit physics results about symmetries—so surely it is physics! Indeed, if we start with a pure state for A+B, that is, if A+B are truly unentangled with C, then the entropy of A and the entropy of B both quantify the entanglement across the A-B boundary. We expect both subsystems to have the same entropy. This is indeed what we find in Section 4.2.2. Conversely, if A+B starts in a mixed state, that is, if A+B starts entangled with C, then the subsystem entropies of A and B will in general be different. The subsystem entropy of A includes entanglement across the A-C boundary, whereas the subsystem entropy of B includes entanglement across the B-C boundary, and these need not be equal. Again, this is what we find, in Sectionn 4.2.1. (In this thesis, I prove these results only for separable states. I conjecture that they can also be proven for non-separable states.)

While Figure 5 is the correct picture, it is still useful for computational purposes to pretend that C doesn't exist (as the hasty physicist thinks). We need not complicate our derivations by acknowledging it.

Note that entropy measures entanglement with the universe, which is not the same thing as *decoherence*. Decoherence requires that the states the system is entangled with are orthogonal in the universe's space. In practice, however, it is often reasonable to assume that the states that the system is entangled with are orthogonal in the universe. This is why it makes sense to describe entropy as quantifying decoherence.

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

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

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.

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

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

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

Plugging this in for the state inside the integral in (3.1), we get the first order approximation

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

Plugging this in to (3.1) again we get the second order approximation

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

In general, we can keep going to achieve higher order approximations. For us, however, the second order approximation (3.3) 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 (3.3).

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 (3.3), so

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

From (3.3) 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,

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

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 (3.4), we see that at some fixed time t we can form asymptotic expansions

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

by taking

$$\hat{\rho}_0 = \hat{\rho}\left(t_0\right)$$

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

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

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

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

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

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

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

Putting this all into (4.2),

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

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 $\overline{\rho}$ 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),

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

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

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

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

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

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

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

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

$$\sum_{n\in I}\sum_{m}\int_{t_0}^{t}\int_{t_0}^{t'}\langle n\ m|\left(\hat{H}_I(t')\hat{H}_I(t'')\ \hat{\rho}_0+\hat{\rho}_0\ \hat{H}_I(t'')\hat{H}_I(t')\right)|n\ m\rangle\ dt''\,dt'$$

$$-\sum_{n\in I}\sum_{m}\int_{t_0}^{t}\int_{t_0}^{t}\langle n\ m|\,\hat{H}_I(t')\,\hat{\rho}_0\,\hat{H}_I(t'')\,|n\ m\rangle\ dt''\,dt'$$

$$\begin{aligned}
&=\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'\\
&\qquad-\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'\\
&\qquad-\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'\\
&\qquad-\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'\\
&\qquad-\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]\\
&\qquad+\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.
\end{aligned}$$

Meanwhile, the third term in (4.11) is

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

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

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

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

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

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 $\lambda^2 \log\frac{1}{\lambda^2}$,

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

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

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

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 $|11\rangle = \frac{1}{\sqrt{2}} (|E_2\rangle + |E_3\rangle)$. 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

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

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

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

We observe that the leading order term for the change in entropy is of order $\lambda^2t^2\log\frac{1}{\lambda^2t^2}$. 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

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

(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 (3.2) 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

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

so

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

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

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

Putting this into (5.5),

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

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

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

In the momentum basis the matrix elements are

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

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

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

Plugging in our result (5.6),

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

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

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

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,

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

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

To be added...