Entropy Growth in Quantum Mechanics

by

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Abstract

When a small perturbation $\lambda\hat{V}$ is added to a Hamiltonian $\hat{H}_0$, the Von Neumann entropy of a subsystem may change as a result. I study this change in entropy. In particular, I derive a general expression for the change in entropy based on perturbative corrections to the eigenvalues of the reduced density operator. It shows that the entropy of a mixed state will never decrease provided (1) there exist component states with zero initial probability that can be transitioned into and (2) initial component states do not have lower-order corrections to their probabilities than states with zero initial probability. I also derive an expression for the change in entropy for an unentangled mixed state that can transition into states with zero initial probability. For such systems, the change in entropy depends only on the transition amplitudes to states with zero initial probability. I consider two simple examples applying my results and speculate on future directions.

Lay Summary

In quantum mechanics, two systems can be fundamentally entwined through a process called entanglement. We may wish to describe the amount of entanglement—we can do so through something called "entanglement entropy." I study how this entanglement entropy changes over time. I derive several formulae for entanglement entropy in different cases of initial conditions. I also develop conditions under which entanglement entropy may never decrease.

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

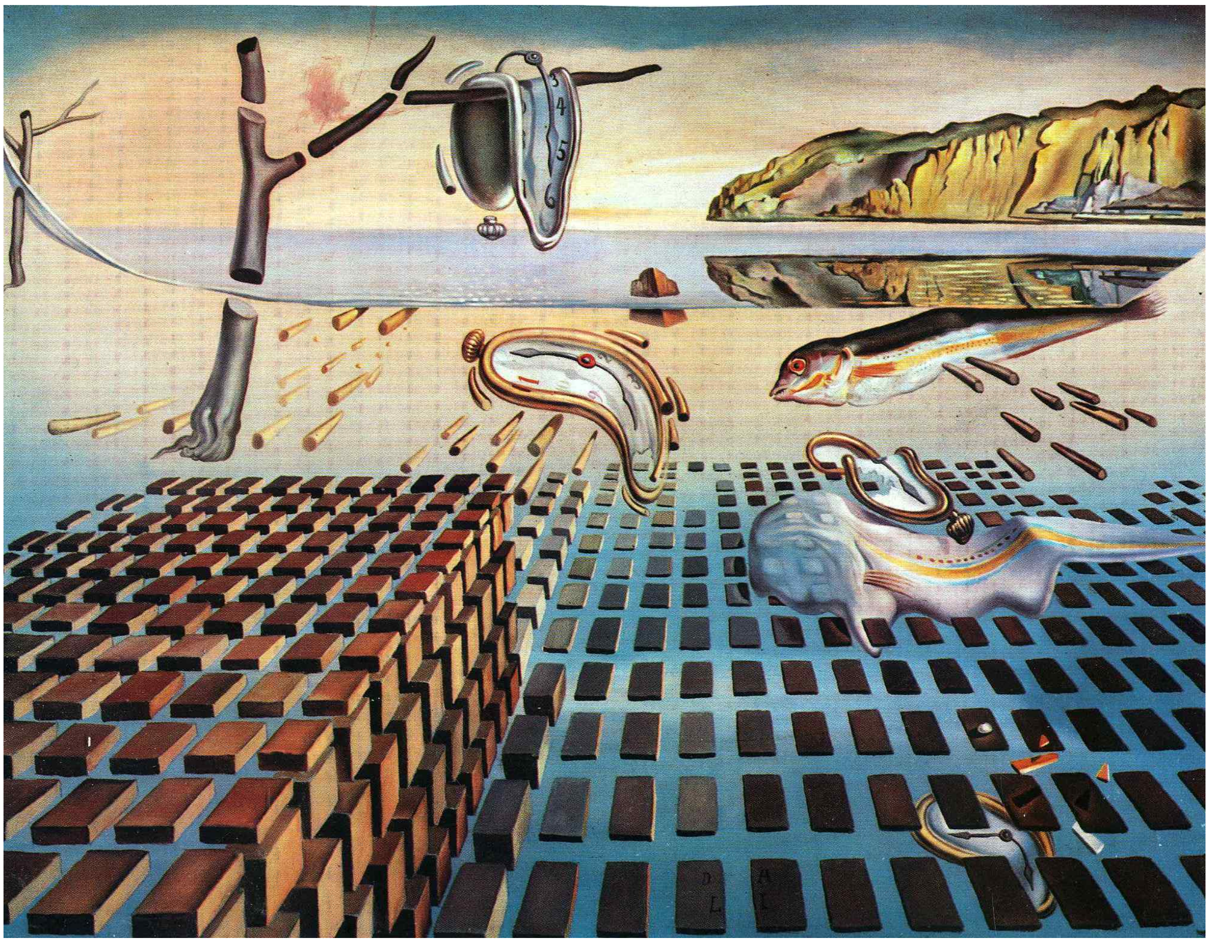

Figure 1: “The Disintegration of the Persistence of Memory” by Salvador Dalí (1952-54). Image from WikiArt. © Salvador Dalí.

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Chapter 1

Introduction

In quantum mechanics, physical laws are written down as expressions describing total energy called "Hamiltonians." I will use a set of techniques called perturbation theory to study Hamiltonians of the form $\hat{H} = \hat{H}_0 + \lambda\hat{V}$ 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 $\lambda\hat{V}$?

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

The physicist reading this thesis may want to jump straight to Chapter 3 because that is where the important results are to be found. The philosopher or casual reader may be more interested in Chapters 1 and 5.

1.1 What is entropy?

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.

The physicist can approach entropy 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 is indeed 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

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

for a situation with N possibilities, each with probability P_i. If $N = 1$, the entropy is zero and we say that the system is in a "pure state." If $N > 1$, the entropy is nonzero and 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 reasonable definition of entropy in quantum mechanics that properly corresponds to Gibbs entropy. [1, 4, 5]

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 $\{|\Psi_i\rangle\}$ 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: $S = -\operatorname{Tr}\left(\hat{\rho}\log\hat{\rho}\right)$.

1.1.1 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 define the reduced density operator

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

that acts on the space $\mathcal{H}_A$. Then the $\mathcal{H}_A$-subsystem entropy is $-\operatorname{Tr}\left(\overline{\hat{\rho}}\log\overline{\hat{\rho}}\right)$.

We can think of $\overline{\hat{\rho}}$ 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 $\overline{\hat{\rho}}$ 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).

But how does subsystem entropy arise, and why is it useful? Let us consider the example of the double slit experiment.

1.1.2 Example: 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 experiments 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 2a).

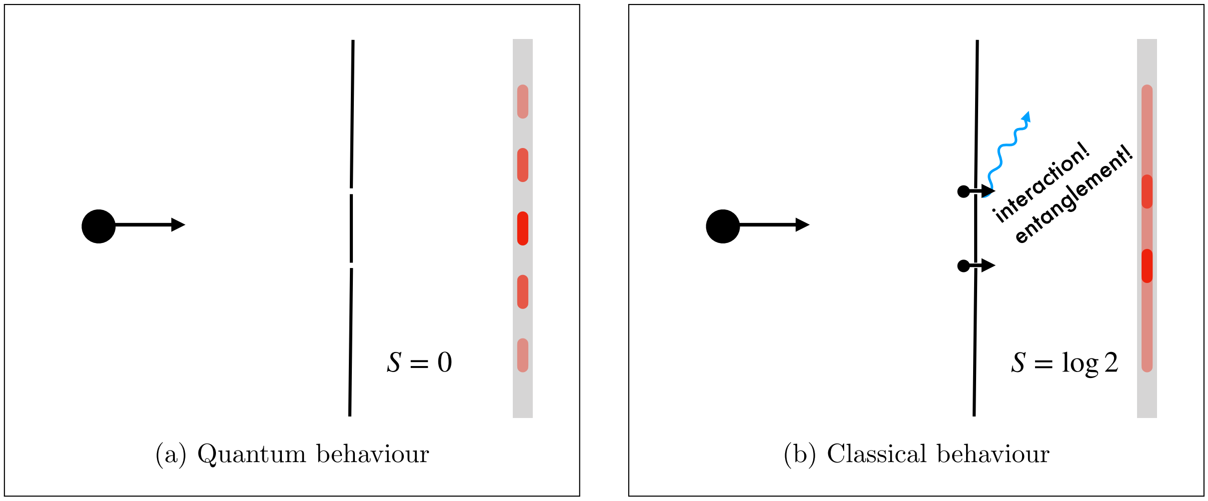
But what happens if we try to measure which slit the particle goes through, for example, by shooting photons at the location in the top slit? Then, we observe the fringe pattern predicted by classical mechanics, where the particle goes through only one slit (Figure 2b). Let's examine this process. To 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 2a. We calculate that the subsystem entropy for the particle is 0.



(a) Quantum behaviour

(b) Classical behaviour

Figure 2: The double slit experiment.

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 2b. The subsystem entropy of the particle is now $\log 2$.

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 will be between 0 and $\log 2$. It seems to quantify the amount of decoherence.

Finally, we note that the key property here was that $\langle\text{photons}\sim|\text{photons}\rangle = 0$. If instead $\langle\text{photons}\sim|\text{photons}\rangle \neq 0$, decoherence will not occur, though the subsystem entropy will still increase in the same way. Thus the subsystem entropy quantifies decoherence only if we assume that $\langle\text{photons}\sim|\text{photons}\rangle = 0$.

1.1.3 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 a 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 which outcome was measured).

This process is exactly the same process as the decoherence that we saw in Section 1.1.2 It is exactly appropriate, therefore, to describe decoherence as "the universe measuring the wavefunction."

(The description here is inspired by the confusingly named "many worlds interpretation" of quantum mechanics, advanced by, for example, Sean Carroll [2].)

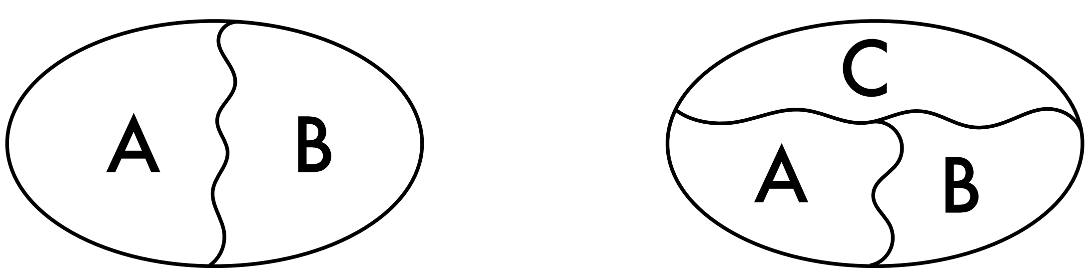
1.1.4 Entropy is entanglement with the universe

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 real one! We can only consider systems like the one in Figure 3a. The subsystem entropy quantifies the amount of entanglement over the boundary between A and B. This, then, is what entropy is: a measure of how entangled a system is with "everything else".

"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. Then you have entropy without entanglement." 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 3b). When we say that A+B is in a classical superposition (mixed state), we really mean that A+B is entangled with C, but we already take the reduced density operator for the A+B system



(a) Conceptualized (b) Reality

Figure 3: A bipartite 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.

"Fair enough," the hasty physicist says, "But now you're talking philosophy, not physics!" This interpretation, though, allows us to intuit *physical* results by symmetries. Indeed, if we start with a pure state for A+B, that is, if A+B is 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 3.4. 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 Section 3.3. (In Sections 3.3 and 3.4, I prove these conclusions only for separable states. I conjecture that they can also be proven for non-separable states.)

While Figure 3b 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 they are orthogonal. This is why it makes sense to describe entropy as quantifying decoherence.

Of course, it is somewhat arbitrary where one draws the boundaries between A, B, and C. Taking the perspective of the whole universe, there is just a wavefunction. We conjure up mixed states due to our imperfect understanding. Henry Adams wrote, "Chaos was the law of nature; order was the dream of man." Perhaps we may now say instead, rather more optimistically, "Order is the law of nature; chaos is the dream of man."

Chapter 2

Theoretical Tools

2.1 Time-dependent perturbation theory in the interaction picture

2.1.1 Time evolution of pure states

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.

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

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 zeroth-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 (2.1), we get the first-order approximation

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

Plugging this in to (2.1) again we get the second-order approximation

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

In general, we can keep going to achieve higher-order approximations. For us, however, the second-order approximation (2.3) is enough.

2.1.2 Time evolution of mixed states

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 (2.3).

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 (2.3), so

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

From (2.3) 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

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

Then

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

2.2 Corrections to eigenvalues of an operator

The goal of this section is to compute the first- and second-order perturbative corrections to the eigenvalues of an operator. We use the approach known as time-independent perturbation theory. (This approach is commonly used in quantum mechanics but surprisingly few textbooks derive higher-order corrections in sufficient generality. One of those is Ref. [7].)

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,

$$\begin{aligned}
\left| \Psi_n \right\rangle &= \sum_{m \in D_n} \left| \Psi_m^{(0)} \right\rangle \left\langle \Psi_m^{(0)} | \Psi_n \right\rangle + \sum_{m \notin D_n} \left| \Psi_m^{(0)} \right\rangle \left\langle \Psi_m^{(0)} | \Psi_n \right\rangle \qquad (2.5) \\
&= \sum_{m \in D_n} \left| \Psi_m^{(0)} \right\rangle \lim_{\delta \to 0} \frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left| \Psi_n^{(0)} \right\rangle}{\sigma_n^{(1)} + \delta} \\
&\quad + \lambda \Bigg(\sum_{m \in D_n} \left| \Psi_m^{(0)} \right\rangle \lim_{\delta \to 0} \left[\frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_2 \left| \Psi_n^{(0)} \right\rangle}{\sigma_n^{(1)} + \delta} + \frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left| \Psi_n^{(1)} \right\rangle}{\sigma_n^{(1)} + \delta} - \frac{\sigma_n^{(2)} \left\langle \Psi_m^{(0)} \right| \hat{\rho}_0 \left| \Psi_n^{(0)} \right\rangle}{\left(\sigma_n^{(1)} + \delta \right)^2} \right] \\
&\qquad + \sum_{m \notin D_n} \left| \Psi_m^{(0)} \right\rangle \frac{\left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left| \Psi_n \right\rangle}{\sigma_n^{(0)} - \sigma_m^{(0)}} \Bigg) \\
&\quad + \mathcal{O}\big(\lambda^2\big)
\end{aligned}$$

In the zeroth order of λ, equation (2.5) 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

$$\boxed{\sigma_n^{(1)} = \left\langle \Psi_n^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle.} \tag{2.6}$$

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

$$\boxed{0 = \left\langle \Psi_k^{(0)}\right| \hat{\rho}_1 \left|\Psi_n^{(0)}\right\rangle, \qquad k\in D_n, \qquad m\neq n.} \tag{2.7}$$

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 (2.5) says

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

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

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

hence

$$\boxed{\sigma_n^{(2)} = \left\langle \Psi_n^{(0)} \right| \hat{\rho}_2 \left| \Psi_n^{(0)} \right\rangle + \sum_{m \notin D_n} \frac{\left| \left\langle \Psi_m^{(0)} \right| \hat{\rho}_1 \left| \Psi_n^{(0)} \right\rangle \right|^2}{\sigma_n^{(0)} - \sigma_m^{(0)}}.} \tag{2.8}$$

Chapter 3

Growth of Von Neumann Entropy due to a Perturbation

3.1 The general case

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

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

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

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

$$\bar{\hat{\rho}} = \sum_n \overline{\sigma_n} \, |\alpha_n\rangle \langle\alpha_n| \,, \tag{3.1}$$

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

$$S = -\sum_n \overline{\sigma_n} \log \overline{\sigma_n}. \tag{3.2}$$

Now, looking at equation (2.4), we see that at some fixed time t we can form asymptotic expansions

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

by taking

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

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

$$\bar{\hat{\rho}}_1 = -\frac{i}{\hbar} \int_{t_0}^{t} \sum_m \left(\cdot \otimes \langle\beta_m|\right) \left[\hat{H}_I(t'),\ \hat{\rho}_0\right] \left(\cdot \otimes |\beta_m\rangle\right) \, dt' \tag{3.3}$$

$$\begin{aligned}
\bar{\hat{\rho}}_2 = &-\frac{1}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t'} \sum_m \left(\cdot \otimes \langle\beta_m|\right) \Big(\hat{H}_I(t')\hat{H}_I(t'')\ \hat{\rho}_0 + \hat{\rho}_0\ \hat{H}_I(t'')\hat{H}_I(t')\Big) \left(\cdot \otimes |\beta_m\rangle\right) \, dt''\, dt' \\
&+ \frac{1}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t} \sum_m \left(\cdot \otimes \langle\beta_m|\right) \hat{H}_I(t')\, \hat{\rho}_0\, \hat{H}_I(t'') \left(\cdot \otimes |\beta_m\rangle\right) \, dt''\, dt'.
\end{aligned} \tag{3.4}$$

From (3.1) we see that

$$\bar{\hat{\rho}}_0 = \sum_n \overline{\sigma_n^{(0)}} \left|\alpha_n^{(0)}\right\rangle \left\langle \alpha_n^{(0)}\right|. \tag{3.5}$$

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

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 can determine $\overline{\sigma_n^{(1)}}$ and $\overline{\sigma_n^{(2)}}$ by combining (2.6), (2.8), (3.3), and (3.4). We get

$$\overline{\sigma_n^{(1)}} = -\frac{i}{\hbar} \int_{t_0}^{t} \sum_m \langle n\ m| \left[\hat{H}_I(t'),\ \hat{\rho}_0\right] |n\ m\rangle\ dt' \tag{3.6}$$

and

$$\begin{aligned}
\overline{\sigma_n^{(2)}} = &\sum_m \int_{t_0}^{t} \int_{t_0}^{t'} \langle n\ m| \left(\hat{H}_I(t')\hat{H}_I(t'')\ \hat{\rho}_0 + \hat{\rho}_0\ \hat{H}_I(t'')\hat{H}_I(t')\right) |n\ m\rangle\ dt''\, dt' \\
&- \sum_m \int_{t_0}^{t} \int_{t_0}^{t} \langle n\ m|\, \hat{H}_I(t')\, \hat{\rho}_0\, \hat{H}_I(t'')\, |n\ m\rangle\ dt''\, dt' \\
&- \sum_{n' \in C_n} \frac{1}{\overline{\sigma_n^{(0)}} - \overline{\sigma_{n'}^{(0)}}} \left| \sum_m \int_{t_0}^{t} \langle n\ m| \left[\hat{H}_I(t'),\ \hat{\rho}_0\right] |n'\ m\rangle\ dt' \right|^2
\end{aligned} \tag{3.7}$$

where $C_n = \left\{n' : \overline{\sigma_{n'}^{(0)}} = \overline{\sigma_n^{(0)}}\right\}$.

We now compute the subsystem entropy at time t. Let us examine the terms in (3.2). If $\sigma_n^{(0)} \neq 0$ (i.e. $n \in I$), let l_n be the lowest positive integer such that $\overline{\sigma_n^{(l_n)}} \neq 0$. Let l be the minimal l_n. (If all corrections are zero, we could say l doesn't exist, but this situation is uninteresting because the system just stays in the initial state. We may as well assume l exists.) We see that

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

On the other hand, if n has $\overline{\sigma_n^{(0)}} = 0$ (i.e. $n \notin I$) and $\overline{\sigma_n} \neq 0$, let k_n be the lowest positive integer such that $\overline{\sigma_n^{(k_n)}} \neq 0$. Let k be the minimal k_n. Then

$$\begin{aligned}\overline{\sigma_n} \log \overline{\sigma_n} &= \left(\lambda^{k_n}\overline{\sigma_n^{(k_n)}} + \mathcal{O}\left(\lambda^{k_n+1}\right)\right) \log\left(\lambda^{k_n}\overline{\sigma_n^{(k_n)}}\left(1+\mathcal{O}(\lambda)\right)\right) \\ &= \lambda^{k_n}\overline{\sigma_n^{(k_n)}} \log\left(\lambda^{k_n}\overline{\sigma_n^{(k_n)}}\right) + \mathcal{O}\left(\lambda^{k_n+1}\right) \\ &= \lambda^{k}\overline{\sigma_n^{(k)}} \log\left(\lambda^{k}\overline{\sigma_n^{(k)}}\right) + \mathcal{O}\left(\lambda^{k+1}\right) \\ &= -\left(\lambda^k \log\frac{1}{\lambda^k}\right)\overline{\sigma_n^{(k)}} + \mathcal{O}\left(\lambda^k\right).\end{aligned}$$

Putting this all into (3.2),

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

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, because $\sum_n \overline{\sigma_n} = 1$ we must have $\sum_{n\in I}\overline{\sigma_n^{(l)}} = -\sum_{n\notin I}\overline{\sigma_n^{(l)}}$. If $l < k$ this vanishes; if $l \geq k$ it can be absorbed into the $\mathcal{O}(\lambda^k)$. Thus the change in entropy due to the perturbation is

$$\boxed{\Delta S = \lambda^l\sum_{n\in I}\overline{\sigma_n^{(l)}}\log\frac{1}{\overline{\sigma_n^{(0)}}} + \left(\lambda^k\log\frac{1}{\lambda^k}\right)\sum_{n\notin I}\overline{\sigma_n^{(k)}} + \mathcal{O}\left(\lambda^{l+1}\right) + \mathcal{O}\left(\lambda^k\right).} \tag{3.8}$$

Here l is the order of the lowest non-vanishing correction $\overline{\sigma_n^{(l)}}$ for $n \in I$ and k is the order of the lowest non-vanishing correction $\overline{\sigma_n^{(k)}}$ for $n \notin I$. In general, l and k will be 1 or 2. We can find them and compute the eigenvalue corrections with (3.6) and (3.7).

Now, what does ΔS mean? 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. Conversely, 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 $\lambda\hat{V}$.

(3.8) is a rather beautiful result. The λ^l term is the leading correction for entropy change within the subspace of $\mathcal{H}_A$ that the system already occupied. The $\lambda^k \log\frac{1}{\lambda^k}$ term is the leading correction for entropy generated due to transitioning to new states.

Because all $\overline{\sigma_n} > 0$, the leading correction to $\overline{\sigma_n}$ must be nonnegative for $n \in I$. Therefore, if $k \leq l$, the second term dominates and the change in entropy is non-negative. **Entropy may only decrease if $l < k$, that is, if there are lower-order corrections in the occupied space ($n \in I$) than in the kernel of $\overline{\rho}_0$ ($n \notin I$).** In particular, if all states have the same order of correction that leads (often true), and if there exist states with zero initial probability that the system can transition to (also often true), then the entropy can only increase.

We will find in Section 3.3 that $l = k = 2$ for separable states. Therefore, if a separable state can transition into new states that initially had probability zero, the entropy will never decrease due to the perturbation. This conclusion is consistent with Ref. [1] which proves that the Von Neumann entropy of separable states does not decrease.

3.2 Case where first-order corrections vanish and new states can be entered

Suppose that some n have $\overline{\sigma_n^{(0)}} = 0$ and $\overline{\sigma_n} \neq 0$. Suppose also that all $\sigma_n^{(1)} = 0$. (In other words, we suppose that $l = k = 2$ and that there are accessible states in the kernel of $\overline{\hat{\rho}_0}$.) Then (3.8) becomes

$$\Delta S = \left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n \notin I} \overline{\sigma_n^{(2)}} + \mathcal{O}(\lambda^2). \tag{3.9}$$

Now, since $\sum_n \overline{\sigma_n^{(2)}} = 0$ we can rewrite (3.9) as

$$\Delta S = -\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n \in I} \overline{\sigma_n^{(2)}} + \mathcal{O}(\lambda^2). \tag{3.10}$$

Substituting in (2.8),

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

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

$$\Delta S = -\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \left(\sum_{n \in I} \left\langle \alpha_n^{(0)} \middle| \overline{\hat{\rho}_2} \middle| \alpha_n^{(0)} \right\rangle + \sum_{n \in I} \sum_{n' \notin I} \frac{\left| \left\langle \alpha_n^{(0)} \middle| \overline{\hat{\rho}_1} \middle| \alpha_{n'}^{(0)} \right\rangle \right|^2}{\overline{\sigma_n^{(0)}}} \right) + \mathcal{O}(\lambda^2). \tag{3.11}$$

Putting in (3.3) and (3.4),

$$\begin{aligned} \Delta S = \frac{1}{\hbar^2} \left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n \in I} \Bigg(& \\ & \sum_m \int_{t_0}^{t} \int_{t_0}^{t'} \langle n\ m| \left(\hat{H}_I(t') \hat{H}_I(t'')\ \hat{\rho}_0 + \hat{\rho}_0\ \hat{H}_I(t'') \hat{H}_I(t') \right) |n\ m\rangle\ dt''\ dt' \\ & - \sum_m \int_{t_0}^{t} \int_{t_0}^{t} \langle n\ m|\ \hat{H}_I(t')\ \hat{\rho}_0\ \hat{H}_I(t'')\ |n\ m\rangle\ dt''\ dt' \\ & - \sum_{n' \notin I} \frac{1}{\overline{\sigma_n^{(0)}}} \left| \sum_m \int_{t_0}^{t} \langle n\ m| \left[\hat{H}_I(t'),\ \hat{\rho}_0 \right] |n'\ m\rangle\ dt' \right|^2 \Bigg) + \mathcal{O}(\lambda^2). \end{aligned} \tag{3.12}$$

This is as far as we will go without making further assumptions. We can, however, relax our requirements about what $|n\ m\rangle$ are. Normally, perturbation theory requires us to choose $\left|\alpha_n^{(0)}\right\rangle$ so that the leading eigenvalue correction matrices are diagonal on degenerate subspaces. We see, however, that we can write 3.12 as

$$\Delta S = \frac{1}{\hbar^2}\left(\lambda^2 \log\frac{1}{\lambda^2}\right) \mathrm{Tr}\left(M_{n,\tilde{n}}\right) + \mathcal{O}\big(\lambda^2\big)$$

where we take $n, \tilde{n} \in I$ and

$$\begin{aligned} M_{n,\tilde{n}} =& \sum_m \int_{t_0}^{t}\int_{t_0}^{t'} \langle n\ m| \left(\hat{H}_I(t')\hat{H}_I(t'')\,\hat{\rho}_0 + \hat{\rho}_0\,\hat{H}_I(t'')\hat{H}_I(t')\right)|\tilde{n}\ m\rangle\ dt''\,dt' \\ &- \sum_m \int_{t_0}^{t}\int_{t_0}^{t} \langle n\ m|\,\hat{H}_I(t')\,\hat{\rho}_0\,\hat{H}_I(t'')\,|\tilde{n}\ m\rangle\ dt''\,dt' \\ &- \sum_{n'\notin I}\frac{1}{\sigma_n^{(0)}}\sum_m \int_{t_0}^{t} \langle n\ m|\left[\hat{H}_I(t'),\ \hat{\rho}_0\right]\left|n'\ m\right\rangle\ dt' \sum_{m'}\int_{t_0}^{t}\left\langle n'\ m'\right|\left[\hat{H}_I(t'),\ \hat{\rho}_0\right]\left|\tilde{n}\ m'\right\rangle\ dt'. \end{aligned}$$

Because the trace of a matrix is invariant under a change of basis, we do not need to use the perturbation-diagonalized basis of $|n\ m\rangle$.

3.3 Case of separable initial state

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

$$\hat{\rho}_0 = \hat{\rho}\left(t_0\right) = \sum_{n,m}\sigma_{n,m}^{(0)}\left(\left|\alpha_n^{(0)}\right\rangle\otimes|\beta_m\rangle\right)\left(\left\langle\alpha_n^{(0)}\right|\otimes\langle\beta_m|\right) \tag{3.13}$$

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".

(3.13) 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

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

The eigenstate/eigenvalue decomposition of an operator is unique up to relabeling once we choose a basis that is appropriately diagonalized on degenerate spaces. Here, for the separable state, we will see that the second-order term dominates, so as observed above we need not diagonalize on degenerate subspaces.

Comparing our equations for the separable state to (3.1) and (3.5), we see that our previous analysis must hold with the notation unchanged. Indeed,

$$\hat{\rho}_0 = \sum_{n,m}\sigma_{n,m}^{(0)}\,|n\ m\rangle\langle n\ m|\,. \tag{3.14}$$

We have

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

so the first-order eigenvalue correction (3.6) vanishes. We will assume that the second-order eigenvalue correction $\overline{\sigma^{(2)}_n}$ does not vanish and turn to (3.12).

The first two terms in (3.12) are

$$\begin{aligned}
&\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'\\
&\quad=\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'\\
&\quad=\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'\\
&\quad=\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'\\
&\quad=\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'\\
&\quad=\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'\\
&\quad=\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 (3.12) is

$$-\sum_{n\in I}\sum_{n'\notin I}\frac{1}{\sigma_n^{(0)}}\left|\sum_m\int_{t_0}^t \langle n\ m|\left[\hat{H}_I(t'),\ \hat{\rho}_0\right]|n'\ m\rangle\ dt'\right|^2$$

$$=-\sum_{n\in I}\sum_{n'\notin I}\frac{1}{\sigma_n^{(0)}}\left|\sum_m\int_{t_0}^t \langle n\ m|\hat{H}_I(t')|n'\ m\rangle\ \left(\sigma_{n,m}^{(0)}-\cancel{\sigma_{n',m}^{(0)}}\right)\ dt'\right|^2\Bigg)$$

$$=-\sum_{n\in I}\sum_{n'\notin I}\frac{1}{\sum_{\tilde{m}}\sigma_{n,\tilde{m}}^{(0)}}\left|\sum_m\sigma_{n,m}^{(0)}\int_{t_0}^t \langle n\ m|\hat{H}_I(t')|n'\ m\rangle\ dt'\right|^2.$$

Putting this all back into (3.12), we obtain the rather interesting result that

$$\boxed{\begin{aligned}\Delta S=\frac{1}{\hbar^2}\left(\lambda^2\log\frac{1}{\lambda^2}\right)\sum_{n\in I}\sum_{n'\notin I}\Bigg(&\sum_m\sigma_{n,m}^{(0)}\sum_{m'}\left|\int_{t_0}^t\langle n\ m|\hat{H}_I(t')|n'\ m'\rangle\ dt'\right|^2\\ &-\frac{1}{\sum_{\tilde{m}}\sigma_{n,\tilde{m}}^{(0)}}\left|\sum_m\sigma_{n,m}^{(0)}\int_{t_0}^t\langle n\ m|\hat{H}_I(t')|n'\ m\rangle\ dt'\right|^2\Bigg)+\mathcal{O}(\lambda^2).\end{aligned}} \tag{3.15}$$

Entropy just depends on the transition amplitudes to states that started with zero initial probability.

In 3.15, the first term $\sum_{n\in I}\sum_{n'\notin I}\sum_m\sigma_{n,m}^{(0)}\sum_{m'}\left|\int_{t_0}^t\langle n\ m|\hat{H}_I(t')|n'\ m'\rangle\ dt'\right|^2$ can be interpreted as the total probability that a transition occurs to a state that had zero probability to start. The second term is harder to interpret; perhaps it is some kind of correction to account for double-counting.

We observe that 3.15 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).

I am not aware of any others having derived (3.15). I think it is a new result.

3.3.1 Upper and lower bounds for entropy growth

We can apply the triangle inequality to (3.15) to obtain an illuminating lower bound on ΔS for separable initial states. We have

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

Applying this to (3.15), we see at order $\lambda^2\log\frac{1}{\lambda^2}$ that

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

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

We can also obtain an upper bound for (3.15) by keeping only the first term. Then, at order $\lambda^2 \log \frac{1}{\lambda^2}$,

$$\begin{aligned} &\frac{1}{\hbar^2}\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n\in I} \sum_{n'\notin I} \sum_{m} \sigma^{(0)}_{n,m} \sum_{m'\neq m} \left| \int_{t_0}^{t} \langle n\ m| \hat{H}_I(t') \left|n'\ m'\right\rangle dt' \right|^2 \\ &\leq \Delta S \leq \frac{1}{\hbar^2}\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n\in I} \sum_{n'\notin I} \sum_{m} \sigma^{(0)}_{n,m} \sum_{m'} \left| \int_{t_0}^{t} \langle n\ m| \hat{H}_I(t') \left|n'\ m'\right\rangle dt' \right|^2 . \end{aligned} \tag{3.16}$$

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

From these expressions, it seems like entropy is proportional to the density of states that start with zero probability but can be transitioned to. If so, one might be able to estimate the rates of decoherence in different systems (e.g., different molecules) based on the density of accessible states.

3.4 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 (3.15) simplifies to

$$\Delta S = \frac{1}{\hbar^2}\left(\lambda^2 \log \frac{1}{\lambda^2}\right) \sum_{n'\neq n} \sum_{m'\neq m} \left| \int_{t_0}^{t} \langle n\ m| \hat{H}_I(t') \left|n'\ m'\right\rangle dt' \right|^2 + \mathcal{O}\big(\lambda^2\big). \tag{3.17}$$

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 $\mathcal{H}_B$.

Equation (3.17) replicates the result of Ref. [6], though we derived it by a different method.

Chapter 4

Examples

4.1 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

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

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

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

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

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

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

[To be continued...]

4.2 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.]

4.2.1 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

$$\left\langle x_1, x_2\right|\hat{V}(t)\left|\psi\right\rangle = \int_{x_1,x_2} d^3x_1\, d^3x_2\; V(x_1-x_2)\left\langle x_1, x_2|\psi\right\rangle. \tag{4.1}$$

(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

$$\langle x_1, x_2 | k_1, k_2\rangle = \frac{1}{(2\pi)^3}\, e^{ik_1\cdot x_1 + ik_2 \cdot x_2}. \tag{4.2}$$

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

$$\hat{U}(t_0, t)\,|k_1, k_2\rangle = e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}{k_1}^2 + \frac{1}{2m_2}{k_2}^2\right)}\,|k_1, k_2\rangle\,. \tag{4.3}$$

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

$$V(x_1 - x_2) = \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^3}\widetilde{V}(p)e^{ip\cdot(x_1 - x_2)}. \tag{4.4}$$

We now consider (2.2) 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 $\langle k_1', k_2'|$,

$$\begin{aligned}\left\langle k_1', k_2' | \Psi_I, \infty\right\rangle &= \left\langle k_1', k_2' | k_1, k_2\right\rangle - \frac{i}{\hbar}\int_{-\infty}^{\infty} \left\langle k_1', k_2'\right| \hat{H}_I(t)\,|k_1, k_2\rangle\; dt \\ &= \delta^3(k_1' - k_1)\delta^3(k_2' - k_2) - \frac{i}{\hbar}\int_{-\infty}^{\infty} \left\langle k_1', k_2'\right| \hat{H}_I(t)\,|k_1, k_2\rangle\; dt.\end{aligned} \tag{4.5}$$

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 (4.3):

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

We see that

$$\begin{aligned}
\langle k_1', k_2'|\, \hat{V}(t)\,|k_1, k_2\rangle &= \langle k_1', k_2'| \left\{ \int_{x_1,x_2} d^3x_1 d^3x_2 \ \ |x_1, x_2\rangle \langle x_1, x_2| \right\} \hat{V}(t)\,|k_1, k_2\rangle \\
&= \int_{x_1,x_2} d^3x_1 d^3x_2 \ \ \langle k_1', k_2'|x_1, x_2\rangle \langle x_1, x_2|\, \hat{V}(t)\,|k_1, k_2\rangle \\
&= \int_{x_1,x_2} \frac{d^3x_1 d^3x_2}{(2\pi)^6}\ e^{-ik_1'\cdot x_1 - ik_2'\cdot x_2} V(x_1 - x_2) e^{ik_1\cdot x_1 + ik_2\cdot x_2} && \text{(by (4.1) and (4.2))} \\
&= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \int_{x_1,x_2} d^3x_1 d^3x_2 \ \ e^{-ik_1'\cdot x_1 - ik_2'\cdot x_2}\, \widetilde{V}(p)\, e^{ip\cdot(x_1-x_2)} e^{ik_1\cdot x_1 + ik_2\cdot x_2} && \text{(by (4.4))} \\
&= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \widetilde{V}(p) \int_{x_1,x_2} d^3x_1 d^3x_2 \ \ e^{i(k_1 - k_1' + p)\cdot x_1} e^{i(k_2 - k_2' - p)\cdot x_2} \\
&= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \widetilde{V}(p)\,(2\pi)^6\, \delta^3(k_1 - k_1' + p)\, \delta^3(k_2 - k_2' - p) \\
&= \frac{1}{(2\pi)^3}\ \widetilde{V}(k_1' - k_1)\ \delta^3(k_1' - k_1 - k_2' + k_2).
\end{aligned}$$

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:

$$\int_{-\infty}^{\infty} dt\ \langle k_1', k_2'|\, \hat{H}_I(t)\,|k_1, k_2\rangle = \frac{\hbar}{(2\pi)^2}\ \widetilde{V}(k_1' - k_1)\, \delta\left(\tfrac{1}{2m_1}{k_1'}^2 + \tfrac{1}{2m_2}{k_2'}^2 - \tfrac{1}{2m_1}{k_1}^2 - \tfrac{1}{2m_2}{k_2}^2\right)\, \delta^3(k_1' - k_1 - k_2' + k_2). \tag{4.6}$$

Putting this into (4.5),

$$\begin{aligned}
\langle k_1', k_2'|\Psi_I, \infty\rangle = \ &\delta^3(k_1' - k_1)\ \delta^3(k_2' - k_2) \\
&- \frac{i}{(2\pi)^2}\ \widetilde{V}(k_1' - k_1)\ \delta^3(k_1' - k_1 - k_2' + k_2)\ \delta\left(\frac{{k_1'}^2}{2m_1} + \frac{{k_2'}^2}{2m_2} - \frac{{k_1}^2}{2m_1} - \frac{{k_2}^2}{2m_2}\right).
\end{aligned} \tag{4.7}$$

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

4.2.2 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

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

In the momentum basis the matrix elements are

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

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

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

Plugging in our result (4.6),

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

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

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

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,

$$\begin{aligned}
\left\langle k_1{}'\right|\hat{\rho}_{\text{reduced}}(\infty) \left|k_1\right\rangle = \Bigg(&\left\langle k_1'\right| \hat{\rho}_{\text{reduced}}(-\infty) \left|k_1\right\rangle\ + \\
&\int_{-\infty}^{\infty} \frac{d^3k_2\, d^3\widetilde{k}_2}{(2\pi)^2}\ \widetilde{V}\left(k_2 - \widetilde{k}_2\right)\ \left(P\left(k_1, k_1' k_2, \widetilde{k}_2\right) D\left(k_1, k_2, \widetilde{k}_2\right) + P^*\left(k_1', k_1, k_2, \widetilde{k}_2\right) D\left(k_1', k_2, \widetilde{k}_2\right)\right)\Bigg)
\end{aligned} \tag{4.8}$$

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 5

Conclusion

We have derived expressions for the change in Von Neumann entropy due to a perturbation, including two beautiful and new expressions (3.8) and (3.15). We have seen that the leading-order perturbative correction to entropy is non-negative if the density operator's eigenvalue corrections for states in the initial density operator's kernel are of similar or lower order as for states not in the kernel. In particular, entropy will not decrease if we start in a separable mixed state such that some component states have zero initial probability but can be transitioned into. In this case, the entropy growth is dependent on the transition amplitudes to these states. We also applied our formulae in two toy examples.

Future work could examine whether it is possible to use the density of accessible kernel states to predict the rate at which systems become entangled. In particular, a system's energy spectrum and selection rules might dictate the rate of decoherence.

In my analysis in Chapter 3, it is possible that the first order-probability corrections $\sigma_n^{(1)}$ vanish if and only if the initial state is separable. I have proven the "if" direction. The "only if" direction should also be proven or falsified by counterexample.

Future work should also investigate applications of entropy. For example, how useful is Von Neumann entropy for quantifying decoherence in quantum computing, and can the formulae derived here be used in such applications?

The approach here could also be replicated for other kinds of entropy, for example, N-Tsallis entropy. Ref. [3] shows that N-Tsallis entropy can decrease when one starts with separable states. We could ask: are these cases where N-Tsallis entropy decreases ones with lower-order corrections in the initial state space than in the zero-initial-probability space? If not, my results would show Von Neumann entropy to increase for the system, giving rise to an important difference between Von Neumann and N-Tsallis entropy.

Finally, physicists should continue to investigate how quantum entropy might give rise to thermodynamical properties. Perhaps one could derive all of thermodynamics starting with only the Schrödinger equation. Ref. [1] and [5] begin this work. It should be continued.

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