

Scattering Notes

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1 Time-dependent perturbation theory

Suppose we have a Hamiltonian of the form

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

where \hat{H}_0 is a well-understood Hamiltonian that does not depend on time and $\hat{V}(t)$ 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

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

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,

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

where we define the interaction Hamiltonian to be

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

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

We now integrate both sides of our expression.

$$\begin{aligned} \int_{t_0}^t \frac{\partial}{\partial t'} |\Psi_I, t'\rangle &= -\frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t') |\Psi_I, t'\rangle dt' \\ |\Psi_I, t\rangle - |\Psi_I, t_0\rangle &= -\frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t') |\Psi_I, t'\rangle dt' \\ |\Psi_I, t\rangle &= |\Psi_I, t_0\rangle - \frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t') |\Psi_I, t'\rangle dt' \end{aligned} \tag{1}$$

This is called the integral form of the Schrödinger equation.

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

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

Plugging this in for the state inside the integral in (1), we get the first order approximation

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

We can plug in again to get the second order approximation

$$|\Psi_I, t\rangle = |\Psi_I, t_0\rangle - \frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t') \left[|\Psi_I, t_0\rangle - \frac{i}{\hbar} \int_{t_0}^{t'} \hat{H}_I(t'') |\Psi_I, t_0\rangle dt'' \right] dt' + \mathcal{O}(\hat{H}_I(t)^3). \quad (3)$$

In general, we can keep going to achieve higher order approximations. For us, however, the first and second order approximations are enough.

2 Application to scattering

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

$$\langle x_1, x_2 | \hat{V}(t) | \psi \rangle = \int_{x_1, x_2} d^3x_1 d^3x_2 V(x_1 - x_2) \langle x_1, x_2 | \psi \rangle. \quad (4)$$

(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

$$\langle x_1, x_2 | k_1, k_2 \rangle = \frac{1}{(2\pi)^3} e^{ik_1 \cdot x_1 + ik_2 \cdot x_2}. \quad (5)$$

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

$$\hat{U}(t_0, t) |k_1, k_2\rangle = e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}k_1^2 + \frac{1}{2m_2}k_2^2\right)} |k_1, k_2\rangle. \quad (6)$$

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

$$V(x_1 - x_2) = \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^3} \tilde{V}(p) e^{ip \cdot (x_1 - x_2)}. \quad (7)$$

We now consider (2) and take the limits $t_0 \rightarrow -\infty$ and $t \rightarrow \infty$ 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 $\langle k'_1, k'_2|$,

$$\begin{aligned} \langle k'_1, k'_2 | \Psi_I, \infty \rangle &= \langle k'_1, k'_2 | k_1, k_2 \rangle - \frac{i}{\hbar} \int_{-\infty}^{\infty} \langle k'_1, k'_2 | \hat{H}_I(t) | k_1, k_2 \rangle dt \\ &= \delta^3(k'_1 - k_1) \delta^3(k'_2 - k_2) - \frac{i}{\hbar} \int_{-\infty}^{\infty} \langle k'_1, k'_2 | \hat{H}_I(t) | k_1, k_2 \rangle dt. \end{aligned} \quad (8)$$

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 (6):

$$\begin{aligned} \langle k'_1, k'_2 | \hat{H}_I(t) | k_1, k_2 \rangle &= \langle k'_1, k'_2 | \hat{U}(t_0, t)^\dagger \hat{V}(t) \hat{U}(t_0, t) | k_1, k_2 \rangle \\ &= \langle k'_1, k'_2 | e^{\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}k_1'^2 + \frac{1}{2m_2}k_2'^2\right)} \hat{V}(t) e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}k_1^2 + \frac{1}{2m_2}k_2^2\right)} | k_1, k_2 \rangle \\ &= e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}k_1'^2 + \frac{1}{2m_2}k_2'^2 - \frac{1}{2m_1}k_1^2 - \frac{1}{2m_2}k_2^2\right)} \langle k'_1, k'_2 | \hat{V}(t) | k_1, k_2 \rangle. \end{aligned}$$

We see that

$$\begin{aligned} \langle k'_1, k'_2 | \hat{V}(t) | k_1, k_2 \rangle &= \langle k'_1, k'_2 | \left\{ \int_{x_1, x_2} d^3x_1 d^3x_2 |x_1, x_2\rangle \langle x_1, x_2| \right\} \hat{V}(t) | k_1, k_2 \rangle \\ &= \int_{x_1, x_2} d^3x_1 d^3x_2 \langle k'_1, k'_2 | x_1, x_2 \rangle \langle x_1, x_2 | \hat{V}(t) | k_1, k_2 \rangle \\ &= \int_{x_1, x_2} \frac{d^3x_1 d^3x_2}{(2\pi)^6} e^{-ik'_1 \cdot x_1 - ik'_2 \cdot x_2} V(x_1 - x_2) e^{ik_1 \cdot x_1 + ik_2 \cdot x_2} \quad (\text{by (4) and (5)}) \\ &= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \int_{x_1, x_2} d^3x_1 d^3x_2 e^{-ik'_1 \cdot x_1 - ik'_2 \cdot x_2} \tilde{V}(p) e^{ip \cdot (x_1 - x_2)} e^{ik_1 \cdot x_1 + ik_2 \cdot x_2} \quad (\text{by (7)}) \\ &= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \tilde{V}(p) \int_{x_1, x_2} d^3x_1 d^3x_2 e^{i(k_1 - k'_1 + p) \cdot x_1} e^{i(k_2 - k'_2 - p) \cdot x_2} \\ &= \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi)^9} \tilde{V}(p) (2\pi)^6 \delta^3(k_1 - k'_1 + p) \delta^3(k_2 - k'_2 - p) \\ &= \frac{1}{(2\pi)^3} \tilde{V}(k'_1 - k_1) \delta^3(k'_1 - k_1 - k'_2 + k_2). \end{aligned}$$

so

$$\langle k'_1, k'_2 | \hat{H}_I(t) | k_1, k_2 \rangle = e^{-\frac{i}{\hbar}(t-t_0)\left(\frac{1}{2m_1}k_1'^2 + \frac{1}{2m_2}k_2'^2 - \frac{1}{2m_1}k_1^2 - \frac{1}{2m_2}k_2^2\right)} \frac{1}{(2\pi)^3} \tilde{V}(k'_1 - k_1) \delta^3(k'_1 - k_1 - k'_2 + k_2)$$

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

$$\int_{-\infty}^{\infty} dt \langle k'_1, k'_2 | \hat{H}_I(t) | k_1, k_2 \rangle = \frac{\hbar}{(2\pi)^2} \tilde{V}(k'_1 - k_1) \delta\left(\frac{1}{2m_1}k_1'^2 + \frac{1}{2m_2}k_2'^2 - \frac{1}{2m_1}k_1^2 - \frac{1}{2m_2}k_2^2\right) \delta^3(k'_1 - k_1 - k'_2 + k_2). \quad (9)$$

Putting this into (8),

$$\begin{aligned} \langle k'_1, k'_2 | \Psi_I, \infty \rangle &= \delta^3(k'_1 - k_1) \delta^3(k'_2 - k_2) \\ &\quad - \frac{i}{(2\pi)^2} \tilde{V}(k'_1 - k_1) \delta^3(k'_1 - k_1 - k'_2 + k_2) \delta\left(\frac{k_1'^2}{2m_1} + \frac{k_2'^2}{2m_2} - \frac{k_1^2}{2m_1} - \frac{k_2^2}{2m_2}\right). \quad (10) \end{aligned}$$

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

3 Mixed states and the density operator

We now consider the same problem but where we allow for mixed states. We will need to describe the system by the density operator $\hat{\rho}(t)$. First, let us derive the time evolution of $\hat{\rho}(t)$ in first order perturbation theory.

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

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

At time t states will have evolved according to (3), so

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

where

$$|\Psi_I, t\rangle = |\Psi_I, t_0\rangle - \frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t') \left[|\Psi_I, t_0\rangle - \frac{i}{\hbar} \int_{t_0}^{t'} \hat{H}_I(t'') |\Psi_I, t_0\rangle dt'' \right] dt' + \mathcal{O}(\hat{H}_I(t)^3).$$

Then

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

so

$$\hat{\rho}(t) = \hat{\rho}(t_0) - \frac{i}{\hbar} \int_{t_0}^t \left[\hat{H}_I(t'), \hat{\rho}(t_0) \right] dt' + \mathcal{O}(\hat{H}_I(t)^2). \quad (11)$$

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

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

In the momentum basis the matrix elements are

$$\langle k'_1 | \hat{\rho}_{\text{reduced}}(t) | k_1 \rangle = \langle k'_1 | \hat{\rho}_{\text{reduced}}(t_0) | k_1 \rangle - \frac{i}{\hbar} \int_{t_0}^t dt' \int_{-\infty}^{\infty} d^3 k_2 \langle k'_1, k_2 | \left[\hat{H}_I(t'), \hat{\rho}(t_0) \right] | k_1, k_2 \rangle + \mathcal{O}(\hat{H}_I(t)^2).$$

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

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

Plugging in our result (9),

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

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

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

where

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

Then, assuming \tilde{V} is an even function,

$$\begin{aligned}
\langle k_1' | \hat{\rho}_{\text{reduced}}(\infty) | k_1 \rangle &= \left(\langle k_1' | \hat{\rho}_{\text{reduced}}(-\infty) | k_1 \rangle + \right. \\
&\quad \left. \int_{-\infty}^{\infty} \frac{d^3 k_2 d^3 \tilde{k}_2}{(2\pi)^2} \tilde{V}(k_2 - \tilde{k}_2) \left(P(k_1, k_1', k_2, \tilde{k}_2) D(k_1, k_2, \tilde{k}_2) + P^*(k_1', k_1, k_2, \tilde{k}_2) D(k_1', k_2, \tilde{k}_2) \right) \right)
\end{aligned} \tag{12}$$

where

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

4 Entropy analysis through perturbation theory

Consider a Hermitian operator \hat{A}_0 with an eigenstate $|\psi_0\rangle$ that has an eigenvalue τ_0 . Consider another operator $\hat{A} = \hat{A}_0 + \lambda \hat{A}_1 + \mathcal{O}(\lambda^2)$ with an eigenstate $|\psi\rangle = |\psi_0\rangle + \lambda |\psi_1\rangle + \mathcal{O}(\lambda^2)$ that has an eigenvalue $\tau = \tau_0 + \lambda \tau_1 + \mathcal{O}(\lambda^2)$. We have

$$\begin{aligned}
(\hat{A}_0 + \lambda \hat{A}_1) (|\psi_0\rangle + \lambda |\psi_1\rangle) &= (\tau_0 + \lambda \tau_1) (|\psi_0\rangle + \lambda |\psi_1\rangle) + \mathcal{O}(\lambda^2) \\
\hat{A}_0 |\psi_1\rangle + \hat{A}_1 |\psi_0\rangle &= \tau_0 |\psi_1\rangle + \tau_1 |\psi_0\rangle + \mathcal{O}(\lambda) \\
\langle \psi_0 | \hat{A}_0 | \psi_1 \rangle + \langle \psi_0 | \hat{A}_1 | \psi_0 \rangle &= \tau_0 \langle \psi_0 | \psi_1 \rangle + \tau_1 \langle \psi_0 | \psi_0 \rangle + \mathcal{O}(\lambda) \\
\tau_0 \langle \psi_0 | \psi_1 \rangle + \langle \psi_0 | \hat{A}_1 | \psi_0 \rangle &= \tau_0 \langle \psi_0 | \psi_1 \rangle + \tau_1 + \mathcal{O}(\lambda) \\
\tau_1 &= \langle \psi_0 | \hat{A}_1 | \psi_0 \rangle + \mathcal{O}(\lambda) \\
\tau_1 &= \langle \psi_0 | \hat{A}_1 | \psi_0 \rangle
\end{aligned}$$

(since we take τ_1 not to depend on λ).

We will apply this result with $\hat{A} = \hat{\rho}_{\text{reduced}}(t)$ and $\hat{A}_0 = \hat{\rho}_{\text{reduced}}(t_0)$. In general, we can write $\hat{\rho}_{\text{reduced}}(t_0)$ in the form

$$\hat{\rho}_{\text{reduced}}(t_0) = \sum_i P_i |\psi_i\rangle \langle \psi_i|.$$

for some $|\psi_i\rangle$ and P_i such that $\sum_i P_i = 1$. It is clear that the eigenstates of $\hat{\rho}_{\text{reduced}}(t_0)$ are then the states $|\psi_i\rangle$; these have eigenvalues P_i . Take $\tilde{V}(p) = \lambda V^*(p)$. Then we can read off the first order corrections for $\hat{\rho}$ from (12).

4(a) Pure initial state

We will first consider the case where the initial state is pure, that is,

$$\hat{\rho}_{\text{reduced}}(t_0) = |\psi_0\rangle \langle \psi_0|$$

for some $|\psi_0\rangle$. Then exactly one eigenvalue is non-zero; it is associated with the non-degenerate eigenstate $|\psi_0\rangle$.

Let $\{\epsilon_i\}$ be the eigenvalues of $\hat{\rho}_{\text{reduced}}(t)$ and choose them so that $\epsilon_1 \approx 1$ and $\epsilon_i \approx 0$ for $i \geq 2$.

The von Neumann entropy is

$$\begin{aligned} S &= -\text{tr}(\hat{\rho}(t) \ln \hat{\rho}(t)) \\ &= -\sum_{i=1}^{\infty} \epsilon_i \ln \epsilon_i \\ &= -\epsilon_1 \ln \epsilon_1 - \sum_{i=2}^{\infty} \epsilon_i \ln \epsilon_i. \end{aligned}$$

Now, $x \ln x \approx x$ if $x \approx 0$, so

$$S \approx -\epsilon_1 \ln \epsilon_1 - \sum_{i=2}^{\infty} \epsilon_i.$$

Also $\epsilon_1 = 1 - \sum_{i=2}^{\infty} \epsilon_i$ so

$$S \approx -\epsilon_1 \ln \epsilon_1 + \epsilon_1 - 1.$$

In particular,