PC4230

Quantum Mechanics III

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1 Introduction

Quantum mechanics is bizarre in the way that we have developed a very sophisticated mathematical framework to describe our world, but when faced with the question of "why does it work?" we have no answer. One example is with the single slit experiment. We know that if we direct a beam of electrons towards the slit we get a diffraction pattern on the screen. However, what is surprising is when we send only a single electron. Why does it land at a particular position of the screen and not another? There seems to be no good answer. Indeed, quantum mechanics does not give us any insight into singular events. We only know about the statistics of repeated events.

The interpretation we adopt is as such

- Quantum systems generally do not possess definite properties.
- States only describe the "potential" of yielding some result after observation.
- Observation collapses the state and creates a result with some probability.
- The probability of observing the system in some eigenstate is given by the Born rule: $P_n = |\langle\Psi|\phi_n\rangle|^2$.

This is also to say that the state does not have any notion about a distribution of position or momentum before any measurement. It is only after measurement that the state has a definite position (with some probability).

A quick review of quantum evolution in Hilbert space. We start with Schrödinger's equation:

$$i\hbar\frac{\partial\left|\Psi\right\rangle}{\partial t} = \hat{H}\left|\Psi\right\rangle$$

Inserting the completeness condition, we have

$$i\hbar\sum_m \left|\psi_m\right\rangle \frac{\partial\left\langle\psi_m|\Psi\right\rangle}{\partial t} = \sum_{m,n}\left|\psi_m\right\rangle\ \left\langle\psi_m|\hat{H}|\psi_n\right\rangle\left\langle\psi_n|\Psi\right\rangle$$

For expansion coefficient m we have the first order equation

$$i\hbar\frac{\partial C_m}{\partial t} = \sum_n \left\langle\psi_m|\hat{H}|\psi_n\right\rangle C_n$$

where $C_n = \langle \psi_n | \Psi \rangle$. The formal solution takes the form of

$$|\Psi(t)\rangle = \exp\left[-\frac{i\hat{H}(t-t_0)}{h}\right]|\Psi(t_0)\rangle \equiv \hat{U}\,|\Psi(t_0)\rangle\,.$$

Here, U is an unitary operator, i.e. $U^\dagger = (U^T)^* = U^{-1}$.

2 Time independent perturbation theory

2.1 Non-degenerate case

Suppose we have a completely solvable Hamiltonian $\hat{H}^0$ in terms of eigenkets $|\psi_n^0\rangle$ and eigenenergies E_n^0. Can we say something about a more general system that has $\hat{H}^0$ as an ideal starting point, and with some perturbation $\lambda\hat{V}$?

Let $\hat{H} = \hat{H}^0 + \lambda\hat{V}$. We will try to express the unknown solution of $\hat{H}$ in terms of the known solution of $\hat{H}^0$. Assume

$$\hat{H}\,|\Psi_n\rangle = (\hat{H}^0 + \lambda\hat{V})\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle\,.$$

As $\lambda \to 0$, we have the known solution:

$$\hat{H}^0\,\big|\psi_n^0\big\rangle = E_n^0\,\big|\psi_n^0\big\rangle\,.$$

The standard trick here is to make a power series expansion of the unknown solution in terms of the perturbation strength λ.

$$\begin{aligned}|\Psi_n\rangle &= \big|\psi_n^0\big\rangle + \lambda\,\big|\psi_n^1\big\rangle + \lambda^2\,\big|\psi_n^2\big\rangle + \cdots \\ E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots\,.\end{aligned}$$

Note a fundamental assumption here is that the states $|\Psi_n\rangle$ exist in the same Hilbert space as the Hamiltonian $\hat{H}^0$. We can also assume that all correction terms are orthogonal to the unperturbed state $|\phi_n^0\rangle$. If some states have components that are not orthogonal to $|\phi_n^0\rangle$, we can simply add them into $|\phi_n^0\rangle$ and re-normalize it. In any case, after plugging in we get:

$$\begin{gathered}\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle \\ (\hat{H}^0 + \lambda\hat{V})\big(\big|\psi_n^0\big\rangle + \lambda\,\big|\psi_n^1\big\rangle + \lambda^2\,\big|\psi_n^2\big\rangle\big) = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2)\big(\big|\psi_n^0\big\rangle + \lambda\,\big|\psi_n^1\big\rangle + \lambda^2\,\big|\psi_n^2\big\rangle\big).\end{gathered}$$

Comparing the different coefficients of λ,

$$\begin{aligned}\hat{H}^0\,\big|\psi_n^0\big\rangle &= E_n^0\,\big|\psi_n^0\big\rangle && (\lambda^0) \\ \hat{H}^0\,\big|\psi_n^1\big\rangle + \hat{V}\,\big|\psi_n^0\big\rangle &= E_n^0\,\big|\psi_n^1\big\rangle + E_n^1\,\big|\psi_n^0\big\rangle && (\lambda^1) \\ \hat{H}^0\,\big|\psi_n^2\big\rangle + \hat{V}\,\big|\psi_n^1\big\rangle &= E_n^0\,\big|\psi_n^2\big\rangle + E_n^1\,\big|\psi_n^1\big\rangle + E_n^2\,\big|\psi_n^0\big\rangle && (\lambda^2).\end{aligned}$$

2.1.1 First order corrections

We break down each of these equations into components of the eigenstates $|\psi_n^0\rangle$ as our basis. We do this by projecting them onto each of the eigenstates. For the first order equation:

$$\langle\psi_m^0|\hat{H}^0|\psi_n^1\rangle + \langle\psi_m^0|\hat{V}|\psi_n^0\rangle = E_n^0\langle\psi_m^0|\psi_n^1\rangle + E_n^1\langle\psi_m^0|\psi_n^0\rangle.$$

Since $\hat{H}^0$ is Hermitian, for $m \neq n$ this gives us

$$\hat{V}_{mn} = \langle\psi_m^0|\hat{V}|\psi_n^0\rangle = (E_n^0 - E_m^0)\langle\psi_m^0|\psi_n^1\rangle.$$

Using the completeness relation, we can find the first order correction to the eigenstate:

$$\begin{aligned}|\psi_n^1\rangle &= \sum_m |\psi_m^0\rangle\langle\psi_m^0|\,|\psi_n^1\rangle \\ &= \sum_{m\neq n} \frac{\hat{V}_{mn}}{(E_n^0 - E_m^0)}|\psi_m^0\rangle.\end{aligned}$$

The $m = n$ state in the summation vanishes due to orthogonality, which we assumed by construction, i.e. $\langle\psi_n^0|\psi_n^1\rangle = 0$.

For $m = n$, the projection

$$\langle\psi_n^0|\hat{V}|\psi_n^0\rangle = E_n^1$$

gives the first order correction to the eigenvalue.

2.1.2 Second order corrections

The approach is identical. First we project onto the basis states:

$$\langle\psi_m^0|\hat{H}^0|\psi_n^2\rangle + \langle\psi_m^0|\hat{V}|\psi_n^1\rangle = E_n^0\langle\psi_m^0|\psi_n^2\rangle + E_n^1\langle\psi_m^0|\psi_n^1\rangle + E_n^2\langle\psi_m^0|\psi_n^0\rangle.$$

For $m \neq n$ we get

$$(E_m^0 - E_n^0)\langle\psi_m^0|\psi_n^2\rangle + \langle\psi_m^0|\hat{V}\left(\sum_{k\neq n}\frac{\hat{V}_{kn}}{E_n^0 - E_k^0}|\psi_k^0\rangle\right) = E_n^1\langle\psi_m^0|\left(\sum_{k\neq n}\frac{\hat{V}_{kn}}{E_n^0 - E_k^0}|\psi_k^0\rangle\right)$$

$$(E_m^0 - E_n^0)\langle\psi_m^0|\psi_n^2\rangle + \sum_{k\neq n}\frac{\hat{V}_{mk}\hat{V}_{kn}}{E_n^0 - E_k^0} = \hat{V}_{nn}\frac{V_{mn}}{E_n^0 - E_m^0}$$

Insert the completeness relation to obtain

$$\begin{aligned}|\psi_n^2\rangle &= \sum_m |\psi_m^0\rangle\langle\psi_m^0|\,|\psi_n^2\rangle \\ &= \sum_m\sum_{k\neq n}|\psi_m^0\rangle\frac{\hat{V}_{mk}\hat{V}_{kn}}{(E_n^0 - E_k^0)(E_m^0 - E_n^0)} - \sum_m|\psi_m^0\rangle\frac{\hat{V}_{nn}\hat{V}_{mn}}{(E_n^0 - E_m^0)^2}.\end{aligned}$$

Actually we are not done yet. For the first order case we have conveniently ignored normalisation because the state is already normalised to the first order:

$$\begin{aligned}\langle\Psi_n|\Psi_n\rangle &= (\langle\psi_n^0| + \lambda\langle\psi_n^1|)(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle) \\ &= 1 + \lambda^2\langle\psi_n^1|\psi_n^1\rangle\end{aligned}$$

However since we are talking about corrections to the second order now, it is no longer normalised:

$$\begin{aligned}\langle\Psi_n|\Psi_n\rangle &= \left(\langle\psi_n^0| + \lambda\langle\psi_n^1| + \lambda^2\langle\psi_n^2|\right)\left(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + |\psi_n^2\rangle\right) \\ &= 1 + \lambda^2\langle\psi_n^1|\psi_n^1\rangle\end{aligned}$$

We have to multiply throughout by a factor of $1/\sqrt{1+\lambda^2\langle\psi_n^1|\psi_n^1\rangle}$, or by truncating up to the second order,

$$|\Psi_n\rangle = \left(1 - \frac{\lambda^2}{2}\langle\psi_n^1|\psi_n^1\rangle\right)\left(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle\right)$$

We skip the substitution since it gets quite tedious.

The correction to the eigenenergy is given by the case of $m = n$:

$$\begin{aligned}E_n^2 &= \langle\psi_m^0|\hat{V}|\psi_n^1\rangle \\ &= \sum_{m\neq n}\langle\psi_n^0|\hat{V}\left(\frac{\hat{V}_{mn}}{E_n^0 - E_m^0}|\psi_m^0\rangle\right) \\ &= \sum_{m\neq n}\frac{V_{mn}^2}{E_n^0 - E_m^0}.\end{aligned}$$

Thus overall up to the second order we have

$$E_n = E_n^0 + \lambda V_{mn} + \lambda^2\sum_{m\neq n}\frac{V_{mn}^2}{E_n^0 - E_m^0}$$

We can see that the curvature $\frac{\partial^2 E_n}{\partial\lambda^2}$ is proportional to λ.

2.1.3 Example: Square well

Recall the exact solution to a particle trapped in an infinite square well with length L:

$$\begin{aligned}|\phi_n^0\rangle &= \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \\ E_n^0 &= \frac{\hbar^2\pi^2 n^2}{2mL^2}\end{aligned}$$

Consider a perturbation that extends the width of the well by some length $\mathrm{d}L$. Is this solvable with perturbation theory? The answer is no, since the two spaces live in different Hilbert spaces. The original exact solution exists in a Hilbert space spanned by states defined by states vanishing at $x = 0$ and $x = L$. The new perturbed state will live in a Hilbert space that is spanned by states vanishing at $x = 0$ and $x = L + \mathrm{d}L$. Therefore there is no way that we are able to make corrections to the original state using our original eigenbasis that can create a new state that satisfies the new boundary conditions. The same goes for a perturbation where we make the well narrower by $\mathrm{d}L$.

Let us consider another problem where we have two non-interacting particles (bosons) in the square well. This is a perturbation of

$$\hat{V} = -aV_0\delta(x_1 - x_2).$$

The ground state is just the product of the states of both particles:

$$\psi_1^0 = \frac{2}{L}\sin\frac{\pi x_1}{L}\sin\frac{\pi x_2}{L}$$

The first order correction is given by

$$\begin{aligned}
E_1^1 &= \left\langle \psi_1^0 \middle| \hat{V} \middle| \psi_1^0 \right\rangle \\
&= -aV_0\frac{4}{a^2}\int_0^L\int_0^L \sin^2\frac{\pi x_1}{L}\sin^2\frac{\pi x_2}{L}\delta(x_1-x_2)\mathrm{d}x_1\mathrm{d}x_2 \\
&= -\frac{4V_0}{a}\int_a^L \sin^4\frac{\pi x}{L}\mathrm{d}x \\
&= -\frac{3}{2}V_0
\end{aligned}$$

2.2 Degenerate case

Our earlier results were based on an assumption of non-degeneracy. Firstly, the first order correction term

$$\left|\psi_n^1\right\rangle = \sum_{m\neq n}\frac{V_{mn}}{E_n^0 - E_m^0}\left|\psi_m^0\right\rangle$$

will blow up due to the denominator. Secondly, any linear combination of degenerate eigenstates remain as an eigenstate of the same eigenvalue. Thus we do not know to which eigenstate the unperturbed state tends to as $\lambda \to 0$.

We will need to consider this case separately. Let the correct state that we approach as $\lambda \to 0$ be $|\psi_n^0\rangle$. More generally, we can write it in terms of all the degenerate states $\left|\tilde{\psi}_{n,d}\right\rangle$:

$$\left|\psi_n^0\right\rangle = \sum_d C_{n,d}\left|\tilde{\psi}_{n,d}^0\right\rangle$$

Returning to a previous result,

$$\hat{H}^0\left|\psi_n^1\right\rangle + \hat{V}\left|\psi_n^0\right\rangle = E_n^0\left|\psi_n^1\right\rangle + E_n^1\left|\psi_n^0\right\rangle.$$

Projecting onto any $\left\langle\tilde{\psi}_{n,d}^n\right|$, we get

$$\hat{V}\left|\psi_n^0\right\rangle = E_n^1\left|\psi_n^0\right\rangle$$

that holds within this degenerate subspace (previously there was no restriction on what we can project it on). So, this tells us that the eigenstates and eigenvalues of $\hat{V}$ are the correct first order corrections. Continuing to work in this degenerate subspace, we simply have to solve a few relations between matrix elements:

$$\begin{aligned}
\left\langle\tilde{\psi}_{n,d'}^0\right|\hat{V}\sum_d C_{n,d}\left|\tilde{\psi}_{n,d}^0\right\rangle &= \left\langle\tilde{\psi}_{n,d'}^0\right| E_n^1\sum_d C_{n,d}\left|\tilde{\psi}_{n,d}^0\right\rangle \\
\sum_d C_{n,d}\left\langle\tilde{\psi}_{n,d'}^0\right|\hat{V}\left|\tilde{\psi}_{n,d}^0\right\rangle &= E_n^1\sum_d C_{n,d}\left\langle\tilde{\psi}_{n,d'}^0\middle|\tilde{\psi}_{n,d}^0\right\rangle
\end{aligned}$$

Consider just a two-fold degeneracy. Let the degenerate subspace be spanned by $|\psi_a^0\rangle$ and $|\psi_b^0\rangle$. Solving for the eigenvalue:

$$\begin{pmatrix} V_{aa} & V_{ab} \\ V_{ba} & V_{bb} \end{pmatrix} \begin{pmatrix} C_a \\ C_b \end{pmatrix} = E^1 \begin{pmatrix} C_a \\ C_b \end{pmatrix}$$

$$\begin{vmatrix} V_{aa} - E^1 & V_{ab} \\ V_{ba} & V_{bb} - E^1 \end{vmatrix} = 0$$

$$\frac{1}{2}\left[V_{aa} + V_{bb} \pm \sqrt{(V_{aa} + V_{bb})^2 + 4|V_{ab}|^2}\right] = E^1$$

Physically, this describes a splitting effect in the eigenenergies.

It is also possible to choose a diagonal basis for the degenerate subspace. In this case, the first order correction will then be given by the diagonal matrix elements. Then the formula will be identical with the non-degenerate case.

Here is a useful theorem. If we find a Hermitian operator $\hat{P}$ that commutes with both the unperturbed Hamiltonian and the perturbations

$$[\hat{P}, \hat{H}^0] = 0 \qquad\qquad [\hat{P}, \hat{V}] = 0,$$

the eigenstates of $\hat{H}^0$ are also eigenstates of $\hat{P}$. If the degenerate states $\left|\tilde{\psi}_a^0\right\rangle$ and $\left|\tilde{\psi}_b^0\right\rangle$ are eigenstates of $\hat{P}$ with different eigenvalues, then $\hat{V}$ will be a diagonal matrix in this eigenbasis. Qualitatively this makes sense as $\hat{V}$ should preserve the symmetry of $\hat{P}$ since they commute. The proof is simple:

$$\left\langle \tilde{\psi}_a^0 \right| \hat{P}\hat{V} \left| \tilde{\psi}_b^0 \right\rangle = \left\langle \tilde{\psi}_a^0 \right| \hat{V}\hat{P} \left| \tilde{\psi}_b^0 \right\rangle$$

$$P_a \left\langle \tilde{\psi}_a^0 \right| \hat{V} \left| \tilde{\psi}_b^0 \right\rangle = P_b \left\langle \tilde{\psi}_a^0 \right| \hat{V} \left| \tilde{\psi}_b^0 \right\rangle$$

where P_a and P_b are the eigenvalues of $\left|\tilde{\psi}_a^0\right\rangle$ and $\left|\tilde{\psi}_b^0\right\rangle$ respectively. Since $P_a \neq P_b$ by assumption, we have $\hat{V}_{ab} = 0$.

2.2.1 Example: Particle on circle

Consider a particle of mass m moving on a ring of radius r. We can describe its position using angle φ. The Hamiltonian is given by

$$\begin{aligned} \hat{H}^0 &= \frac{\hbar^2}{2I}\hat{L}_z^2 \\ &= -\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\varphi^2} \end{aligned}$$

The eigenvector is given by a plane wave $\left\langle \varphi \middle| \tilde{\psi}_n^0 \right\rangle = \frac{1}{\sqrt{2\pi}} e^{in\varphi}$ with eigenvalue $E_n^0 = \frac{n^2\hbar^2}{2mr^2}$. There is two fold degeneracy in this system because you can rotate clockwise and counter-clockwise corresponding to $\pm n$ states.

Now consider a perturbation $\hat{V} = \epsilon f(\varphi)$ with $f(\varphi) = f(-\varphi)$. We can solve this manually, or we can notice that both the Hamiltonian and the perturbation preserves the parity symmetry. In other words they commute with the parity operator. Let us choose

$$\left|\psi^0_{\pm n}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\tilde{\psi}^0_n\right\rangle \pm \left|\tilde{\psi}^0_{-n}\right\rangle\right)$$

as the basis states of the degenerate subspace. Then the eigenstates

$$\left\langle\varphi\middle|\tilde{\psi}^0_{n+}\right\rangle = \sqrt{\frac{1}{\pi}}\cos(n\varphi) \qquad\qquad \left\langle\varphi\middle|\tilde{\psi}^0_{n-}\right\rangle = \sqrt{\frac{1}{\pi}}\sin(n\varphi)$$

are also eigenstates of the parity operator, with eigenvalues ± 1. Therefore, in this new basis the perturbation matrix is diagonal. The first order energy correction can thus be evaluated in the same way as for the non-degenerate case:

$$\begin{aligned}
E^1_{n+} &= \left\langle\tilde{\psi}^0_{n+}\middle|\hat{V}\middle|\tilde{\psi}^0_{n+}\right\rangle \\
&= \frac{\epsilon}{\pi}\int_{-\pi}^{\pi}\cos^2(n\varphi)f(\varphi)\mathrm{d}\varphi \\
E^1_{n-} &= \left\langle\tilde{\psi}^0_{n-}\middle|\hat{V}\middle|\tilde{\psi}^0_{n-}\right\rangle \\
&= -\frac{\epsilon}{\pi}\int_{-\pi}^{\pi}\sin^2(n\varphi)f(\varphi)\mathrm{d}\varphi
\end{aligned}$$

2.2.2 Example: Fine structure relativistic correction

Consider a hydrogen atom with Hamiltonian

$$\hat{H}^0 = \frac{P^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r}$$

n	l	m	degeneracy
1	0	0	1
2	0	0	4
	1	$0, \pm 1$	
3	0	0	9
	1	$0, \pm 1$	
	2	$0, \pm 1, \pm 2$	

The degeneracy goes as n^2. For large n it becomes quickly impossible to solve the perturbation with brute force. Consider the relativistic correction as a perturbation given by

$$\hat{V} = -\frac{\hat{P}^4}{8m_e^3c^2}.$$

Notice how we can rewrite the perturbation as

$$\hat{V} = -\frac{1}{c^2}\left[\hat{H}^0 + \frac{e^2}{4\pi\epsilon_0 r}\right]^2$$

The unperturbed Hamiltonian possesses rotational symmetry. In fact, the degeneracy originates from this rotational symmetry. From the rewriting, we can see that $\hat{V}$ is also rotationally symmetric. So they both commute with $\hat{L}^2$ (and also L_z). Thus, the first order correction is just given by the expected value of the perturbation on the radial eigenvalues:

$$\begin{aligned} E^1_{n,l,m} &\propto \left\langle \tilde{\psi}^0_{n,l,m} \middle| \hat{P}^4 \middle| \tilde{\psi}^0_{n,l,m} \right\rangle \\ &\propto \left\langle \tilde{\psi}^0_{n,l,m} \middle| (\hat{H}_0 - V_{\text{coulumb}})^2 \middle| \tilde{\psi}^0_{n,l,m} \right\rangle \\ &\propto \left[(E^0_{n,l,m})^2 + 2kE^0_{n,l,m} \left\langle \frac{1}{r} \right\rangle + k^2 \left\langle \frac{1}{r^2} \right\rangle \right] \\ &= -\frac{(E^0_{n,l,m})^2}{2m_e c^2} \left[\frac{4n}{l+1/2} - 3 \right] \end{aligned}$$

where $k = e^2/4\pi\epsilon_0$. Expectation values are evaluated on the unperturbed hydrogen wavefunctions, and are just integrals. So we have simplified a problem with a high degeneracy. This also illustrates the power of symmetry.

3 Discrete variable representation

In preparation for developing a computational approach to solving problems in quantum physics, we will develop a system for discretising continuous variables. We will first focus on time-independent 1D problems.

We discretise the space coordinates by first confining ourselves to a region of interest. This region is chosen with the assumption that the states essentially vanish at the boundaries. Then we simply divide this region into N intervals with width Δx. The width is chosen so that the maximum momentum of interest would be around $\hbar/\Delta x$ (obtained from the de Broglie wavelength). This gives us $N-1$ non-trivial points, which also sets a limit on the dimension of our Hilbert space.

For each cell centred around the i-th point with position x_i, we define the discretised position eigenstate

$$|i\rangle \to \frac{1}{\sqrt{\Delta x}} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} |x\rangle \, \mathrm{d}x.$$

It is a equally weighted uniform distribution of all states in the cell. They are orthogonal and normalisable:

$$\begin{aligned} \langle i|j\rangle &= \frac{1}{\Delta x} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} \langle x| \int_{x_j - \Delta x/2}^{x_j + \Delta x/2} |x'\rangle \, \mathrm{d}x \mathrm{d}x' \\ &= \frac{1}{\Delta x} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} \int_{x_j - \Delta x/2}^{x_j + \Delta x/2} \delta(x - x') \mathrm{d}x \mathrm{d}x' \\ &= \delta_{ij} \end{aligned}$$

Recall that the Hamiltonian is given by $\hat{H} = \hat{T} + \hat{V}$. We show that $\hat{V}$ is still diagonal in this basis. Assuming that the wavefunction is fairly smooth within each cells, we can perform a

mid-point approximation on some of the integrals without too much error.

$$\begin{aligned}
\langle i|V|j\rangle &= \frac{1}{\Delta x}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2}\int_{x_j-\Delta x/2}^{x_j+\Delta x/2}\langle x|V|x'\rangle\,\mathrm{d}x\mathrm{d}x' \\
&= \frac{1}{\Delta x}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2}\int_{x_j-\Delta x/2}^{x_j+\Delta x/2}V(x)\,\langle x|x'\rangle\,\mathrm{d}x\mathrm{d}x' \\
&= \frac{1}{\Delta x}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2}V(x)\int_{x_j-\Delta x/2}^{x_j+\Delta x/2}\delta(x-x')\mathrm{d}x\mathrm{d}x' \\
&\approx V(x_i)\delta_{ij}
\end{aligned}$$

Note that we can use the same method to solve for perturbations. For example

$$\begin{aligned}
\left\langle\psi_n^0\middle|V_p\middle|\psi_m^0\right\rangle &= \sum_{i,j}\left\langle\psi_n^0\middle|i\right\rangle\,\langle i|V_p|j\rangle\,\left\langle j\middle|\psi_m^0\right\rangle \\
&= \sum_{i,j}\left\langle\psi_n^0\middle|i\right\rangle V_{p(x_i)}\delta_{ij}\left\langle j\middle|\psi_m^0\right\rangle \\
&= \sum_{i}\left|\left\langle i\middle|\psi_n^0\right\rangle\right|^2 V_p(x_i)
\end{aligned}$$

However we could have also just included the perturbation directly into V.

Next consider the kinetic energy matrix $\hat{T}$. Similarly, we can do some mid-point approximations on the integrals.

$$\begin{aligned}
\langle i|T|x'\rangle &= \frac{1}{\Delta x}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2}\int_{x_j-\Delta x/2}^{x_j+\Delta x/2}\langle x|T|x'\rangle\,\mathrm{d}x\mathrm{d}x' \\
&= \frac{1}{\Delta x}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2}\int_{x_j-\Delta x/2}^{x_j+\Delta x/2}\langle x|T|x'\rangle\,\mathrm{d}x\mathrm{d}x' \\
&\approx \frac{1}{\Delta x}\,\langle x_i|T|x_j\rangle\int_{x_i-\Delta x/2}^{x_i+\Delta x/2}\int_{x_j-\Delta x/2}^{x_j+\Delta x/2}\mathrm{d}x\mathrm{d}x' \\
&= \Delta x\,\langle x_i|T|x_j\rangle\,.
\end{aligned}$$

Our wavefunction under consideration vanishes at the endpoints. Hence we are able to use the solutions for a particle in a infinite square well as basis states.

$$\langle x|\phi_n\rangle = \sqrt{\frac{2}{L}}\sin\frac{n\pi(x-a)}{L}$$

They must also be eigenstates of $\hat{T}$.

$$\hat{T}\,|\phi_n\rangle = \frac{n^2\hbar^2\pi^2}{2mL^2}\,|\phi_n\rangle$$

We can now put in the completeness condition

$$\begin{aligned}
\langle x_i|\hat{T}|x_j\rangle &= \sum_{\substack{n=1\\n'=1}}^{N-1}\langle x_i|\phi_n\rangle\,\langle\phi_n|\hat{T}|\phi_{n'}\rangle\,\langle\phi_{n'}|x_j\rangle \\
&= \sum_{\substack{n=1\\n'=1}}^{N-1}\sqrt{\frac{2}{L}}\sin\frac{n\pi(x_i-a)}{L}\,\frac{n^2\hbar^2\pi^2}{2mL^2}\,\langle\phi_n|\phi_{n'}\rangle\,\sqrt{\frac{2}{L}}\sin\frac{n\pi(x_j-a)}{L} \\
&= \sum_{n=1}^{N-1}\frac{2}{L}\frac{n^2\hbar^2\pi^2}{2mL^2}\sin\frac{n\pi(x_i-a)}{L}\sin\frac{n\pi(x_j-a)}{L}.
\end{aligned}$$

Notice how we sum only up to the resolution limit $N-1$. This should be a infinite sum, but we can truncate it early because we will not have the resolution to capture the structure given by any higher order terms.

3.1 Reduced units

It will help in both simplifying our calculation and also reducing floating point errors if we use reduced units. It would be bad if we were multiplying something as small as $\hbar$ everywhere.

This involves making position and momentum dimensionless. Consider the following scaling

$$\hat{x} = \bar{x}\sqrt{\frac{\hbar}{m\omega}} \qquad\qquad \hat{p} = \bar{p}\sqrt{m\omega\hbar}.$$

Here, $\bar{x}$ and $\bar{p}$ are our new dimensionless coordinates and momentum. Why this strange scaling? Some simple calculations will show:

$$[\bar{x}, \bar{p}] = i = \frac{[\hat{x}, \hat{p}]}{\hbar}.$$

This means this scaling is equivalent to setting $\hbar = 1$. What is ω? Here ω is the characteristic frequency scale of the system.

Recall the harmonic oscillator with Hamiltonian given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

Substituting in our scaled position and momentum,

$$\begin{aligned}\hat{H} &= \frac{\bar{p}^2}{2}\hbar\omega + \frac{1}{2}\omega^2\bar{x}^2\frac{\hbar}{\omega} \\ &= \left(\frac{\bar{p}^2}{2} + \frac{1}{2}\bar{x}^2\right)\hbar\omega.\end{aligned}$$

So we have something like a new scaled Hamiltonian given by $\bar{H} = \frac{\bar{p}^2}{2} + \frac{1}{2}\bar{x}^2$, and $\hbar\omega$ is an energy scaling. This also means that this scaling is as though $m = 1$.

We can also apply it to the time dependent Schödinger equation

$$\begin{aligned}i\hbar\frac{\partial\,|\psi\rangle}{\partial t} &= \hat{H}\,|\psi\rangle = \bar{H}(\hbar\omega)\,|\psi\rangle \\ i\frac{\partial\,|\psi\rangle}{\partial \omega t} &= \bar{H}\,|\psi\rangle\end{aligned}$$

In summary, the new units of our new scaled variables are listed below.

$\bar{x}$	$\sqrt{\frac{\hbar}{m\omega}}$
$\bar{p}$	$\sqrt{\hbar m\omega}$
$\bar{H}$	$\hbar\omega$
$\bar{t}$	$\frac{1}{\omega}$

In our calculations, we will proceed with $\hbar = 1$ and $m = 1$, and this will give us results in terms of the dimensionless variables. To convert them back to real units (meters, seconds, etc.) we multiply them with the scale listed above.

3.2 Limitations

Imagine we are computationally solving for the n-th eigenstate of the harmonic oscillator. We know that

$$\bar{p}^2 \propto (n - \frac{1}{2})$$
$$\bar{p} \propto \sqrt{n}$$

Therefore we should have a resolution of around $\frac{1}{\sqrt{n}}$. So $\frac{L}{N} < \frac{1}{\sqrt{n}}$.

We also have

$$\frac{1}{2}\bar{x}^2 \propto \frac{n - \frac{1}{2}}{2}$$
$$\bar{x} \propto \sqrt{n}$$

Therefore we also have another constraint of $\sqrt{n} < L$.

When will our computation fail? Assume $n \approx N$. Then, the two conditions will say

$$\sqrt{N} < L \qquad\qquad L < \sqrt{N}$$

which contradicts each other. So our computation is only valid if $n \ll N$.

3.3 Methodology

Knowing these limitations, how do we get started without knowing the exact solutions? Let us consider another problem and pretend that we don't know how to solve it:

$$\hat{H} = \frac{\hat{p}^2}{2m} + D[1 - \exp(-\alpha(x - x_0))]^2$$

First, we should find an appropriate value for ω. Performing a series expansion, we have

$$\hat{H} \approx D\left[1 - \left(1 - \alpha(x - x_0) + \frac{\alpha^2}{2}(x - x_0)^2\right)\right]$$

In a harmonic approximation,

$$D\alpha^2(x - x_0)^2 \approx \frac{1}{2}m\omega^2(x - x_0)^2$$

and obtain that $\omega = \sqrt{2D\alpha^2/m}$. Rewrite the Hamiltonian with our scaled units:

$$\begin{aligned}\hat{H} &= \frac{\bar{p}^2}{2m}\hbar m\omega + D\left[1 - \exp\left(-\alpha\sqrt{\frac{\hbar}{m\omega}}(\bar{x} - \bar{x}_0)\right)\right]^2 \\ &= \left\{\frac{\bar{p}^2}{2} + \frac{D}{\hbar\omega}[1 - \exp(\bar{\alpha}(\bar{x} - \bar{x}_0))]^2\right\}\hbar\omega\end{aligned}$$

where $\bar{\alpha} = \alpha\sqrt{\hbar/m\omega}$. Our $\bar{H}$ is given by the terms in the curly braces.

4 Time evolution

4.1 Introduction

All wave equations have time evolutions. Therefore just studying the time evolution of the Schrödinger equation is not very interesting. What is more interesting is the interplay between time evolution and measurement.

Take the time dependent Schrödinger equation

$$i\hbar\frac{\partial\left|\Psi\right\rangle}{\partial t}=\hat{H}\left|\Psi\right\rangle.$$

Note the two responsibilities of the Hamiltonian. Firstly, it gives you the energy as its eigenvalues. Secondly, it is also the generator of the time evolution. We know that the equation has solution of the form

$$|\Psi(t)\rangle=\exp\left[-\frac{i\hat{H}(t-t_0)}{\hbar}\right]|\Psi(t_0)\rangle$$

where $\hat{U}=\exp\left[-\frac{i\hat{H}(t-t_0)}{\hbar}\right]$ is an unitary operator. Unitary operators do not change the length of vectors and the inner product between vectors. Plugging the solution back to the Schödinger equation, we have

$$i\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t}=\hat{H}\hat{U}(t,t_0).$$

This is the most general setting, because we do not care about initial state. For a time independent Hamiltonian, we have the solution above. For a time dependent Hamiltonian, the solution reads

$$\begin{aligned}\int_{t_0}^{t}i\hbar\frac{\partial\hat{U}(t',t_0)}{\partial t}\mathrm{d}t'&=\int_{t_0}^{t}\hat{H}(t')\hat{U}(t',t_0)\mathrm{d}t'\\ i\hbar\Big(\hat{U}(t,t_0)-\hat{U}(t_0,t_0)\Big)&=\int_{t_0}^{t}\hat{H}(t')\hat{U}(t',t_0)\mathrm{d}t\\ \hat{U}(t,t_0)&=1-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\hat{U}(t',t_0)\mathrm{d}t'\end{aligned}$$

Below are some properties of $\hat{U}$:

- $\hat{U}(t_0,t_0)=1$.
- $\hat{U}(t_3,t_2)\hat{U}(t_2,t_1)=\hat{U}(t_3,t_1)$.
- $\hat{U}(t_1,t_2)\hat{U}(t_2,t_1)=\hat{U}(t_1,t_1)=1$. In other words, $\hat{U}^{\dagger}(t_2,t_1)=\hat{U}^{-1}(t_2,t_1)=\hat{U}(t_1,t_2)$.

There is a group structure being exhibited here.

Time independent operators can be transformed via the application of $\hat{U}$ to make them time dependent:

$$\begin{aligned} i\hbar\frac{\partial U^\dagger(t,t_0)\hat{O}U(t,t_0)}{\partial t} &= i\hbar\frac{\partial U^\dagger}{\partial t}\hat{O}\hat{U} + i\hbar\hat{U}^\dagger\hat{O}\frac{\partial\hat{U}}{\partial t} \\ &= -\hat{U}^\dagger\hat{H}\hat{O}\hat{U} + \hat{U}^\dagger\hat{O}\hat{H}\hat{U} \\ &= \hat{U}^\dagger\hat{O}\hat{U}\hat{U}^\dagger\hat{H}\hat{O}\hat{U} + \hat{U}^\dagger H\hat{U}\hat{U}^\dagger\hat{O}\hat{H}\hat{U} \\ &= \Big[\hat{U}^\dagger\hat{O}\hat{U}, \hat{U}^\dagger\hat{H}\hat{U}\Big]. \end{aligned}$$

We used the following identities above:

$$\begin{aligned} \Big(\hat{H}\hat{O}\Big)^\dagger &= \hat{O}^\dagger\hat{H} \\ i\hbar\frac{\partial\hat{U}}{\partial t} &= \hat{H}\hat{U} \\ -i\hbar\frac{\partial\hat{U}^\dagger}{\partial t} &= \hat{U}^\dagger\hat{H} \end{aligned}$$

If $\hat{O}$ is time dependent, then we could do the above again, but with an extra term of $i\hbar\hat{U}\frac{\partial\hat{O}}{\partial t}\hat{U}$.

4.2 Quantum Zeno effect

Consider an initial state $|\phi\rangle$. The state after a small time Δt is given by $\exp\Big(-i\hat{H}\Delta t/\hbar\Big)\,|\phi\rangle$. What is the probability of the system remaining in the initial state?

$$\begin{aligned} &\left|\left\langle\phi\middle|\exp\left(-\frac{i\hat{H}\Delta t}{\hbar}\right)\middle|\phi\right\rangle\right|^2 \\ &\quad\approx \left\langle\phi\middle|1+\frac{i\hat{H}\Delta t}{\hbar}-\frac{\hat{H}^2\Delta t^2}{2\hbar^2}\middle|\phi\right\rangle\left\langle\phi\middle|1-\frac{i\hat{H}\Delta t}{\hbar}-\frac{\hat{H}^2\Delta t^2}{2\hbar^2}\middle|\phi\right\rangle \\ &\quad= \left(1+\frac{i\Delta t}{\hbar}\left\langle\phi|\hat{H}|\psi\right\rangle-\frac{\Delta t^2}{2\hbar^2}\left\langle\psi|\hat{H}^2|\psi\right\rangle\right)\left(1-\frac{i\Delta t}{\hbar}\left\langle\phi|\hat{H}|\psi\right\rangle-\frac{\Delta t^2}{2\hbar^2}\left\langle\psi|\hat{H}^2|\psi\right\rangle\right) \\ &\quad= 1+\frac{\Delta t^2}{\hbar^2}\Big(\left\langle\psi|\hat{H}|\psi\right\rangle\Big)^2-\frac{\Delta t^2}{\hbar^2}\left\langle\psi|\hat{H}^2|\psi\right\rangle \\ &\quad= 1-\frac{\Delta t^2}{\hbar^2}\left\langle\psi\middle|\left\langle\hat{H}^2\right\rangle-\left\langle\hat{H}\right\rangle\middle|\psi\right\rangle \\ &\quad= 1-\frac{\Delta t^2}{\hbar^2}\Big(\Delta\hat{H}\Big)^2 \end{aligned}$$

where $\Delta\hat{H}$ denotes the variance. After N measurements, the probability of the system remaining in the same initial state is given by

$$\left(1-\frac{\Delta t^2}{\hbar^2}\Big(\Delta\hat{H}\Big)^2\right)^N.$$

Suppose that these measurements were made in the duration of total time T, with $\Delta t = T/N$. We can rewrite the probability

$$\left(1 - \frac{T^2}{N^2\hbar^2}\left(\Delta\hat{H}\right)^2\right)^N.$$

As $N \to \infty$, this probability goes to 1, and this is the quantum Zeno effect. This is something that cannot be derived from the time evolution of the Schrödinger equation.

5 Time dependent perturbation theory

5.1 Heisenberg representation

What we have been using so far is the Schrödinger representation. This is where we let the states evolve in time according to some unitary operator. In the Heisenberg representation, we let observables evolve and keep the states fixed.

In the Schrödinger representation, the expectation value of an observable at some time is

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

If we define the operator in the Heisenberg representation as

$$\hat{O}_H(t) = \hat{U}^\dagger(t,t_0)\hat{O}_S(t)\hat{U}(t,t_0)$$

then we will get the same result

$$\langle\Psi(t)|\hat{O}_S(t)|\Psi(t)\rangle = \langle\Psi(t_0)|\hat{O}_H(t)|\Psi(t_0)\rangle$$

Heisenberg's equation of motion is then given by

$$\begin{aligned} i\hbar\frac{\partial\hat{O}_H(t)}{\partial t} &= i\hbar\frac{\partial\hat{U}^\dagger\hat{O}_S(t)\hat{U}}{\partial t} \\ &= \left[\hat{U}^\dagger\hat{O}_S\hat{U}, U^\dagger\hat{H}_S\hat{U}\right] + i\hbar\hat{U}^\dagger\frac{\partial\hat{O}_S}{\partial t}\hat{U} \\ &= \left[\hat{O}_H, \hat{H}_H\right] + i\hbar\frac{\partial\hat{O}_S}{\partial t}_H. \end{aligned}$$

What about Born's rule? Consider the operator $\hat{O}_S$ with eigenstate $|\phi\rangle$ in the Schrödinger representation. The probability of finding the system $\hat{U}|\Psi(t_0)\rangle$ with eigenvalue ϕ is given by $\left|\langle\phi|\hat{U}|\Psi(t_0)\rangle\right|^2$. In the Heisenberg representation, the eigenstate is given by $\hat{U}^\dagger|\phi\rangle$. The system is given by simply $|\Psi(t_0)\rangle$, and Born's rule says $\left|\langle\phi|\hat{U}|\Psi(t_0)\rangle\right|^2$.

5.2 Interaction representation

Let us divide the Hamiltonian $\hat{H}$ into a time independent $\hat{H}_0$ and a time dependent perturbation $\hat{V}(t)$. The time evolution of the unperturbed system is usually known, by choosing the appropriate $\hat{H}_0$. How do we find the evolution in the presence of perturbation $\hat{V}$?

Let us factorise the unitary evolution operator into two parts, $\hat{U}_0$ without the perturbation and $\hat{U}_I$ which is an additional correction due to the perturbation:

$$\hat{U}(t,t_0) = \hat{U}_0(t,t_0)\hat{U}_I(t,t_0).$$

Then we can write

$$\begin{aligned}\langle\Psi(t)|\hat{O}_s(t)|\Psi(t)\rangle &= \langle\Psi(t_0)|\,\hat{U}_I(t,t_0)\hat{U}_0^\dagger(t,t_0)\hat{O}(t)\hat{U}_0(t,t_0)\hat{U}_I(t,t_0)\,|\Psi(t_0)\rangle \\ &= \langle\Psi_I(t_0)|\hat{O}_I(t)|\Psi_I(t_0)\rangle\end{aligned}$$

where $\hat{O}_I = \hat{U}_0^\dagger\hat{O}\hat{U}_0$ and $|\Psi_I\rangle = \hat{U}_I\,|\Psi\rangle$. This also explains why the interaction representation is also called an intermediate representation. Operators will transform by $\hat{U}_0$ and states will transform by $\hat{U}_I$.

Now we need to figure out what $\hat{U}_I$ is doing.

$$\begin{aligned}i\hbar\frac{\partial\hat{U}_I}{\partial t} &= i\hbar\frac{\partial\hat{U}_0^\dagger\hat{U}}{\partial t} \\ &= i\hbar\frac{\partial\hat{U}_0^\dagger}{\partial t}\hat{U} + i\hbar\hat{U}_0^\dagger\frac{\partial\hat{U}}{\partial t} \\ &= -\hat{U}_0^\dagger\hat{H}_0\hat{U} + \hat{U}_0^\dagger\hat{H}\hat{U} \\ &= -\hat{U}_0^\dagger\hat{H}_0\hat{U}_0\hat{U}_I + \hat{U}_0^\dagger\hat{H}\hat{U}_0\hat{U}_I \\ &= \hat{U}_0^\dagger\Big(\hat{H} - \hat{H}_0\Big)\hat{U}_0\hat{U}_I \\ &= \hat{V}_I(t)U_I\end{aligned}$$

We are interested in solving this equation. We shall solve it perturbatively:

- Zeroth order: $i\hbar\frac{\partial\hat{U}_I}{\partial t} = 0$, meaning $\hat{U}_I = 1$.
- First order: $i\hbar\frac{\partial\hat{U}_I}{\partial t} = \hat{V}_I(t)$, where we have plugged in $\hat{U}_I = 1$. Integrating both sides we have

$$\begin{aligned}\int_{t_0}^{t}\frac{\partial\hat{U}_I}{\partial t}\,\mathrm{d}t' &= \int_{t_0}^{t}\frac{1}{i\hbar}\hat{V}_I(t')\,\mathrm{d}t' \\ \hat{U}_I(t,t_0) &= 1 + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(t')\,\mathrm{d}t'\end{aligned}$$

- Second order: again we plug the first order solution back in, and get

$$\hat{U}_I = 1 + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(t')\,\mathrm{d}t' + \left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}\hat{V}_I(t')\int_{t_0}^{t'}\hat{V}_I(t'')\,\mathrm{d}t'\,\mathrm{d}t''$$

We can see the general form. Every next order will add a new term with an extra integral. However second order will suffice for our purposes.

Some rearrangement gives us an interesting interpretation of this procedure. Consider the first

order solution:

$$\begin{aligned}\hat{U} &= \hat{U}_0\hat{U}_I \\ &= \hat{U}_0 + \hat{U}_0\frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(t')\,\mathrm{d}t' \\ &= \hat{U}_0(t,t_0) + \hat{U}_0(t,t_0)\frac{1}{i\hbar}\int_{t_0}^{t}\hat{U}_0^\dagger(t',t_0)\hat{V}(t')\hat{U}_0(t',t_0)\,\mathrm{d}t' \\ &= \hat{U}_0(t,t_0) + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{U}_0(t,t')\hat{V}(t')\hat{U}_0(t',t_0)\,\mathrm{d}t'\end{aligned}$$

So this describes a free evolution from time t_0 to t', then we meet the potential, followed by another free evolution to time t, and we do this for all possible t'. We can do the same for the second order solution (only looking at the extra term):

$$\begin{aligned}&\hat{U}_0(t,t_0)\left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,\hat{V}_I(t')\hat{V}_I(t'') \\ &\quad= \left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,\hat{U}_0(t,t')\hat{V}(t')\hat{U}_0(t',t'')\hat{V}(t'')\hat{U}_0(t'',t_0)\end{aligned}$$

which shows us encountering the potential twice. This expansion is also called the Dyson series.

5.3 First order result

Let us walk through how we would use first order perturbation in our calculations. Recall for first order we have $\hat{U}_I(t,t_0) = 1 + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(t')\,\mathrm{d}t'$, and in the interaction picture $\hat{V}_I = \hat{U}_0^\dagger V\hat{U}_0$. Using the eigenstates of $\hat{H}_0$ to express the matrix elements,

$$\begin{aligned}\left\langle\psi_n^0\middle|\hat{U}_I(t,t_0)\middle|\psi_m^0\right\rangle &= \delta_{mn} + \frac{1}{i\hbar}\int_{t_0}^{t}\mathrm{d}t'\left\langle\psi_n^0\middle|\exp\left(\frac{i\hat{H}_0(t'-t_0)}{\hbar}\right)\hat{V}(t')\exp\left(\frac{i\hat{H}_0(t_0-t')}{\hbar}\right)\middle|\psi_m^0\right\rangle \\ &= \delta_{mn} + \frac{1}{i\hbar}\int_{t_0}^{t}\left\langle\psi_n^0\right|\hat{V}(t_1)\left|\psi_m^0\right\rangle\exp\left(\frac{i(E_n^0-E_m^0)(t_1-t_0)}{\hbar}\right).\end{aligned}$$

Transition amplitudes are then given by

$$\begin{aligned}\left\langle\psi_n^0\middle|\hat{U}(t,t_0)\middle|\psi_m^0\right\rangle &= \left\langle\psi_n^0\middle|\hat{U}_0(t,t_0)\hat{U}_I(t,t_0)\middle|\psi_m^0\right\rangle \\ &= \exp\left(\frac{iE_n^0(t_0-t)}{\hbar}\right)\left\langle\psi_n^0\middle|\hat{U}_I(t,t_0)\middle|\psi_m^0\right\rangle\end{aligned}$$

Finally, the transition probability (for $m \neq n$) is given by

$$\begin{aligned}P_{m\to n} &= \left|\left\langle\psi_n^0\middle|\hat{U}(t,t_0)\middle|\psi_m^0\right\rangle\right|^2 \\ &= \left|\left\langle\psi_n^0\middle|\hat{U}_I(t,t_0)\middle|\psi_m^0\right\rangle\right|^2 \\ &= \frac{1}{\hbar^2}\left|\int_{t_0}^{t}\left\langle\psi_n^0\middle|\hat{V}(t_1)\middle|\psi_m^0\right\rangle\exp\left(\frac{i(E_n^0-E_m^0)(t'-t_0)}{\hbar}\right)\mathrm{d}t'\right|^2\end{aligned}$$

Apart from some constant factors, the transition probability given by the first order perturbation is proportional to the Fourier transform of the matrix element of the matrix element $\hat{V}_{nm}$ evaluated at the frequency determined by $\omega_{nm} = \frac{E_n^0-E_m^0}{\hbar}$.

5.4 Example: constant perturbation

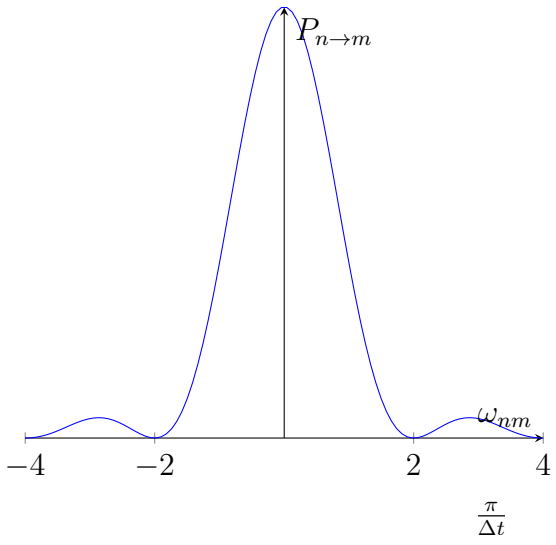
We start with Hamiltonian $\hat{H}^0$, and turn on a constant perturbation V starting at time t_0. We have

$$\begin{aligned} P_{m\to n} &= \frac{1}{\hbar^2}|V_{mn}|^2\left|\int_{t_0}^{t}\exp(i\omega_{nm}(t'-t_0))\,\mathrm{d}t'\right|^2 \\ &= \frac{|V_{nm}|^2}{\hbar^2}\left|\frac{e^{i\omega_{nm}(t-t_0)}-1}{i\omega_{nm}}\right|^2 \\ &= \frac{|V_{nm}|^2}{\omega_{nm}^2\hbar^2}\left|e^{i\omega_{nm}(t-t_0)/2}\right|^2\left|e^{i\omega_{nm}(t-t_0)/2}-e^{-i\omega_{nm}(t-t_0)/2}\right|^2 \\ &= \frac{4|V_{nm}|^2}{\omega_{nm}^2\hbar^2}\sin^2\left(\frac{i\omega_{nm}(t-t_0)}{2}\right) \end{aligned}$$

Some rearrangement allows us to write it as so:

$$P_{m\to n} = \frac{4|V_{nm}|^2}{\omega_{nm}^2\hbar^2}\operatorname{sinc}^2\left(\frac{i\omega_{nm}\Delta t}{2}\right)\Delta t^2$$

The following is a sketch of the function:



Roughly speaking, this shows that the transition probability is significant for $\Delta E\Delta t \approx \hbar$, which is some kind of uncertainty principle. For small Δt, it is possible for the system to transition to another energy. As $\Delta t \to \infty$, the function approaches a Dirac delta, and $\Delta E \to 0$. This means that energy is conserved, but only at very long Δt, and it is possible to go against the law due to the uncertainty principle.

5.5 Periodic perturbation

Consider a perturbation of the form

$$\hat{V}(t) = v[\exp(i\omega t) + \exp(-i\omega t)]$$

with $\omega > 0$. The matrix element is given by

$$\left\langle \psi_n^0 \middle| \hat{V}(t) \middle| \psi_m^0 \right\rangle = v_{nm}[\exp(i\omega t) + \exp(-i\omega t)].$$

The probability amplitude is simply (setting $t_0 = 0$):

$$\begin{aligned} P_{m\to n} &= \frac{1}{\hbar^2}\left|\int_0^t \left\langle \psi_n^0 \middle| \hat{V}(t_1) \middle| \psi_m^0 \right\rangle \exp(i\omega_{nm}(t' - t_0))\,\mathrm{d}t'\right|^2 \\ &= \frac{|v_{nm}|^2}{\hbar^2}\left|\int_0^t \exp[i(\omega + \omega_{nm})t'] + \exp[i(\omega_{nm} - \omega)t']\,\mathrm{d}t'\right|^2 \\ &= \frac{|v_{nm}|^2}{\hbar^2}\left|\frac{\exp[i(\omega + \omega_{nm})t] - 1}{\omega + \omega_{nm}} + \frac{\exp[i(\omega_{nm} - \omega)t] - 1}{\omega_{nm} - \omega}\right|^2. \end{aligned}$$

If ω is quite close to $|\omega_{nm}|$, the denominator might go to zero. In this case we make the following approximation:

- If $\omega_{nm} < 0$ (meaning $E_n^0 < E_m^0$), then the first term dominates.
- If $\omega_{nm} > 0$ (meaning $E_n^0 > E_m^0$), then the second term dominates.

To justify this, let us consider the first case. In this case, performing a Taylor expansion to the first order gives

$$\frac{\exp[i(\omega + \omega_{nm})t'] - 1}{\omega + \omega_{nm}} \approx \frac{1 + i(\omega + \omega_{nm})t - 1}{\omega + \omega_{nm}} \propto t.$$

Meanwhile, the other term is oscillating with t, and will contribute less to the amplitude. This approximation is also known as the *rotating wave approximation*. All in all, in this case we get

$$P_{m\to n} \approx \frac{|v_{nm}|^2 t^2}{\hbar^2}\,\mathrm{sinc}^2\left(\frac{(\omega + \omega_{nm})t}{2}\right).$$

If the perturbation is caused by a single photon, then this means that after a long time, then $\omega_{nm} \approx \omega$, so the system will have either captured or emitted a photon.

For the other case, the expression is very similar:

$$P_{m\to n} \approx \frac{|v_{nm}|^2 t^2}{\hbar^2}\,\mathrm{sinc}^2\left(\frac{(\omega_{nm} - \omega)t}{2}\right).$$

Interestingly, our results also means that an oscillating field can bring a quantum state down to lower energy levels.

5.6 Two photon processes

Since we have seen that first order perturbation theory can describe single photon processes, we would naturally expect second order perturbation theory to be able to describe two photon processes. Assume we have two eigenstates with energies $E_n - E_m \approx 2\hbar\omega$. The perturbation as usual is $\hat{V}(t) = v\cos(\omega t)$. The driving frequency is far from the single photon resonance so our previous results will not be applicable here.

Let us assume that $m \neq n$ and that the first order term does not really contribute any effect since again ω is too small to cause a transition. Then,

$$
\begin{aligned}
&\langle \psi_n^0 | \hat{U}_I | \psi_m^0 \rangle \\
&= \left(\frac{1}{i\hbar}\right)^2 \langle \psi_n^0 | \int_0^t \hat{V}_I(t') \int_0^{t'} \hat{V}_I(t'') \, \mathrm{d}t' \, \mathrm{d}t'' \, | \psi_m^0 \rangle \\
&= \left(\frac{1}{i\hbar}\right)^2 \langle \psi_n^0 | \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \, \hat{U}_0^\dagger v \cos(\omega t') \hat{U}_0 \hat{U}_0^\dagger v \cos(\omega t'') \hat{U}_0 \, | \psi_m^0 \rangle \\
&= \left(\frac{1}{i\hbar}\right)^2 \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \\
&\quad \exp\left(\frac{iE_n^0 t'}{\hbar}\right) \langle \psi_n^0 | \, v \cos(\omega t') \hat{U}_0 \sum_k | \psi_k^0 \rangle\langle \psi_k^0 | \, \hat{U}_0^\dagger v \cos(\omega t'') \exp\left(\frac{iE_m^0 t''}{\hbar}\right) | \psi_m^0 \rangle \\
&= \left(\frac{1}{i\hbar}\right)^2 \sum_k \langle \psi_n^0 | v | \psi_k^0 \rangle \, \langle \psi_k^0 | v | \psi_m^0 \rangle \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \\
&\quad \exp\left(\frac{iE_n^0 t'}{\hbar}\right) \cos(\omega t') \exp\left(\frac{-iE_k^0 t'}{\hbar}\right) \exp\left(\frac{iE_k^0 t''}{\hbar}\right) \cos(\omega t'') \exp\left(\frac{iE_m^0 t''}{\hbar}\right) \\
&= \left(\frac{1}{i\hbar}\right)^2 \sum_k \langle \psi_n^0 | v | \psi_k^0 \rangle \, \langle \psi_k^0 | v | \psi_m^0 \rangle \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \\
&\quad e^{i\omega_{nk} t'} \left[\frac{1}{2} e^{i\omega t'} + \frac{1}{2} e^{-i\omega t'}\right] e^{i\omega_{km} t''} \left[\frac{1}{2} e^{i\omega t''} + \frac{1}{2} e^{-i\omega t''}\right] \\
&= \frac{1}{4} \left(\frac{1}{i\hbar}\right)^2 \sum_k \langle \psi_n^0 | v | \psi_k^0 \rangle \, \langle \psi_k^0 | v | \psi_m^0 \rangle \\
&\quad \int_0^t \frac{e^{i(\omega_{nm}+2\omega)t'} - e^{i(\omega_{nk}+\omega)t'}}{\omega_{km} + \omega} + \frac{e^{i\omega_{nm}t'} - e^{i(\omega_{nk}-\omega)t'}}{\omega_{km} + \omega} \\
&\qquad + \frac{e^{i\omega_{nm}t'} - e^{i(\omega_{nk}+\omega)t'}}{\omega_{km} - \omega} + \frac{e^{i(\omega_{nm}-2\omega)t'} - e^{i(\omega_{nk}-\omega)t'}}{\omega_{km} - \omega} \, \mathrm{d}t' \, .
\end{aligned}
$$

In the above we use $\omega_{nm} = (E_n - E_m)/\hbar$ as shorthand. Given the condition that $2\omega \approx \omega_{nm}$, we see that only the seventh exponential will not be oscillating as much. Hence it will end up being the dominating term. This gives us the final result:

$$
\langle \psi_n^0 | \hat{U}_I | \psi_m^0 \rangle \approx \frac{1}{4} \left(\frac{1}{i\hbar}\right)^2 \sum_k \langle \psi_n^0 | v | \psi_k^0 \rangle \, \langle \psi_k^0 | v | \psi_m^0 \rangle \, \frac{e^{i(\omega_{nm}-2\omega)t} - 1}{(\omega_{km} - \omega)(\omega_{nm} - 2\omega)}.
$$

Hence the probability amplitude is given by

$$
P_{m \to n} = \frac{1}{16} \frac{1}{\hbar^4} \left| \sum_k \langle \psi_n^0 | v | \psi_k^0 \rangle \, \langle \psi_k^0 | v | \psi_m^0 \rangle \, t^2 \, \mathrm{sinc}^2 \left(\frac{(\omega_{nm} - 2\omega)t}{2} \right) \right|^2
$$

6 Computational studies of quantum dynamics

In this section we are interested in simulating time dependent problems

6.1 Discrete Fourier transform

We have already introduced the discrete variable transformation. Since the Fourier transform plays an important role in quantum mechanics, it kind of follows that we would need a discrete implementation of the Fourier transform. As we will see, the Fourier transform used to switch between position and momentum representations can help us solve some problems faster [1].

Given a function f and a periodic boundary condition $f(n) = f(n-N)$, we have the discrete Fourier transform

$$g(m) = \sum_{n=0}^{N-1} \exp\left(-\frac{2i\pi nm}{N}\right) f(n)$$

and the inverse transform

$$f(n) = \frac{1}{N} \sum_{m=0}^{N-1} \exp\left(\frac{2i\pi mn}{N}\right) g(m).$$

Consider a discrete variable representation of a function ψ on a lattice starting at some position x_0 with a separation between points of Δx. Define $x_n = n\Delta x$, and $\psi(n) = \psi(x_n - x_0)$. The Fourier transform is given by

$$\phi(m) = \sum_{n=0}^{N-1} \exp\left(-\frac{2i\pi n\Delta x}{N\Delta x} m\right) \psi(x_n - x_0).$$

Denote $\bar{x}_n = x_n - x_0$ and the total length $L = N\Delta x$. Rewriting,

$$\Phi(p_j) = \phi(m) = \sum_{n=0}^{N-1} \exp\left(-\frac{ip_j \bar{x}_n}{\hbar}\right) \psi(\bar{x}_n).$$

where $p_j = \hbar k_j = 2\pi m\hbar/L$. Thus the Fourier transform is clearly a transformation from position space to momentum space.

Note that the possible range of momentum we have here is always positive ranging from 0 to $(N-1)2\pi\hbar/L$. Also, due to periodicity, we have $\Phi(p_j) = \Psi(p_j - 2\pi\hbar/\Delta x)$. We have argued before that due to a resolution limit, we are usually not interested in high momentum states. However here we see that $\Psi(0)$ is large. This is not very physical. Very simply, we just decrease the right half of the momentum lattice by N units. So, the lattice should instead range from:

$$0, \frac{2\pi\hbar}{L}, 2\frac{2\pi\hbar}{L}, \ldots \left(\frac{N}{2} - 1\right)\frac{2\pi\hbar}{L}, \left(\frac{N}{2} - N\right)\frac{2\pi\hbar}{L}, \left(\frac{N}{2} + 1 - N\right)\frac{2\pi\hbar}{L}, \ldots, -\frac{2\pi\hbar}{L}.$$

So, instead of considering high momentum values, we shift it into the negative regime. Again, this is purely a matter of interpretation which occurs due to the implicitly assumed periodic condition imposed by the Fourier transform, which is fine for a position representation but is not physical (without modification) in the momentum representation.

[1] Recall the calculation of the matrix elements of the $\hat{T}$ matrix in discrete variable transformation. It is troublesome because it is not diagonal in the position representation, but is diagonal in the momentum (energy) representation.

6.2 Split operator method

As mentioned at the start of the section we want to switch between position and momentum representations to avoid finding eigenvalues and eigenvectors.

Imagine if we have operator A which is diagonal in momentum representation and B which is diagonal in position representation. Then $A + B$ is not easily evaluated in either position or momentum representation. Indeed it can be hard to obtain $\exp(A + B)$ if it is not diagonal.

We can make use of something called the Baker-Camper-Hausdorff (BCH) formula, which says that

$$\exp(i\delta A)\exp(i\delta B) = \exp(i\delta Z)$$

where Z is given by

$$Z = A + B + \frac{i\delta}{2}[A, B] - \frac{\delta^2}{12}([A, [A, B]] + [B, [B, A]]) + \dots.$$

For small δ, taking a BCH approximation up to second order, we have

$$\exp(i\delta(A + B)) = \exp\left(\frac{i\delta}{2}A\right)\exp(i\delta B)\exp\left(\frac{i\delta}{2}A\right) + O(\delta^3).$$

What follows is a proof of this statement. First consider

$$\exp(i\delta B)\exp\left(\frac{i\delta}{2}A\right) \approx \exp(i\delta Z_1)$$

where the BCH formula gives $Z_1 = B + A/2 + i\delta/2[B, A/2]$. Next, consider

$$\exp(i\delta/2A)\exp(i\delta Z_1) \approx \exp(i\delta Z_2).$$

The BCH formula gives

$$\begin{aligned} Z_2 &= \frac{A}{2} + Z_1 + \frac{i\delta}{2}\left[\frac{A}{2}, Z_1\right] \\ &\approx \frac{A}{2} + \frac{A}{2} + B + \frac{i\delta}{2}\left[B, \frac{A}{2}\right] + \frac{i\delta}{2}\left[\frac{A}{2}, B + \frac{A}{2}\right] \\ &= A + B \end{aligned}$$

Thus substituting the first equation into the second gives us our claim.

Therefore, we can now write

$$\exp\left(\frac{-i\delta t}{\hbar}(T + V)\right) \approx \exp\left(\frac{-i\delta t}{2\hbar}T\right)\exp\left(\frac{-i\delta t}{\hbar}V\right)\exp\left(\frac{-i\delta t}{2\hbar}T\right)$$

or

$$\exp\left(\frac{-i\delta t}{\hbar}(T + V)\right) \approx \exp\left(\frac{-i\delta t}{2\hbar}V\right)\exp\left(\frac{-i\delta t}{\hbar}T\right)\exp\left(\frac{-i\delta t}{2\hbar}V\right)$$

which allow us to handle only diagonal matrices in either momentum or position representation, which we can easily switch between using Fourier transforms. Not only is it easier to compute,

the matrices are also sparser, saving both time and memory. As usual accuracy can be improved by increasing resolution of δt.

The final time evolution operator is thus given by

$$\begin{aligned} U(t_{\text{total}}, 0) &\approx \prod_{j=1}^{N} \exp\left(\frac{-i\delta t H(t_j)}{\hbar}\right) \\ &\approx \prod_{j=1}^{N} \exp\left(\frac{-i\delta t}{2\hbar} V(t_j)\right) \exp\left(\frac{-i\delta t}{\hbar} T(t_j)\right) \exp\left(\frac{-i\delta t}{2\hbar} V(t_j)\right) \end{aligned}$$

If the Hamiltonian is not time dependent then this simplifies to just taking a power of N. Thus the strategy for evaluation would be

1. Start with ψ in position representation
2. Multiply with $\exp(V \ldots)$
3. FFT ψ into momentum representation
4. Multiply with $\exp(T \ldots)$
5. IFFT ψ back into position representation
6. Multiply with $\exp(V \ldots)$
7. Move to next time step

7 Adiabatic approximation

7.1 Introduction

We consider a process as adiabatic if the change in the Hamiltonian is slow. The "slowness" is determined by comparing the time scales between the change versus the time scale of the system itself. This is known as a separation of time scales. For example, a vibrating molecule induces a time dependent Hamiltonian on the electrons in the molecule. However, this vibration is much slower than the speed at which the electrons are moving at, even though the vibration may be extremely fast relative to a human scale.

We will write our Hamiltonian in terms of a set of time dependent parameters $\lambda(t) = \{\lambda_1(t), \ldots, \lambda_n(t)\}$, for example these could be mass, position, colour of an incident laser beam, etc.

$$i\hbar \frac{\partial \left|\Psi(t)\right\rangle}{\partial t} = \hat{H}[\lambda(t)] \left|\Psi(t)\right\rangle .$$

The instantaneous eigenvalues and eigenfunctions are assumed to be as usual:

$$\hat{H}(\lambda) \left|\psi_n(\lambda)\right\rangle = E_n(\lambda) \left|\psi_n(\lambda)\right\rangle .$$

Note that the $|\psi\rangle$ states here have no relation with the $|\Psi\rangle$ state. The $|\Psi\rangle$ state is a solution to the initial value problem, while the eigenstate $|\psi\rangle$ is only the solution to a time-independent

solution given by an fixed point of time. We can connect the two with a time dependent unitary operator $U_R(t)$

$$|\Psi(t)\rangle = U_R(t)\,|\psi(t)\rangle\,.$$

Plugging this back into the Schrödinger equation,

$$\begin{aligned}
i\hbar\frac{\partial U_R(t)\,|\psi(t)\rangle}{\partial t} &= H[\lambda(t)]U_R(t)\,|\psi(t)\rangle \\
i\hbar\frac{\partial U_R(t)}{\partial t}\,|\psi(t)\rangle + i\hbar U_R(t)\frac{\partial\,|\psi(t)\rangle}{\partial t} &= H[\lambda(t)]U_R(t)\,|\psi(t)\rangle \\
i\hbar U_R^{-1}\frac{\partial U_R}{\partial t}\,|\psi(t)\rangle + i\hbar\frac{\partial\,|\psi(t)\rangle}{\partial t} &= U_R^{-1}H[\lambda(t)]U_R\,|\psi(t)\rangle \\
i\hbar\frac{\partial\,|\psi(t)\rangle}{\partial t} &= \left(U_R^{-1}H[\lambda(t)]U_R - i\hbar U_R^{-1}\frac{\partial U_R}{\partial t}\right)|\psi(t)\rangle\,.
\end{aligned}$$

Notice that the last term in the brackets form a effective Hamiltonian H_{eff} in this representation. Notice that if we choose $U_R = U$, the true unitary evolution of the system, we recover the Heisenberg representation. Indeed if we worked it out we would obtain $H_{\text{eff}} = 0$, meaning the states are not evolving. If we choose $U_R = U_0$, we recover the interaction representation.

For our purposes, we will define U_R as

$$U_R = \sum_n |\psi_n(\lambda(t))\rangle\langle\psi_n(\lambda(0))|\,.$$

To see what it does, consider the action of this operator on an initial state $|\psi_m(\lambda(0))\rangle$:

$$|\Psi(t)\rangle = U_R\,|\psi_m(\lambda(0))\rangle = |\psi_m(\lambda(t))\rangle\,.$$

It maps an initial eigenstate to the same eigenstate, but with the new parameters. For example, if we move the potential of a harmonic oscillator slowly, the ground state should follow. If the movement was fast however, this would not be true, the new state would be a very messy superposition of the new eigenstates. It is a good exercise to simulate this with the computational methods we have discussed so far.

Plugging in our U_R into H_{eff},

$$\begin{aligned}
H_{\text{eff}} &= U_R^{-1}H[\lambda(t)]U_R - i\hbar U_R^{-1}\frac{\partial U_R}{\partial t} \\
&= \sum_n |\psi_n(\lambda(0))\rangle\langle\psi_n(\lambda(t))|\,H(\lambda(t))\sum_n |\psi_n(\lambda(t))\rangle\langle\psi_n(\lambda(0))| \\
&\quad - i\hbar\sum_n |\psi_n(\lambda(0))\rangle\langle\psi_n(\lambda(t))|\sum_m \frac{\partial\,|\psi_m(\lambda(t))\rangle}{\partial t}\,\langle\psi_m(\lambda(0))| \\
&= \sum_n |\psi_n(\lambda(0))\rangle\,E_n(\lambda(t))\,\langle\psi_n(\lambda(0))| \\
&\quad - i\hbar\sum_{n,m} |\psi_n(\lambda(0))\rangle\,\langle\psi_m(\lambda(0))|\,\langle\psi_n(\lambda(t))|\,\frac{\partial\,|\psi_m(\lambda(t))\rangle)}{\partial t}.
\end{aligned}$$

Substituting this into the Schrödinger equation,

$$\begin{aligned}
i\hbar\frac{\partial\,|\psi(t)\rangle}{\partial t} = \Big[&\sum_n |\psi_n(\lambda(0))\rangle\,E_n(\lambda(t))\,\langle\psi_n(\lambda(0))| \\
&- i\hbar\sum_{n,m} |\psi_n(\lambda(0))\rangle\,\langle\psi_m(\lambda(0))|\,\langle\psi_n(\lambda(t))|\,\frac{\partial\,|\psi_m(\lambda(t))\rangle)}{\partial t}\Big]\,|\psi(t)\rangle
\end{aligned}$$

Again, keep in mind the difference between $|\psi(t)\rangle$, $|\Psi(t)\rangle$, and $|\psi(\lambda(t))\rangle$. Project this onto $\langle\psi_k(\lambda(0))|$, and denote $D_k = \langle\psi_k(\lambda(0))|\psi(t)\rangle$:

$$i\hbar\frac{\partial D_k}{\partial t} = E_k(\lambda(t))D_k - i\hbar\sum_m D_k \langle\psi_k(\lambda(t))| \frac{\partial |\psi_m(\lambda(t))\rangle}{\partial t}$$

We now need to solve this. If we only consider the first part:

$$i\hbar\frac{\partial D_k}{\partial t} = E_k(\lambda(t))D_k$$

The solution is standard:

$$D_k = \exp\left[\frac{-i}{\hbar}\int E_k(\lambda(t))\,\mathrm{d}t\right].$$

This motivates an ansatz

$$D_k = C_k(t)\exp\left[\frac{-i}{\hbar}\int E_k(\lambda(t))\,\mathrm{d}t\right].$$

Plugging the ansatz back in, and define $\theta_k = \frac{-1}{\hbar}\int E_k(\theta(t))\,\mathrm{d}t$ as the dynamical phase. We have

$$i\hbar\frac{\partial C_k(t)}{\partial t}e^{i\theta_k} = -i\hbar\sum_m \langle\psi_k(\lambda(t))| \frac{\partial |\psi_m(\lambda(t))\rangle}{\partial t}C_k(t)e^{i\theta_m}$$

$$\frac{\partial C_k(t)}{\partial t} = -\sum_m \langle\psi_k(\lambda(t))| \frac{\partial |\psi_m(\lambda(t))\rangle}{\partial t}C_k(t)e^{i(\theta_m-\theta_k)}$$

We split the summation into two cases:

$$-\frac{\partial C_k(t)}{\partial t} = \langle\psi_k(\lambda(t))| \frac{\partial |\psi_k(\lambda(t))\rangle}{\partial t}C_k(t) + \sum_{m\neq n} \langle\psi_k(\lambda(t))| \frac{\partial |\psi_m(\lambda(t))\rangle}{\partial t}C_k(t)e^{i(\theta_m-\theta_k)}$$

It turns out that for adiabatic processes, because we are integrating over a long period of time, and the second term contains an oscillating term, we can safely approximate it away. This will be valid as long as along the process E_m and E_k do not get close to each other:

$$\theta_m - \theta_k = \frac{-1}{\hbar}\int E_m(\lambda(t)) - E_k(\lambda(t))\,\mathrm{d}t\,.$$

The solution of

$$-\frac{\partial C_k(t)}{\partial t} \approx \langle\psi_k(\lambda(t))| \frac{\partial |\psi_k(\lambda(t))\rangle}{\partial t}C_k(t)$$

is given by

$$C_k(t) = C_k(0)e^{i\gamma_k(t)}$$

where we defined the geometric phase as

$$\gamma_m(t) = i\int_0^t \langle\psi_m(\lambda(t'))| \frac{\partial |\psi_m(\lambda(t))\rangle}{\partial t'}\,\mathrm{d}t'$$

Therefore, finally, we have

$$\begin{aligned}|\Psi(t)\rangle &= U_R\,|\psi(t)\rangle \\ &= U_R\sum_n C_n(0)e^{i\gamma_n(t)}e^{i\theta_n(t)}\,|\psi_n(\lambda(0))\rangle \\ &= \sum_n C_n(0)e^{i\gamma_n(t)}e^{i\theta_n(t)}\,|\psi_n(\lambda(t))\rangle\,.\end{aligned}$$

Thus, if the initial state starts off as the k-th eigenstate, it will also end up as the k-th eigenstate with some phase factors.

7.2 Aside

The term "adiabatic" used in this context seems to be different from the same term defined in statistical mechanics. However, as we see, since the k-th state goes to the k-th state, the occupational probability for each state remains the same. Therefore, the informational entropy remains a constant, which is analogous to the thermodynamic entropy remaining constant in statistical mechanics.

The dynamical phase θ_m comes from the eigenenergies and it is expected that they will contribute to an overall phase (recall the phase for a stationary system). What is the meaning behind the geometric phase γ_m?

$$\begin{aligned}\gamma_m(t) &= i\int_0^t \langle\psi_m(\lambda(t'))|\,\frac{\partial\,|\psi_m(\lambda(t))\rangle}{\partial t'}\,\mathrm{d}t' \\ &= i\int_0^t \left\langle \psi_m(\lambda(t'))\middle|\sum_i \frac{\partial\psi_m(\lambda_i(t))}{\partial t'}\right\rangle \frac{\mathrm{d}\lambda_i}{\mathrm{d}t'}\,\mathrm{d}t' \\ &= i\int_{\lambda(0)}^{\lambda(t)} \left\langle \psi_m(\lambda(t'))\middle|\sum_i \frac{\partial\psi_m(\lambda_i(t))}{\partial t'}\right\rangle \mathrm{d}\lambda\end{aligned}$$

and this is why it is called a geometric phase. It is a line integral along the path taken by the adiabatic process in the λ-parameter phase.

If the eigenfunction along a path in the parameter space is always real in a certain representation, then the geometric phase must be zero. This is simply because the geometric phase itself is always real. This in turn is because of the normalisation condition which means

$$\frac{\partial\,\langle\psi_m|\psi_n\rangle}{\partial t} = 0$$

which then results in

$$\langle\psi_m(\lambda)|\,\frac{\partial\,|\psi_m(\lambda)\rangle}{\partial t} = -\frac{\partial\,\langle\psi_m(\lambda)|}{\partial t}\,|\psi_m(\lambda)\rangle$$

so $\gamma_m^* = \gamma_m$.

7.3 Example: transport without transit

We start off with an example from [1]. Consider a system with three potential wells. The tunnelling rate from well i to j is given by Ω_{ij}. We simplify our calculations greatly if we model this as a three level system. We have a model Hamiltonian given by

$$H_{\text{eff}} = \hbar\begin{pmatrix} 0 & \Omega_{12} & 0 \\ \Omega_{12}^* & 0 & \Omega_{23} \\ 0 & \Omega_{23}^* & 0 \end{pmatrix}.$$

The tunnelling rates can be adjusted by adjusting the laser intensity that forms the wells. Thus, we are going to investigate the dynamics of the system when we change the tunnelling rates very slowly.

For a fixed Ω_{12} and Ω_{23}, we can solve for the eigenvalues:

$$\begin{vmatrix} -E & \Omega_{12} & 0 \\ \Omega_{12}^* & -E & \Omega_{23} \\ 0 & \Omega_{23}^* & -E \end{vmatrix} = 0$$
$$-E(E^2 - |\Omega_{23}|^2) - |\Omega_{12}|^2 E = 0.$$

The solutions are given by $E_0 = 0$ and $E_\pm = \pm\hbar\Omega_M$ where $\Omega_M = \sqrt{|\Omega_{12}|^2 + |\Omega_{23}|^2}$. The eigenvector for $E_0 = 0$ is given by (up to normalization)

$$|\psi_0\rangle = \begin{pmatrix} \Omega_{23} \\ 0 \\ -\Omega_{12}^* \end{pmatrix}.$$

In the case where $|\Omega_{23}| \gg |\Omega_{12}|$, we can approximate this with $(1, 0, 0)$. Similarly when $|\Omega_{23}| \ll |\Omega_{12}|$, we can approximate it with $(0, 0, 1)$. Thus, our idea here is to modify Ω_{12} and Ω_{23} slowly to evolve the system between these two eigenstates. This would result in the trapped particle moving from well 1 to well 3.

What is surprising here is that the system will never be found in well 2. Also, as long as we maintain $|\Omega_{23}| \gg |\Omega_{12}|$, the system will remain in well 1 despite being able to tunnel into well 2.

7.4 Example: laser atom interaction

Now consider a three level system. We have a pump laser field that excites atoms from the ground state (state 1) into an excited state (state 2), and a Stokes field that entices the atoms down from the excited state into a middle state (state 3)between the ground and excited state. In this case, the coupling strength (Rabi frequency) is given by

$$\hbar\Omega_p = \langle\psi_1| - \mathbf{d}\cdot\mathbf{E}_p\,|\psi_2\rangle$$
$$\hbar\Omega_s = \langle\psi_2| - \mathbf{d}\cdot\mathbf{E}_s\,|\psi_3\rangle\,.$$

Qualitatively, the following three configurations have the same energy:

1. atom on state 1, with one free pump field photon,
2. atom on state 2, with one less pump field photon,
3. atom on state 3, with one more photon in the Stokes field.

However, configurations 1 and 2 are coupled, and configurations 2 and 3 are coupled. So the whole situation is analogous to the three-well problem above. For convenience, set $E_2 = 0$. The effective Hamiltonian is thus

$$H_{\text{eff}} = \frac{\hbar}{2}\begin{pmatrix} 0 & \Omega_p & 0 \\ \Omega_p^* & 0 & \Omega_s \\ 0 & \Omega_s^* & 0 \end{pmatrix}.$$

We will do something counter-intuitive. We will turn on the Stoke field first then transition into the pumping field. This is a transition from a state of $|\Omega_s| \gg |\Omega_p|$ into $|\Omega_s| \ll |\Omega_p|$. By

a similar reasoning as the previous section, atoms transition from state 1 to 3 without going through state 2. This is useful in certain cases, such as when the excited state is too energetic and so decays too quickly.

If we kept $|\Omega_s| \gg |\Omega_p|$ throughout the evolution, the atom will remain at the ground state. This is kind of surprising, because this means that the atoms are not going to absorb the pumping field, even if it is at a resonant frequency. This means that we are able to turn a opaque medium transparent. This is called Electromagnetically Induced Transparency.

7.5 Example: Landau-Zener process

Consider the Hamiltonian

$$H_{LZ} = \begin{pmatrix} -\gamma & \Delta \\ \Delta & \gamma \end{pmatrix}.$$

We want to find out what happens when we change the bias parameter γ from $+\infty$ to $-\infty$. Firstly, the eigenvalues are given by $E_\pm = \pm\sqrt{\Delta^2 + \gamma^2}$. The eigenvectors are (up to normalization):

$$\begin{pmatrix} \Delta \\ E_\pm + \gamma \end{pmatrix}.$$

Let us only worry about the case for E_+. When $\gamma = +\infty$, the resulting state will be $(0, 1)$ and when $\gamma = -\infty$, the resulting state will be $(1, 0)$. The eigenvector for E_- will be orthogonal to the eigenvector for E_+. Thus at $\gamma = +\infty$ the system is at $(1, 0)$, and at $\gamma = -\infty$ the system is at $(0, 1)$. So this is a way to implement a NOT gate. One big advantage of this operation (and similarly for all adiabatic processes) is that the system is not sensitive to the duration of the operation.

8 Berry phase

Suppose we have parameters $\lambda_1, \lambda_2, \ldots$ and our Hamiltonian is parametrised by them. If we let the system adiabatically evolve through a closed loop in the parameter space, what is the resultant geometric phase of the system after it has finished the loop? The obtained phase for this process is called the Berry phase.

In a closed loop in the λ space the geometric phase can be written as

$$\gamma_m = i \oint \langle \psi_m(\lambda) | \boldsymbol{\nabla} | \psi_m(\lambda) \rangle \cdot \mathrm{d}\lambda \,.$$

Using Stoke's theorem,

$$\gamma_m = i \int_S \boldsymbol{\nabla} \times \langle \psi_m(\lambda) | \boldsymbol{\nabla} | \psi_m(\lambda) \rangle \cdot \mathrm{d}\lambda \,.$$

We have previously shown that the geometric phase is zero if the eigenfunction can be chosen to always be real. Then in this case the Berry phase will also be zero. Moreover, the Berry phase

is independent of how we choose the overall phases of the eigenstates that are continuous over the parameters. This is known as the gauge invariance of the Berry phase. To see this, consider the eigenstate $e^{if_n(\lambda)}|\psi_n(\lambda)\rangle$. The new Berry phase is

$$\begin{aligned}
\gamma_m &= i\oint \langle\psi_m(\lambda)|\, e^{-if_m(\lambda)}\boldsymbol{\nabla}\left|\left[e^{if_m(\lambda)}\psi_m(\lambda)\right]\right\rangle \cdot \mathrm{d}\lambda \\
&= i\oint \langle\psi_m(\lambda)|\, e^{-if_m(\lambda)}\left[i(\boldsymbol{\nabla} f_m(\lambda))e^{if_m(\lambda)}\,|\psi_m(\lambda)\rangle + e^{if_m(\lambda)}\boldsymbol{\nabla}\,|\psi_m(\lambda)\rangle\right]\cdot \mathrm{d}\lambda \\
&= i\oint \boldsymbol{\nabla} f_m(\lambda)\cdot \mathrm{d}\lambda + i\oint \langle\psi_m(\lambda)|\,\boldsymbol{\nabla}\,|\psi_m(\lambda)\rangle\cdot \mathrm{d}\lambda
\end{aligned}$$

The first integral is zero since we are integrating over a closed loop. Thus the phase change does not affect the Berry phase.

In differential geometry, The "parallel" in parallel transport means that the inner product is maintained locally to be unity. The loose analogue of this in quantum mechanics is to change states while maintaining the inner product at unity:

$$\begin{aligned}
\langle\psi_n(\lambda)|\psi_n(\lambda+\mathrm{d}\lambda)\rangle &= 1 \\
\left\langle\psi_n(\lambda)\middle|\psi_n(\lambda)+\frac{\mathrm{d}|\psi_n(\lambda)}{\mathrm{d}\lambda}\right\rangle &= 1 \\
1+\langle\psi_n(\lambda)|\,\frac{\mathrm{d}\,|\psi_n(\lambda)\rangle}{\mathrm{d}\lambda} &= 1 \\
\langle\psi_n(\lambda)|\,\frac{\mathrm{d}\,|\psi_n(\lambda)\rangle}{\mathrm{d}\lambda} &= 0.
\end{aligned}$$

Substituting in a state with a relative phase,

$$\begin{aligned}
\langle\psi_n(\lambda)|\,e^{-if_n(\lambda)}\frac{\mathrm{d}}{\mathrm{d}\lambda}\left[e^{if_n(\lambda)}\,|\psi_n(\lambda)\rangle\right] &= 0 \\
\langle\psi_n(\lambda)|\,e^{-if_n(\lambda)}\left[i\frac{\mathrm{d}f}{\mathrm{d}\lambda}e^{if_n(\lambda)}\,|\psi_n(\lambda)\rangle + e^{if_n(\lambda)}\frac{\mathrm{d}\,|\psi_n(\lambda)\rangle}{\mathrm{d}\lambda}\right] &= 0 \\
\frac{\mathrm{d}f}{\mathrm{d}\lambda} &= i\,\langle\psi_n(\lambda)|\,\frac{\mathrm{d}\,|\psi_n(\lambda)\rangle}{\mathrm{d}\lambda}
\end{aligned}$$

is exactly the expression for the Berry phase. Local parallel transport does not preserve local phase.

8.1 Example: particle in magnetic field

Consider a spin $\frac{1}{2}$ particle in a slowly rotating magnetic field with components

$$B_x = B\sin\theta\cos\phi \qquad B_y = B\sin\theta\sin\phi \qquad B_z = B\cos\theta$$

The Hamiltonian is given by

$$\begin{aligned}
H &= -\gamma\mathbf{B}\cdot\mathbf{S} \\
&= -\frac{\gamma\hbar}{2}(B_x\sigma_x + B_y\sigma_y + B_z\sigma_z) \\
&= -\frac{\gamma\hbar}{2}B\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}
\end{aligned}$$

The ground state is given by the spin up state

$$\chi_+(\theta,\phi) = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}.$$

Consider the simple loop with constant θ and ϕ goes from 0 to 2π. The Berry phase is given by

$$\begin{aligned} i\int_0^{2\pi} \langle\chi_+| \frac{\mathrm{d}\,|\chi_+\rangle}{\mathrm{d}\phi}\,\mathrm{d}\phi &= i\int_0^{2\pi} \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix} \begin{pmatrix} 0 \\ ie^{i\phi}\sin\frac{\theta}{2}\end{pmatrix}\mathrm{d}\phi \\ &= i^2\int_0^{2\pi}\sin^2\frac{\theta}{2}\,\mathrm{d}\phi \\ &= \pi(\cos\theta - 1). \end{aligned}$$

For an arbitrary loop, we can use the curl form:

$$\begin{aligned} i\iint_S \boldsymbol{\nabla}\times \begin{pmatrix} \langle\chi_+|\frac{\mathrm{d}}{\mathrm{d}\theta}|\chi_+\rangle \\ \langle\chi_+|\frac{\mathrm{d}}{\mathrm{d}\phi}|\chi_+\rangle \\ 0\end{pmatrix}\cdot \mathrm{d}\theta\,\mathrm{d}\phi &= -\iint_S \frac{\mathrm{d}}{\mathrm{d}\theta}\sin^2\frac{\theta}{2}\,\mathrm{d}\theta\,\mathrm{d}\phi \\ &= -\frac{1}{2}\iint_S \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,. \end{aligned}$$

The integral is just the expression for a solid angle on the Bloch sphere traced out by the loop. Hence, we see how the geometric phase actually relates to some kind of interpreted geometry in the parameter phase. The integral is also a flux integral, and the curl looks like some kind of fictitious magnetic field. Thus this is an analogue of a magnetic field that has magnetic monopoles, since it has flux.

9 Transitionless quantum driving

We have previously derived that adiabatic processes bring the k-th eigenstate of the initial Hamiltonian to the k-eigenstate of the new Hamiltonian. Can we do this precisely and rapidly? In other words, given an initial state $|\Psi(0)\rangle = |\psi_k(\lambda(0))\rangle$ which evolves later to $|\Psi(t)\rangle = e^{i\theta_k(t)}e^{i\gamma_k(t)}\,|\psi_k(\lambda(t))\rangle$, how do we make this into an exact solution of a system with some Hamiltonian $H(t)$.

Let us recall evaluate a few terms that will be used later:

$$\begin{aligned} \theta_k &= -\frac{1}{\hbar}\int_0^t E_k(\lambda(t'))\,\mathrm{d}t' \\ \dot\theta_k &= -\frac{1}{\hbar}E_k(\lambda(t)) \\ \gamma_k &= i\int_0^t \langle\psi(\lambda(t'))|\frac{\mathrm{d}\,|\psi(\lambda(t'))\rangle}{\mathrm{d}t'}\,\mathrm{d}t' \\ \dot\gamma_k &= i\,\langle\psi_k(\lambda(t))|\frac{\mathrm{d}\,|\psi_k(\lambda)\rangle}{\mathrm{d}\lambda}\dot\lambda \end{aligned}$$

We know that the following unitary operator maps the initial state to the final state:

$$U(t,0) = \sum_k e^{i\theta_k(t)}e^{i\gamma_k(t)}\,|\psi_k(\lambda(t))\rangle\langle\psi_k(\lambda(0))|\,.$$

What kind of Hamiltonian can realise U? From the Schroödinger equation, the Hamiltonian is given by

$$\begin{aligned}
H &= i\hbar \frac{\partial U}{\partial t} U^{-1} \\
&= i\hbar \left[\sum_k i(\dot{\theta}_k + \dot{\gamma}_k) e^{i\theta_k} e^{i\gamma_k} \left|\psi_k(\lambda(t))\right\rangle\!\left\langle\psi_k(\lambda(0))\right| + e^{i\theta_k} e^{i\gamma_k} \frac{\partial \left|\psi_k(\lambda(t))\right\rangle}{\partial \lambda} \dot{\lambda} \left\langle\psi_k(\lambda(0))\right| \right] \\
&\quad \left[\sum_j e^{-i\theta_j} e^{-i\gamma_j} \left|\psi_j(\lambda(0))\right\rangle\!\left\langle\psi_k(\lambda(t))\right| \right] \\
&= i\hbar \left[\sum_k i(\dot{\theta}_k + \dot{\gamma}_k) \left|\psi_k(\lambda(t))\right\rangle\!\left\langle\psi_k(\lambda(0))\right| + \dot{\lambda} \frac{\partial \left|\psi_k(\lambda(t))\right\rangle}{\partial \lambda} \left\langle\psi_k(\lambda(t))\right| \right] \\
&= i\hbar \Big[\sum_k i \left(-\frac{1}{\hbar} E_k(\lambda(t)) + i \left\langle\psi_k(\lambda(t))\right| \frac{\partial \left|\psi_k(\lambda(t))\right\rangle}{\partial \lambda} \dot{\lambda} \right) \left|\psi_k(\lambda(t))\right\rangle\!\left\langle\psi_k(\lambda(0))\right| \\
&\quad + \dot{\lambda} \frac{\partial \left|\psi_k(\lambda(t))\right\rangle}{\partial \lambda} \left\langle\psi_k(\lambda(t))\right| \Big] \\
&= H(\lambda(t)) + i\hbar\dot{\lambda} \sum_k \left[- \left|\psi_k(\lambda)\right\rangle\!\left\langle\psi_k(\lambda)\right| \left\langle\psi_k(\lambda)\right| \frac{\partial \left|\psi_k(\lambda)\right\rangle}{\partial \lambda} + \frac{\partial \left|\psi_k(\lambda)\right\rangle}{\partial \lambda} \left\langle\psi_k(\lambda)\right| \right] \\
&= H(\lambda(t)) + i\hbar\dot{\lambda} \sum_{m \neq k} \frac{\left\langle\psi_m(\lambda)\right| \frac{\mathrm{d}H(\lambda)}{\mathrm{d}\lambda} \left|\psi_k(\lambda)\right\rangle}{E_k(\lambda) - E_m(\lambda)} \left|\psi_m(\lambda)\right\rangle \left\langle\psi_k(\lambda)\right| .
\end{aligned}$$

The last step was achieved by inserting the completeness condition into the second term in the summation, and by using the fact that

$$\left\langle\psi_m\right| \frac{\mathrm{d} \left|\psi_n(\lambda)\right\rangle}{\mathrm{d}\lambda} = \frac{\left\langle\psi_m(\lambda)\right| \frac{\mathrm{d}H(\lambda)}{\mathrm{d}\lambda} \left|\psi_n(\lambda)\right\rangle}{E_n(\lambda) - E_m(\lambda)}.$$

Now, going back to our derivation, notice that in the adiabatic limit $\dot{\lambda} \to 0$, the second term goes to zero, which supports the initial claim made by adiabatic approximation. Also it is evident that the cost we pay for speed is the complexity of creating a system that obey this new Hamiltonian.

9.1 Example: application to Landau-Zener process

Recall the Hamiltonian

$$H_{LZ} = \begin{pmatrix} -\gamma & \Delta \\ \Delta & \gamma \end{pmatrix}$$

We showed that an adiabatic Landau-Zener process can realise a NOT operation. Since the wavefunction can always be chosen to be real, the geometric phase is zero. So for our case

$$U = \sum_{k=1,2} e^{i\theta_k(t)} \left|\psi_k(\gamma(t))\right\rangle\!\left\langle\psi_k(\gamma(0))\right|$$

where the two eigenstates are given by

$$\left|\psi_1(\gamma)\right\rangle = \begin{pmatrix} \sin\frac{\beta}{2} \\ \cos\frac{\beta}{2} \end{pmatrix} \qquad\qquad \left|\psi_2(\gamma)\right\rangle = \begin{pmatrix} -\cos\frac{\beta}{2} \\ \sin\frac{\beta}{2} \end{pmatrix}$$

where $\beta = \operatorname{arccot}(\gamma/\Delta)$. This parametrisation simplifies normalisation. The results we have derived give us an alternative Hamiltonian. The following computation is obtained not from the last result in the derivation above, but from the third line.

$$\begin{aligned}
H &= H_{LZ} + i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\sin\frac{\beta}{2}\\ \cos\frac{\beta}{2}\end{pmatrix}\begin{pmatrix}\sin\frac{\beta}{2} & \cos\frac{\beta}{2}\end{pmatrix} + i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}-\cos\frac{\beta}{2}\\ \sin\frac{\beta}{2}\end{pmatrix}\begin{pmatrix}-\cos\frac{\beta}{2} & \sin\frac{\beta}{2}\end{pmatrix}\\
&= H_{LZ} + i\hbar\frac{\dot\beta}{2}\begin{pmatrix}-\cos\frac{\beta}{2}\sin\frac{\beta}{2} & \cos^2\frac{\beta}{2}\\ -\sin^2\frac{\beta}{2} & -\sin\frac{\beta}{2}\cos\frac{\beta}{2}\end{pmatrix} + i\hbar\frac{\dot\beta}{2}\begin{pmatrix}-\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin^2\frac{\beta}{2}\\ -\cos^2\frac{\beta}{2} & \cos\frac{\beta}{2}\sin\frac{\beta}{2}\end{pmatrix}\\
&= H_{LZ} + i\hbar\frac{\dot\beta}{2}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\\
&= H_{LZ} - \frac{\dot\beta\hbar}{2}\sigma_y
\end{aligned}$$

This Hamiltonian is comparatively easy to create. All we need to do is to apply a field along the y direction with a time dependence matching $\dot\beta$.

10 Open quantum systems

The motivation behind this section is that all quantum systems are in the presence of some environment. Thus it is necessary to understand what happens to a quantum system in this situation. Previously we have always assumed that the system and environment is one and the same, described by some Hamiltonian, etc. Now we have to be very clear what we are interested and not interested in.

Consider entanglement. We have two systems. Once they interact, the total wavefunction in general will no longer be a direct product of their individual wavefunctions and this is what we call "entanglement". In principle, the entire universe must be described by one whole entity as a highly entangled wavefunction.

What is the difference between classical and quantum correlation? Suppose Alice and Bob have a total of \$100. Then by knowing the amount of money Alice has, we will know the money Bob has. Now consider an entangled system

$$\frac{1}{\sqrt{2}}[|\uparrow\rangle_A|\downarrow\rangle_B - |\downarrow\rangle_A|\uparrow\rangle_B]$$

By measuring particle A we will know the state of B since they are of opposite spin by construction. This is exactly like classical correlation, and there is nothing to be excited of. However, wavefunctions do not describe reality, but potentiality. Observations depend on how measurement is performed. Consider the following rewriting of the same wavefunction:

$$\frac{1}{\sqrt{2}}\left[\frac{|\uparrow\rangle_A + |\downarrow\rangle_A}{\sqrt{2}}\otimes\frac{-|\uparrow\rangle_B + |\downarrow\rangle_B}{\sqrt{2}} + \frac{|\uparrow\rangle_A - |\downarrow\rangle_A}{\sqrt{2}}\otimes\frac{|\uparrow\rangle_B + |\downarrow\rangle_B}{\sqrt{2}}\right]$$

Thus a different measurement on A will cause different properties to emerge on B. Entanglement is thus correlations about potentiality, without having reality first. How system B's reality emerges depends on how we go about measuring particle A.

10.1 Density matrices

A pure state is a system that is described by a wavefunction. So far, all that we have learned is regarding pure states. If a system is in state $|\psi\rangle$ then we define the *density matrix* (or *density operator*)

$$\hat{\rho} = |\psi\rangle\langle\psi| \,.$$

We have the von Neumann equation

$$\begin{aligned} i\hbar\frac{\partial\hat{\rho}}{\partial t} &= i\hbar\frac{\partial\,|\psi\rangle}{\partial t}\,\langle\psi| + |\psi\rangle\, i\hbar\frac{\partial\,\langle\psi|}{\partial t} \\ &= H\,|\psi\rangle\langle\psi| + |\psi\rangle\,[H\,|\psi\rangle]^\dagger \\ &= H\hat{\rho} - \hat{\rho}H \\ &= [H,\hat{\rho}]. \end{aligned}$$

We can also do the same in the interaction representation,

$$\hat{\rho}_I(t) = |\psi_I(t)\rangle\langle\psi_I(t)|$$

and

$$i\hbar\frac{\partial\hat{\rho}_I}{\partial t} = [V_I,\hat{\rho}_I]$$

recalling

$$i\hbar\frac{\partial\hat{U}_I(t,t_0)}{\partial t} = \hat{V}_I(t)\hat{U}_I(t,t_0).$$

In a particular representation $|\psi\rangle = \sum_i c_i\,|\psi_i\rangle$, then we have the matrix

$$\begin{aligned} \hat{\rho} &= \sum_{ij} c_i c_j^*\,|\psi_i\rangle\langle\psi_j| \\ &= \begin{pmatrix} |c_1|^2 & & c_ic_j^* \\ & |c_2|^2 & \\ & \ddots & \\ c_i^*c_j & & |c_n|^2 \end{pmatrix}. \end{aligned}$$

This also tells us why we call it a density matrix. The diagonal terms gives us the population in a certain representation, and the off diagonal terms are something called "coherence" that are cross terms during expansion and intuitively measure the interference between states.

10.1.1 Trace of density matrices

By normalisation it follows that

$$\operatorname{tr}\hat{\rho} = 1.$$

We also have

$$\begin{aligned}\operatorname{tr}\hat{\rho}^2 &= \operatorname{tr}(|\psi\rangle\langle\psi|\psi\rangle\langle\psi|)\\ &= \operatorname{tr}|\psi\rangle\langle\psi|\\ &= 1\end{aligned}$$

Suppose we have an observable $\hat{A}$ with eigenstates $|\psi_i\rangle$ such that $\hat{A}|\psi_i\rangle = A_i|\psi_i\rangle$. The expectation value is given by

$$\begin{aligned}\langle\psi|\hat{A}|\psi\rangle &= \sum_i A_i|\langle\phi_i|\psi\rangle|^2\\ &= \sum_i \langle\phi_i|\psi\rangle\ \langle\psi|A_i|\phi_i\rangle\\ &= \sum_i \langle\phi_i|\,\hat{\rho}\hat{A}\,|\phi_i\rangle\\ &= \operatorname{tr}\hat{\rho}\hat{A}\end{aligned}$$

Here it may be helpful to point out that $\operatorname{tr} AB = \operatorname{tr} BA$.

10.1.2 Mixed state density operators

Consider the following experimental setup. We make a spin measurement on a particle, and if it has spin up, we produce a state $|\psi_1\rangle$, and if it has spin down, we produce a state $|\psi_2\rangle$. Now how do we describe the entire ensemble as a whole?

The system produced is $|\psi_k\rangle$, with probability P_k. Then the ensemble average

$$\begin{aligned}\left\langle\hat{A}\right\rangle &= \sum_k P_k\langle\psi_k|\hat{A}|\psi_k\rangle\\ &= \sum_k P_k \operatorname{tr}|\psi_k\rangle\langle\psi_k|\,\hat{A}\\ &= \operatorname{tr}\sum_k P_k|\psi_k\rangle\langle\psi_k|\,\hat{A}\end{aligned}$$

This naturally gives rise to the definition of the mixed state density operator

$$\rho^{\text{mix}} = \sum_k P_k|\psi_k\rangle\langle\psi_k|\,.$$

It is also easy to determine some properties of the trace

$$\begin{aligned}\operatorname{tr}\hat{\rho}^2 &= \operatorname{tr}\sum_k P_k^2|\psi_k\rangle\langle\psi_k|\\ &= \sum_k P_k^2 \operatorname{tr}|\psi_k\rangle\langle\psi_k|\\ &= \sum_k P_k^2\end{aligned}$$

Thus, if $\operatorname{tr}\hat{\rho}^2 = 1$, then we have a pure state. Otherwise, it is a mixed state.

There is a difference between mixed states and superposition states. For instance, the pure state $|\psi\rangle = c_1 |\psi_1\rangle + c_2 |\psi_2\rangle$ will be measured at state $|\psi_1\rangle$ with probability $|c_1|^2$ and state $|\psi_2\rangle$ with probability $|c_2|^2$. However, this is an entirely quantum description. The state is prepared exactly in the state $|psi\rangle$. This does not mean that the system is *at* state $|\psi_1\rangle$ with probability $|c_1|^2$ and state $|\psi_2\rangle$ with probability $|c_2|^2$. To further highlight the difference, consider the density operators for the pure and mixed situations:

$$\hat{\rho} = \begin{pmatrix} |c_1|^2 & c_1 c_2^* \\ c_1^* c_2 & |c_2|^2 \end{pmatrix} \qquad \hat{\rho}^{\text{mix}} = \begin{pmatrix} |c_1|^2 & 0 \\ 0 & |c_2|^2 \end{pmatrix}.$$

Here is a puzzle to highlight this further. Let there be a macroscopic ball of mass M rolling back and forth on a U-shaped curve. We may assume that this could be described as a mixed state of different energy eigenstates

$$\rho_{\text{ball}} = \sum_k P_k(t) \, |E_k\rangle\langle E_k| \, ,$$

because we do not expect the massive particle to exhibit any quantum interference effects. Let us calculate the expectation value of position x:

$$\begin{aligned} \operatorname{tr}\left[\hat{x} \sum_k P_k(t) \, |E_k\rangle\langle E_k|\right] &= \int \langle x| \, \hat{x} \sum_k P_k(t) \, |E_k\rangle\langle E_k| \, |x\rangle \, \mathrm{d}x \\ &= \int \langle E_k|x\rangle \; \langle x|\hat{x} \sum_k P_k(t) |E_k\rangle \, \mathrm{d}x \\ &= \sum_k \langle E_k|\hat{x}|E_k\rangle \, P_k(t) \\ &= 0 \end{aligned}$$

Thus the particle never moves if it is described as a mixed state. Even at macroscopic levels, quantum interference effects still play a role. This is actually not surprising, because stationary states are stationary apart from some phase change. To have meaningful time dependent behaviour, we cannot avoid interference between stationary states.

10.1.3 Reduced density matrix

We have a system A which is of interest and a system B which comprises of all other degrees of freedom, including the environment. The likely observables will look something like $\hat{O}_{\text{A}} \otimes \mathbf{I}_{\text{b}}$ where $\mathbf{I}_{\text{B}}$ is the identity operator on system B. In this case, we will see that we do not need the density matrix of the entire system.

Let the basis of system A be $|\psi_l\rangle$ and the basis of system B be $|\phi_k\rangle$. The entire system has basis $|\psi_l\rangle \, |\phi_k\rangle$. The trace of some operator $\hat{O}_{\text{AB}}$ in this system is hence

$$\sum_{l,k} \langle\psi_l| \, \langle\phi_k| \, \hat{O}_{\text{AB}} \, |\phi_k\rangle \, |\psi_l\rangle = \sum_l \langle\psi_l| \left(\sum_k \langle\phi_k| \, \hat{O}_{\text{AB}} \, |\phi_k\rangle \right) |\psi_l\rangle$$

where the term in brackets is called a partial trace.

As an example, the trace of the density operator is given by

$$\begin{aligned}\operatorname{tr}\hat{\rho}_{\mathrm{AB}} &= \sum_l \langle\psi_l| \left(\sum_k \langle\phi_k| \hat{\rho}_{\mathrm{AB}} |\phi_k\rangle\right) |\psi_l\rangle \\ &= \sum_l \langle\psi_l| \hat{\rho}_A |\psi_l\rangle \\ &= \operatorname{tr}_A \hat{\rho}_A\end{aligned}$$

where we have defined $\hat{\rho}_A$ as the partial trace. This term is our reduced density matrix.

To see the usefulness of this definition, consider the expectation of our operator $\hat{O}_{\mathrm{A}} \otimes \mathbf{I}_{\mathrm{B}}$.

$$\begin{aligned}\operatorname{tr}\Big(\hat{\rho}_{\mathrm{AB}}\hat{O}_{\mathrm{AB}} \otimes \mathbf{I}_{\mathrm{B}}\Big) &= \sum_{k,l} \langle\psi_l| \langle\phi_k| \hat{\rho}_{\mathrm{AB}} |\phi_k\rangle \hat{O}_{\mathrm{A}} |\psi_l\rangle \\ &= \sum_l \langle\psi_l| \sum_k \langle\phi_k| \hat{\rho}_{\mathrm{AB}} |\phi_k\rangle \hat{O}_{\mathrm{A}} |\psi_l\rangle \\ &= \sum_l \langle\psi_l| \hat{\rho}_{\mathrm{A}}\hat{O}_{\mathrm{A}} |\psi_l\rangle \\ &= \operatorname{tr}_{\mathrm{A}} \hat{\rho}_{\mathrm{A}}\hat{O}_{\mathrm{A}}\end{aligned}$$

10.2 Quantum measurement

What happens during measurement? von Neumann proposed that measurement is implemented by physical interaction. A apparatus could be thought of as something that tries to map a system's state onto say a needle's state:

$$|\mathrm{system}_i\rangle \left|\mathrm{apparatus}_{\mathrm{ready}}\right\rangle \to |\mathrm{system}_i\rangle |\mathrm{apparatus}_i\rangle$$

What if the initial system is in a superposition?

$$\sum_i c_i |s_i\rangle |a_{\mathrm{ready}}\rangle \to \sum_i c_i |s_i\rangle |a_i\rangle$$

At the end of measurement, the system and apparatus becomes entangled. Let us compute the reduced density matrix of the apparatus. The total density matrix is

$$\hat{\rho}_{sa} = \sum_i c_i |s_i\rangle |a_i\rangle \sum_j c_j^* \langle a_j| \langle s_j|$$

The reduced density matrix is

$$\begin{aligned}\hat{\rho}_a &= \operatorname{tr}_s \hat{\rho}_{sa} \\ &= \operatorname{tr}_s \left[\sum_{ij} c_i c_j^* |a_i\rangle\langle a_j| |s_i\rangle\langle s_j|\right] \\ &= \sum_{ij} c_i c_j^* |a_i\rangle\langle a_j| \langle s_j|s_i\rangle \\ &= \sum_i |c_i|^2 |a_i\rangle\langle a_i|\end{aligned}$$

In the end the apparatus is a mixed state, which seems like it has been prepared in state i with probability $|c_i|^2$. This agrees with Born's rule. We can do the same for the system, and get

$$\hat{\rho}_s = \sum_i |c_i|^2 |s_i\rangle\langle s_i| .$$

This is why we say that the act of measurement destroys the state.

10.2.1 Wigner's friend paradox

Here is a thought experiment called Wigner's friend. Wigner's friend measures the state of Schrödingers' cat.

$$\frac{1}{\sqrt{2}}(|\text{alive}\rangle + |\text{dead}\rangle)\,|\text{ready}\rangle \to \frac{1}{\sqrt{2}}(|\text{alive}\rangle\,|\text{happy}\rangle + |\text{dead}\rangle\,|\text{sad}\rangle)$$

Wigner thinks that before he asks his friend, his friend does not have an answer as his friend is entangled with the cat. However, from his friend's point of view, no matter if Wigner asks him or not, he has already performed the measurement, and the superposition has collapsed. Which is the correct state? There is still no easy answer. To perhaps resolve the so called paradox, we should keep in mind that the wavefunction is not a description of reality, but is only able to tell us statistics of measurements. Thus if Wigner and his friend took multiple measurements and took the ensemble average, they will agree. It is natural for them to disagree about the exact state with just a single measurement.

10.2.2 Which way information in double slit experiment

Consider the double slit experiment but now we have a detector at one slit to peek at which slit the particle has gone through.

$$\frac{1}{\sqrt{2}}(|\psi_R\rangle + |\psi_L\rangle)\,|\text{ready}\rangle \to \frac{1}{\sqrt{2}}(|\psi_R\rangle\,|\text{excited}\rangle + |\psi_L\rangle\,|\text{ground}\rangle)$$

Our reduced density is a mixed state density

$$\rho_{\text{atom}} = \frac{1}{2}(|\psi_R\rangle\langle\psi_R| + |\psi_L\rangle\langle\psi_L|)$$

The probability density distribution is given by

$$\text{tr}_{\text{atom}}\left[\rho_{\text{atom}}\,|x\rangle\langle x|\right] = \frac{1}{2}\big(|\psi_R(x)|^2 + |\psi_L(x)|^2\big).$$

The cross terms are gone so there is no longer any interference patterns. This is even if the detectors were just left alone without any observation. So long as the information of the travel path is available, it is enough to kill the superposition.

Now let us consider that we just set up the double slit experiment as usual (without any detectors), but with some environment between the slit and the detector, such as air molecules.

$$\frac{1}{\sqrt{2}}(|\psi_R\rangle + |\psi_L\rangle)\,|E_0\rangle \to \frac{1}{\sqrt{2}}(|\psi_R\rangle\,|E_R\rangle + |\psi_L\rangle\,|E_L\rangle)$$

The system's reduced density is given by

$$\hat{\rho}_s = \frac{1}{2}(|\psi_R\rangle\langle\psi_R| + |\psi_L\rangle\langle\psi_L| + \langle E_L|E_R\rangle\,|\psi_R\rangle\langle\psi_L| + \langle E_R|E_L\rangle\,|\psi_L\rangle\langle\psi_R|).$$

If the inner product $\langle E_L|E_R\rangle$ is small, then interference will vanish. If the environment is somehow insensitive to the path the atom takes, such that the inner product is still close to 1, then the interference will remain. The value $|\langle E_R|E_L\rangle|$ is often called the decoherence factor. Typically, the decoherence factor decays fast with time. That is, the information quickly leaks out and the environment is effectively measuring or collapsing the wavefunction.

10.2.3 Weak adiabatic measurement

In this measurement model, the wavefunction of the system under measurement is not collapsed. There is almost no entanglement between the system of interest and the measurement device, which is the culprit for causing wavefunction collapse in the von Neumann model. We will be using adiabatic evolution to imprint the expectation value of interest onto the quantum state of a measurement device. The device is then measured as per normal and the expectation value is estimated without collapsing the original system's wavefunction.

Consider a weak measurement model

$$H_s + \lambda A_s P_m$$

where H_s is the system Hamiltonian, A_s is some operator of the system, and P_m is the momentum operator of the device. Traditionally measurement would collapse the system onto some eigenstate of A_s, which is not what we want. We let the system couple very weakly to the device and slowly turn up λ.

Suppose the system is has an original eigenstate $H_s\,|\psi_n^0\rangle = E_n^0\,|\psi_n^0\rangle$. With weak coupling, the new eigenstate $|\psi_n(\lambda)\rangle \approx |\psi_n^0\rangle$ is still close to the original eigenstate. The energy is given by

$$E_n(\lambda) = E_n^0 + \left\langle\psi_n^0\right|\lambda A_s P_m\left|\psi_n^0\right\rangle$$

The second term is proportional to the expectation value of the operator $\langle\psi_n^0|A_s|\psi_n^0\rangle$.

The Heisenberg equation of motion

$$\begin{aligned}\frac{\mathrm{d}X_m}{\mathrm{d}t} &= \frac{i}{\hbar}\left[\left\langle\psi_n^0\right|\lambda A_s P_m\left|\psi_n^0\right\rangle, X_m\right] \\ &= \lambda\left\langle\psi_n^0\right|A_s\left|\psi_n^0\right\rangle\frac{i}{\hbar}[P_m, X_m] \\ &= \lambda\left\langle\psi_n^0\right|A_s\left|\psi_n^0\right\rangle\end{aligned}$$

This means that the expectation value of A_s can be deduced by measuring X_m, without collapsing the state of the system.

10.3 Decoherence

We will explore an exactly solvable decoherence model. Before we do that, we will further explore the idea of coherence.

Consider a symmetric double well system and we are only interested in the ground state $|\psi_g\rangle$ and first excited state $|\psi_e\rangle$, with respective eigenenergies E_0 and E_1. Start with a superposition state $\frac{1}{\sqrt{2}}(|\psi_g\rangle + |\psi_e\rangle)$. The density matrix of this system is

$$\hat{\rho}_s = \frac{1}{2}[|\psi_g\rangle\langle\psi_g| + |\psi_e\rangle\langle\psi_e| + |\psi_g\rangle\langle\psi_e| + |\psi_e\rangle\langle\psi_g|].$$

The spatial profile of the system is given by the expectation value

$$\langle x|\hat{\rho}_s|x\rangle = \frac{1}{2}[|\psi_g(x)|^2 + |\psi_e(x)|^2 + \psi_g(x)\psi_e^*(x) + \psi_e(x)\psi_g^*(x)].$$

After some time, each of the eigenstates will acquire some phase, and the state becomes $\frac{1}{\sqrt{2}}\left(e^{-iE_0t}|\psi_g\rangle + e^{-iE_1t}|\psi_e\rangle\right)$. Then the expectation value now becomes

$$\langle x|\hat{\rho}_s|x\rangle = \frac{1}{2}[|\psi_g(x)|^2 + |\psi_e(x)|^2 + e^{i(E_1-E_0)t}\psi_g(x)\psi_e^*(x) + e^{i(E_0-E_1)t}\psi_e(x)\psi_g^*(x)].$$

Thus, the phase difference creates something like a beat signal in the interference terms. The wave packet moves from the left well to the right well periodically. This is a simple description quantum tunnelling due to the interference between $|\psi_g\rangle$ and $|\psi_e\rangle$.

Suppose we now include an environment, such that $|\psi_g\rangle$ evolves to $|\psi_g\rangle|E_g\rangle e^{-iE_0t}$, and $|\psi_e\rangle$ evolves to $|\psi_e\rangle|E_e\rangle e^{-iE_1t}$. The expectation value becomes

$$\begin{aligned}&\langle x|\hat{\rho}_s|x\rangle \\ &= \frac{1}{2}[|\psi_g(x)|^2 + |\psi_e(x)|^2 + e^{i(E_1-E_0)t}\psi_g(x)\psi_e^*(x)\langle E_e|E_g\rangle + e^{i(E_0-E_1)t}\psi_e(x)\psi_g^*(x)\langle E_g|E_e\rangle].\end{aligned}$$

The particle's average position will oscillate, but this oscillation will slowly decay. The rate of decay depends on how fast the two branches diverge, or in other words depending on how fast the inner product decays.

10.4 Exactly solvable decoherence model

The ensemble is made up of a particle's spin interacting with a bath of harmonic oscillators. The system of interest has Hamiltonian

$$\hat{H}_s = \frac{1}{2}\omega_0\sigma_z$$

and the environment has Hamiltonian

$$\hat{H}_e = \sum_i \left(\frac{1}{2m_i}\hat{p}_i^2 + \frac{1}{2}m_i\omega_i^2\hat{q}_i^2\right).$$

We will introduce a specially tailored coupling between the two that allows us to solve the system precisely. This coupling has the following Hamiltonian:

$$\hat{H}_c = \hat{\sigma}_z \otimes \sum_i c_i\hat{q}_i.$$

For each oscillator, the system is linearly coupled to the position of the operator.

The position $\hat{q}$ and momentum $\hat{p}$ operators can be written in terms of creation and annihilation operators

$$\hat{p}_i = -i\sqrt{\frac{m_i\omega_i}{2}}\left(\hat{a}_i - \hat{a}_i^\dagger\right) \qquad\qquad \hat{q}_i = \sqrt{\frac{1}{2m_i\omega_i}}\left(\hat{a}_i + \hat{a}_i^\dagger\right).$$

The total Hamiltonian thus reads

$$\hat{H} = \underbrace{\frac{1}{2}\omega\hat{\sigma}_z}_{\hat{H}_s} + \underbrace{\sum_i \omega_i \hat{a}_i^\dagger \hat{a}_i}_{\hat{H}_e} + \underbrace{\hat{\sigma}_z \otimes \sum_i \left(g_i\hat{a}_i^\dagger + g_i^*\hat{a}_i\right)}_{\hat{H}_c}$$

Note that Hamiltonian commutes with σ_z. Furthermore, the environment is modelled as harmonic oscillators, which are easier to solve for. Finally, the coupling is linear in terms of $\hat{a}_i$ and $\hat{a}_i^\dagger$. These are some of the reasons why this problem can be solved exactly.

Let us work in the interaction representation. The Hamiltonian can be divided into the time dependent component comprising of the coupling $\hat{H}_c$ and the time independent component which is made up of the other two terms which we will call $\hat{H}_0$. We have the following relations:

$$\begin{aligned}
\frac{\mathrm{d}\hat{\sigma}_z}{\mathrm{d}t} &= i[\hat{H}_0, \hat{\sigma}_z] = 0 \\
\frac{\mathrm{d}\hat{a}_i^\dagger}{\mathrm{d}t} &= i[\hat{H}_0, \hat{a}_i^\dagger] = i\left[\sum_j \omega_j \hat{a}_j^\dagger \hat{a}_j, \hat{a}_i^\dagger\right] = i\omega\hat{a}_i^\dagger \\
\frac{\mathrm{d}\hat{a}_i}{\mathrm{d}t} &= i[\hat{H}_0, \hat{a}_i] = i\left[\sum_j \omega_j \hat{a}_j^\dagger \hat{a}_j, \hat{a}_i\right] = -i\omega\hat{a}_i
\end{aligned}$$

where all the operators above are in the interaction representation. This tells us that

$$\hat{\sigma}_{z\,I} = \sigma_z \qquad\qquad \hat{a}_{i\,I}^\dagger = e^{i\omega_i t}a_i^\dagger \qquad\qquad \hat{a}_{i\,I} = e^{-i\omega_i t}a_i$$

Thus, in the interaction representation

$$\hat{H}_{c\,I}(t) = \hat{\sigma}_z \otimes \sum_i \left[g_i\hat{a}_i^\dagger e^{i\omega t} + g_i^*\hat{a}_i e^{-i\omega t}\right]$$

Luckily, this problem is exactly solvable.

10.4.1 Magnus expansion solution

We introduce the Magnus expansion. Ordinarily for a problem such as

$$Y'(t) = A(t)Y(t)$$

where Y is a vector and A is a matrix. The regular approach is to use the Dyson series. There is another approach, where the solution can be written as

$$Y(t) = \exp\Omega(t, t_0)Y_0$$

where the operators

$$\begin{aligned}
\Omega(t) &= \sum_{k=1}^{\infty} \Omega_k(t) \\
\Omega_1(t) &= \int_0^t A(t_1)\,\mathrm{d}t_1 \\
\Omega_2(t) &= \frac{1}{2}\int_0^t \int_0^{t_1} [A(t_1), A(t_2)]\,\mathrm{d}t_2\,\mathrm{d}t_1 \\
\Omega_3(t) &= \frac{1}{6}\int_0^t \int_0^{t_1} \int_0^{t_2} [A(t_1), [A(t_2), A(t_3)]] + [A(t_3), [A(t_2), A(t_1)]\,\mathrm{d}t_3\,\mathrm{d}t_2\,\mathrm{d}t_1
\end{aligned}$$

Applying this to our problem

$$i\frac{\partial U_I}{\partial t} = H_I U_I,$$

make the ansatz

$$U_I = \exp\bigl(-iH_I^{\text{eff}} t\bigr)$$

with

$$\begin{aligned}
H_I^{\text{eff}} &= \sum_k B_k \\
B_1 &= \frac{1}{t}\int_0^t H_I(t_1)\,\mathrm{d}t_1 \\
B_2 &= -\frac{1}{2t}\int_0^t \int_0^{t_1} [H_I(t_1), H_I(t_2)]\,\mathrm{d}t_2\,\mathrm{d}t_1
\end{aligned}$$

and so on. As we will find out, $[H_I(t_1), H_I(t_2)]$ turns out to be a number. This means that all the commutators in the higher orders will go to 0, which means that the solution is exactly the series taken up to the second order. Evaluate the commutator:

$$\begin{aligned}
[H_I(t_1), H_I(t_2)] &= \left[\sum_i g_i \hat{a}_i^\dagger e^{i\omega_i t_1} + g_i^* \hat{a}_i e^{-i\omega_i t_1}, \sum_j g_j \hat{a}_j^\dagger e^{i\omega_j t_2} + g_j^* \hat{a}_j e^{-i\omega_j t_2}\right] \\
&= \sum_i g_i g_i^* [\hat{a}_i^\dagger, \hat{a}_i] e^{i\omega_i(t_1 - t_2)} + g_i g_i^* [\hat{a}_i, \hat{a}_i^\dagger] e^{-i\omega_i(t_1 - t_2)} \\
&= \sum_i |g_i|^2 \bigl(e^{-i\omega_i(t_1 - t_2)} - e^{i\omega_i(t_1 - t_2)}\bigr)
\end{aligned}$$

which is just a number. Furthermore, we see that B_2 will just produce some overall phase and so is not of our interest. We will hence focus on B_1, which is a time average of the Hamiltonian

in the interaction representation. The final solution, up to some phase, is

$$\begin{aligned}
U_I &= \exp\left(-i\int_0^t H_I(t')\,\mathrm{d}t'\right) \\
&= \exp\left(-i\sigma_z \otimes \sum_i \int_0^t g_i a_i^\dagger e^{i\omega_i t'} + g_i^* a_i e^{-i\omega_i t'}\,\mathrm{d}t'\right) \\
&= \exp\left[\sigma_z \sum_i \left(\frac{g_i a_i^\dagger (e^{i\omega_i t}-1)}{\omega_i} + \frac{g_i^* a_i (e^{-i\omega_i t}-1)}{-\omega_i}\right)\right] \\
&= \exp\left[\frac{\sigma_z}{2}\sum_i \left(a_i^\dagger \lambda_i(t) - a_i \lambda_i^*(t)\right)\right]
\end{aligned}$$

where

$$\lambda_i(t) = \frac{2g_i}{\omega_i}(1 - e^{i\omega_i t})$$

Let us test the solution with the state $|s\rangle = [a\,|\uparrow\rangle + b\,|\downarrow\rangle] \otimes |E_0\rangle$.

$$\begin{aligned}
&U_i(t)\,|s\rangle \\
&= a\exp\left[\frac{1}{2}\sum_i \left(a_i^\dagger \lambda_i(t) - a_i\lambda_i^*(t)\right)\right]|\uparrow\rangle\,|E_0\rangle + b\exp\left[-\frac{1}{2}\sum_i \left(a_i^\dagger \lambda_i(t) - a_i\lambda_i^*(t)\right)\right]|\downarrow\rangle\,|E_0\rangle \\
&= a\,|\uparrow\rangle \prod_i \exp\left[\frac{1}{2}\left(a_i^\dagger \lambda_i(t) - a_i\lambda_i^*(t)\right)\right]|E_0\rangle + b\,|\downarrow\rangle \prod_i \exp\left[-\frac{1}{2}\left(a_i^\dagger \lambda_i(t) - a_i\lambda_i^*(t)\right)\right]|E_0\rangle \\
&= a\,|\uparrow\rangle\,|\varepsilon_+(t)\rangle + b\,|\downarrow\rangle\,|\varepsilon_-(t)\rangle
\end{aligned}$$

Let

$$|\lambda\rangle = \exp\left[\lambda\hat{a}^\dagger - \lambda^*\hat{a}\right]|E_0\rangle\,.$$

This is known as a coherent state in quantum optics, because it can be shown that it is an eigenstate of $\hat{a}$. Then we can write

$$|\varepsilon_\pm\rangle = \prod_i \left|\pm\frac{\lambda_i}{2}\right\rangle.$$

It is not too important for us right now, but it can be expanded as

$$|\lambda\rangle = \exp\left(-\frac{|\lambda|^2}{2}\right)\sum_{n=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}\,|n\rangle$$

which gives us a relation between two coherent states:

$$\langle\lambda|\mu\rangle = \exp\left(-\frac{1}{2}|\lambda|^2 - \frac{1}{2}|\mu|^2 + \lambda^*\mu\right)$$

and so the decoherence factor is given by

$$\begin{aligned}
\langle\varepsilon_-|\varepsilon_+\rangle &= \prod_i \exp\left(-\frac{1}{2}|\lambda_i|^2\right) \\
&= \exp\left(-\sum_i \frac{4|g_i|^2}{\omega_i^2}(1-\cos\omega_i t)\right) \\
&\approx \exp\left(-\sum_i 2|g_i|^2 t^2\right)
\end{aligned}$$

The last step uses the approximation $\cos\omega_i t \approx 1 - \omega_i^2 t^2/2$. The decoherence factor exhibits Gaussian decay.

We are still in the interaction representation. To change back into the Schrödinger representation, we multiply the state with U_0. However, when computing the density matrix, U_0 and $U_0^\dagger$ will cancel. $\hat{\rho} = U_0 \hat{\rho}_I U_0^\dagger$ is simply a rotation. The key factor that determines the rate of decay is still the decoherence factor.

10.4.2 BCH formula solution

Again, we want to solve for the propagator

$$i\frac{\partial U_I}{\partial t} = \hat{H}_{cI} U_I$$

with

$$\hat{H}_{eI}(t) = \hat{\sigma}_z \otimes \sum_i \left[g_i \hat{a}_i^\dagger e^{i\omega t} + g_i^* \hat{a}_i e^{-i\omega t} \right].$$

Recall the BCH formula

$$\exp(i\delta A)\exp(i\delta B) = \exp(i\delta Z)$$

where

$$Z = A + B + \frac{i\delta}{2}[A,B] - \frac{\delta^2}{12}([A,[A,B]] + [B,[B,A]]) + \ldots.$$

Notice that if the commutator $[A,B]$ is a number, the later commutators will vanish.

We can split the evolution into many small time intervals. For example, let us just begin with the following:

$$U_I(t,0) = e^{-iH_I(t_3)\Delta t} e^{-iH_I(t_2)\Delta t} e^{-iH_I(t_1)\Delta t}.$$

We have previously shown that $[H_I(t), H_I(t')]$ is just a number. Using the BCH formula we can combine the last two exponentials:

$$U_I(t,0) = \exp(-iH_I(t_3)\Delta t)\exp(-i[H_I(t_2)+H_I(t_1)]\Delta t)\exp\left(-\frac{1}{2}[H_I(t_2),H_I(t_1)]\Delta t^2\right).$$

Applying it again:

$$U_I(t,0) = \exp(-i[H_I(t_3)+H_I(t_2)+H_I(t_1)]\Delta t)\exp\left(-\frac{1}{2}[H_I(t_3),H_I(t_2)+H_I(t_1)]\Delta t^2\right)\cdots$$

Generalising this for an arbitrary number of terms, we will have

$$U_I(t,0) = \exp\left(-i\sum_{j=1}^{n} H_I(t_j)\Delta t\right)\exp\left(-\frac{1}{2}\sum_{m=2}^{n}\left[H_I(t_m), \sum_{j=1}^{m-1} H_I(t_j)\right]\Delta t^2\right)$$

When we make $\Delta t \to 0$, the sums turn into integrals, and we have

$$U_I(t,0) = \exp\left(-i\int_0^t H_I(t')\,\mathrm{d}t'\right)\exp\left(-\frac{1}{2}\int_0^t\left[H_I(t'), \int_0^{t'} H_I(t'')\,\mathrm{d}t''\right]\mathrm{d}t'\right)$$

This looks like our solution given by the Magnus expansion.

10.5 Dynamical decoupling for suppression of decoherence

We have learned about decoherence and how it makes life hard when designing quantum systems. It is usually more difficult to affect the environment. Therefore, in this section we will learn how to affect the system instead to suppress the coupling between the system and environment.

Let us return to the pure dephasing model in the previous question.

$$\hat{H} = \frac{1}{2}\omega\hat{\sigma}_z + \sum_i \omega_i \hat{a}_i^\dagger \hat{a}_i + \hat{\sigma}_z \otimes \sum_i \left(g_i \hat{a}_i^\dagger + g_i^* \hat{a}_i\right) + \hat{H}_c(t)$$

Our goals is to find a control Hamiltonian $\hat{H}_c$ that may suppress the system-environment coupling. A basic idea we can come up with here is to make the spin flip rapidly about the z-axis. This makes σ_z averaged out to 0 from the environment's point of view, effectively decoupling the system and environment.

Let $\hbar = 1$. Since we have

$$i\frac{\mathrm{d}U_c(t)}{\mathrm{d}t} = \hat{H}_c(t)U_c(t),$$

finding U_c is equivalent to finding $\hat{H}_c$. Let us work in a representation rotated by U_c, or equivalently, by choosing U_c as the U_0 in the interaction representation. We denote operators in this representation with a tilde. Then, the effective Hamiltonian in this representation,

$$\begin{aligned}
\tilde{H} &= U_c^\dagger[H_s + H_e + H_{\text{int}} + H_c]U_c - iU_c^\dagger\frac{\mathrm{d}U_c}{\mathrm{d}t} \\
&= U_c^\dagger[H_s + H_e + H_{\text{int}} + H_c]U_c - U_c^\dagger H_c U_c \\
&= \tilde{H}_s + \hat{H}_e + \tilde{H}_{\text{int}}
\end{aligned}$$

The last step is because the environment operators commute with all system operators. U_c is only applied to the system and so $\tilde{H}_e = \hat{H}_e$.

Let us assume a periodic U_c with a period t_c, i.e. $U_c(t + t_c) = U_c(t)$. If t_c is small, then it sets a very small characteristic system. This period will affect $\tilde{H}$ as well, since its time dependence comes from U_c. Thus the unitary evolution operator induced by $\tilde{H}$ will also be periodic. Hence we only need to worry calculate the dynamics up to t_c:

$$U(Nt_c, 0) = U_c(Nt_0, 0)\tilde{U}(Nt_c, 0) = 1 \cdot \tilde{U}(t_0, 0)^N$$

So now we need to solve

$$i\frac{\mathrm{d}\tilde{U}}{\mathrm{d}t} = \tilde{H}\tilde{U}.$$

Applying Magnus expansion to the total propagator,

$$\begin{aligned}
\tilde{U}(t_c, 0) &\approx \exp\Big[-it_c(\tilde{H}_0 + \tilde{H}_1 + \dots)\Big] \\
\tilde{H}_0 &= \frac{1}{t_c}\int_0^{t_c} \tilde{H}(t_1)\,\mathrm{d}t_1 \\
\tilde{H}_1 &= \frac{-i}{2t_c}\int_0^{t_c}\int_0^{t_1} \Big[\tilde{H}(t_1), \tilde{H}(t_2)\Big]\,\mathrm{d}t_2\,\mathrm{d}t_1
\end{aligned}$$

Since the integrals are always from 0 to t_c, we can see that $\tilde{H}_0$ is of zeroth order of t_c, and $\tilde{H}_1$ is of first order of t_c. So if t_c is small enough, we can truncate the expansion up to the zeroth order. Furthermore, if

$$\int_0^{t_c} \tilde{H}_{\text{int}}(t)\,\mathrm{d}t = 0,$$

we have

$$\begin{aligned}
\tilde{U}(t_c, 0) &\approx \exp\left[-i\int_0^{t_c} \tilde{H}_s(t) + \hat{H}_e(t) + \tilde{H}_{\text{int}}(t)\,\mathrm{d}t\right] \\
&= \exp\left[-i\int_0^{t_c} \tilde{H}_s(t) + \hat{H}_e(t)\,\mathrm{d}t\right] \\
&= \exp\left[-i\int_0^{t_c} U_c^\dagger \hat{H}_s(t) U_c\,\mathrm{d}t\right] \otimes \exp\Big[-i\hat{H}_e t_c\Big].
\end{aligned}$$

This means that the final state will not be an entangled state.

So now our efforts are focused on finding a correct U_c that makes the integral vanish. Let us go back to the original pure dephasing model. $\hat{H}_{\text{int}}$ is essentially σ_z for our purposes since we cannot touch the environment part of the Hamiltonian. Propose $U_c = \exp\Big(-i\frac{2\pi t}{t_c}\sigma_x\Big)$.

$$\begin{aligned}
\int_0^{t_c} \exp\left(i\frac{2\pi t}{t_c}\sigma_x\right)\sigma_z \exp\left(-i\frac{2\pi t}{t_c}\sigma_x\right)\mathrm{d}t &= \int_0^{t_c} \sigma_z \exp\left(-i\frac{4\pi t}{t_c}\sigma_x\right)\mathrm{d}t \\
&= \sigma_z \int_0^{t_c} \cos\frac{4\pi t}{t_c} - i\sigma_x \sin\frac{4\pi t}{t_c}\,\mathrm{d}t \\
&= 0
\end{aligned}$$

Where we made use of the following relations.

$$\sigma_x\sigma_z = -\sigma_z\sigma_x \qquad\qquad \exp(i(\hat{\mathbf{n}}\cdot\sigma)\alpha) = \cos\alpha + i(\hat{\mathbf{n}}\cdot\sigma)\sin\alpha$$

Finally,

$$\begin{aligned}
H_c &= i\frac{\mathrm{d}U_c}{\mathrm{d}t}U_c^{-1} \\
&= \frac{2\pi}{t_c}\sigma_x
\end{aligned}$$

This answer is very natural! The easiest way to rotate the spin is to apply a field along the x-axis such that the spin precesses.

Could we create a more general U_c such that this scheme would work in a general situation? In other words, what if the coupling depends on all σ_x, σ_y, and σ_z? One thing we could try is to rotate the spin about two axes

$$U_c = \exp\left(i\frac{2\pi t}{t_c}n_y\sigma_y\right)\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)$$

Check with σ_y as coupling:

$$\begin{aligned}
&\int_0^{t_c} \exp\left(-i\frac{2\pi t}{t_c}n_y\sigma_y\right)\exp\left(-i\frac{2\pi t}{t_c}n_x\sigma_x\right)\sigma_y \exp\left(i\frac{2\pi t}{t_c}n_y\sigma_y\right)\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)\mathrm{d}t \\
&= \int_0^{t_c} \sigma_y \exp\left(i\frac{4\pi t}{t_c}n_x\sigma_x\right)\mathrm{d}t \\
&= 0
\end{aligned}$$

Check with σ_x as coupling:

$$\begin{aligned}
&\int_0^{t_c} \exp\left(-i\frac{2\pi t}{t_c}n_y\sigma_y\right)\exp\left(-i\frac{2\pi t}{t_c}n_x\sigma_x\right)\sigma_x\exp\left(i\frac{2\pi t}{t_c}n_y\sigma_y\right)\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)\mathrm{d}t\\
&=\int_0^{t_c} \exp\left(-i\frac{2\pi t}{t_c}n_y\sigma_y\right)\sigma_x\exp\left(i\frac{4\pi t}{t_c}n_y\sigma_y\right)\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)\mathrm{d}t\\
&=\int_0^{t_c} \sigma_x\exp\left(-i\frac{2\pi t}{t_c}n_y\sigma_y\right)\left[\cos\frac{4\pi t}{t_c}n_y+i\sigma_y\sin\frac{4\pi t}{t_c}n_y\right]\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)\mathrm{d}t\\
&=\sigma_x\int_0^{t_c} \sigma_y\exp\left(i\frac{2\pi t}{t_c}n_y\sigma_y\right)\left[i\sin\frac{4\pi t}{t_c}n_y\right]\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)\mathrm{d}t\\
&=i\sigma_x\sigma_y\int_0^{t_c} \sin\frac{4\pi t}{t_c}n_y\exp\left(i\frac{4\pi t}{t_c}n_x\sigma_x\right)\mathrm{d}t\\
&=i\sigma_x\sigma_y\int_0^{t_c} \sin\frac{4\pi t}{t_c}n_y\left[\cos\frac{4\pi t}{t_c}n_x+i\sigma_x\sin\frac{4\pi t}{t_c}n_x\right]\mathrm{d}t
\end{aligned}$$

This integral is 0 if $n_x \neq n_y$.

What is H_c?

$$\begin{aligned}
&H_c\\
&=i\frac{\mathrm{d}U_c}{\mathrm{d}t}U_c^{-1}\\
&=-\left[\frac{2\pi}{t_c}n_y\sigma_y\exp\left(i\frac{2\pi t}{t_c}n_y\sigma_y\right)\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)+\exp\left(i\frac{2\pi t}{t_c}n_y\sigma_y\right)\frac{2\pi}{t_c}n_x\sigma_x\exp\left(i\frac{2\pi t}{t_c}n_x\sigma_x\right)\right]\\
&\quad\exp\left(-i\frac{2\pi t}{t_c}n_x\sigma_x\right)\exp\left(-i\frac{2\pi t}{t_c}n_y\sigma_y\right)\\
&=-\frac{2\pi}{t_c}n_y\sigma_y-\frac{2\pi}{t_c}n_x\sigma_x\exp\left(-i\frac{4\pi t}{t_c}n_y\sigma_y\right)\\
&=-\frac{2\pi}{t_c}n_y\sigma_y-\frac{2\pi}{t_c}n_x\sigma_x\left[\cos\frac{4\pi t}{t_c}n_y-i\sigma_y\sin\frac{4\pi t}{t_c}n_y\right]
\end{aligned}$$

Notice how we have fields along all axes, recall $\sigma_x\sigma_y = -\sigma_z$.

10.6 Quantum Born-Markov master equation

This section will focus on the derivation of an equation of motion for the reduced density matrix of a system. More specifically, we are looking for a propagator for

$$\hat{\rho}_s(t) = \mathrm{tr}_e\,\rho_{se}(t) = \mathrm{tr}_e(\hat{U}\hat{\rho}_{se}(0)\hat{U}^\dagger).$$

We will be considering a total Hamiltonian of the form

$$\begin{aligned}
\hat{H} &= \hat{H}_s + \hat{H}_e + \hat{H}_c\\
&= \hat{H}_0 + \sum_\alpha \hat{S}_\alpha \otimes \hat{E}_\alpha
\end{aligned}$$

All terms are assumed to be time-independent.

If there is no environment, then

$$\frac{\mathrm{d}\hat{\rho}_s(t)}{\mathrm{d}t} = i[\hat{H}'_s, \hat{\rho}_s]$$

Here H' is to indicate possible modifications to the effective Hamiltonian due to the environment. If there is some system-environment coupling, we expect

$$\frac{\mathrm{d}\hat{\rho}_s(t)}{\mathrm{d}t} = -i[H'_s, \hat{\rho}_s] + D(\hat{\rho}_s),$$

which is a sum of some unitary evolution and additional environment effects.

We start off from

$$\frac{\mathrm{d}\hat{\rho}_I(t)}{\mathrm{d}t} = -i[\hat{H}_{eI}(t), \hat{\rho}_I(t)]$$

Here this density matrix is for the entire ensemble. Integrating the above

$$\hat{\rho}_I(t) = \hat{\rho}(0) - i\int_0^t [\hat{H}_{eI}(t), \hat{\rho}_I(t')]\,\mathrm{d}t'$$

Put the integral back into the original equation,

$$\begin{aligned}\frac{\mathrm{d}\hat{\rho}_I(t)}{\mathrm{d}t} &= -i\left[\hat{H}_{cI}(t), \hat{\rho}(0) - i\int_0^t [\hat{H}_{eI}(t), \hat{\rho}_I(t')]\,\mathrm{d}t'\right] \\ &= -i\Big[\hat{H}_{cI}(t), \hat{\rho}(0)\Big] - \int_0^t \left[\hat{H}_{eI}(t), \left[\hat{H}_{eI}(t), \hat{\rho}_I(t')\right]\right]\mathrm{d}t'\end{aligned}$$

We have $\hat{\rho}_{sI}(t) = \mathrm{tr}_e\,\hat{\rho}_I(t)$. Thus

$$\frac{\mathrm{d}\hat{\rho}_{sI}(t)}{\mathrm{d}t} = -i\,\mathrm{tr}_e\left[\hat{H}_{cI}(t), \hat{\rho}(0)\right] - \int_0^t \mathrm{tr}_e\left[\hat{H}_{eI}(t), \left[\hat{H}_{eI}(t), \hat{\rho}_I(t')\right]\right]\mathrm{d}t'$$

We will begin to make some approximations. First, we assume that at time $t = 0$, the system and environment are not entangled:

$$\hat{\rho}(0) = \hat{\rho}_s(0) \otimes \hat{\rho}_e(0).$$

Now,

$$\begin{aligned}\mathrm{tr}_e\,\hat{H}_{eI}(t)\hat{\rho}_I(0) &= \mathrm{tr}_e\left[\sum_\alpha S_\alpha(t)E_\alpha(t)\hat{\rho}_{eI}\right]\hat{\rho}_{sI}(0) \\ &= \sum_\alpha \mathrm{tr}_e[E_\alpha\hat{\rho}_{eI}]S_\alpha\hat{\rho}_{sI}(0) \\ &= \sum_\alpha \mathrm{tr}_e[e^{iH_e(t)}E_\alpha e^{-iH_e t}\hat{\rho}_{eI}]S_\alpha\hat{\rho}_{sI}(0) \\ &= \sum_\alpha \mathrm{tr}_e[E_\alpha\hat{\rho}_{eI}]S_\alpha\hat{\rho}_{sI}(0)\end{aligned}$$

The last step results from observing that from statistical mechanics we have $\rho_e = e^{-\beta H_e}/Z$ [2] and so they commute, and also the cyclic property of trace $\mathrm{tr}(AB) = \mathrm{tr}(BA)$. The trace turns

[2] Boltzmann distribution means that the state $|\psi_k\rangle$ with eigenvalue E_k occurs with probability $e^{-\beta E_k}/Z$. If the environment is at thermal equilibrium, then it is at a mixed state $\sum_k |\psi_k\rangle\langle\psi_k|\, e^{-\beta E_k}/Z = e^{-\beta H_e}/Z \sum_k |\psi_k\rangle\langle\psi_k| = e^{-\beta H_e}/Z$.

out to be time independent. We can easily set it to 0, and this is also known as the centring condition:

$$\mathrm{tr}_e\left[\hat{H}_{cI}(t), \hat{\rho}(0)\right] = 0.$$

So far up to the second order we have

$$\frac{\mathrm{d}\hat{\rho}_{sI}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{tr}_e\left[\hat{H}_{eI}(t), \left[\hat{H}_{eI}(t'), \hat{\rho}_I(t')\right]\right] \mathrm{d}t'$$

To simplify this, we make another approximation that

$$\hat{\rho}_I(t) = \hat{\rho}_{sI}(t) \otimes \hat{\rho}_e.$$

That is, the environment state is not perturbed by the system. We may worry that this approximation is too aggressive. However, it can be justified since we are already at the second order. Most of the interaction will be captured by the first two terms in the commutator. Their correlation is not assumed to be important any more. Thus,

$$\frac{\mathrm{d}\hat{\rho}_{sI}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{tr}_e\left[\hat{H}_{eI}(t), \left[\hat{H}_{eI}(t'), \hat{\rho}_{sI}(t') \otimes \hat{\rho}_e\right]\right] \mathrm{d}t'$$

Now,

$$\begin{aligned}
\hat{H}_{cI}(t) &= U_0^\dagger \hat{H}_c U_0 \\
&= e^{i(H_s+H_e)t} \sum_\alpha S_\alpha E_\alpha e^{-i(H_s+H_e)t} \\
&= \sum e^{iH_s t} S_\alpha e^{iH_s t} e^{iH_e t} E_\alpha e^{iH_e t} \\
&= \sum_\alpha S_{\alpha I} \otimes E_{\alpha I}
\end{aligned}$$

Let us simplify the commutators first.

$$\begin{aligned}
\mathrm{tr}_e\left[S_{\alpha I} \otimes E_{\alpha I}, \left[S'_{\beta I} \otimes E'_{\beta I}, \hat{\rho}'_{sI} \otimes \hat{\rho}_e\right]\right] &= \mathrm{tr}_e\left[S_{\alpha I} E_{\alpha I}, S'_{\beta I} E'_{\beta I} \hat{\rho}'_{sI} \hat{\rho}_e - \hat{\rho}'_{sI} \hat{\rho}_e S'_{\beta I} E'_{\beta I}\right] \\
&= \mathrm{tr}_e[S_{\alpha I} E_{\alpha I} S'_{\beta I} E'_{\beta I} \hat{\rho}'_{sI} \hat{\rho}_e - S_{\alpha I} E_{\alpha I} \hat{\rho}'_{sI} \hat{\rho}_e S'_{\beta I} E'_{\beta I} \\
&\qquad - S'_{\beta I} E'_{\beta I} \hat{\rho}'_{sI} \hat{\rho}_e S_{\alpha I} E_{\alpha I} + \hat{\rho}'_{sI} \hat{\rho}_e S'_{\beta I} E'_{\beta I} S_{\alpha I} E_{\alpha I}] \\
&= \mathrm{tr}_e[E_{\alpha I} E'_{\beta I} \hat{\rho}_e]\Big(S_{\alpha I} S'_{\beta I} \hat{\rho}'_{sI} - S'_{\beta I} \hat{\rho}'_{sI} S_{\alpha I}\Big) \\
&\qquad + \mathrm{tr}_e[E'_{\beta I} E_{\alpha I} \hat{\rho}_e]\Big(\hat{\rho}'_{sI} S'_{\beta I} S_{\alpha I} - S_{\alpha I} \hat{\rho}'_{sI} S'_{\beta I}\Big)
\end{aligned}$$

Here, the prime denotes using t' as argument versus t. Define the environment self correlation function as

$$\begin{aligned}
C_{\alpha\beta}(t-t') &= \mathrm{tr}_e[E_{\alpha I} E'_{\beta I} \hat{\rho}_e] \\
&= \left\langle E_{\alpha I} E'_{\beta I} \right\rangle_{\hat{\rho}_e}
\end{aligned}$$

We are close, except that on the left side of our equation we have $\hat{\rho}_{sI}(t)$, and on the other side we have $\hat{\rho}_{sI}(t')$. Finally we apply the Markov approximation. This means that the current rate of change does not depend on the entire history of the system. This is expressed by making the

correlator $C_{\alpha\beta}(t-t')$ decay very fast, since this would mean that the observables at t and t' are not correlated. We can also extend the lower limit of the integral to $-\infty$ because of this. This is mainly to result in a indefinite integral that looks nice. Rewrite $\tau = t - t'$. Furthermore, assuming the correlation function $C_{\alpha\beta}(\tau)$ is very short, we can replace the history $\hat{\rho}_{sI}(t-\tau)$ by the current $\hat{\rho}_{sI}(t)$. The final integral reads

$$\begin{aligned}\frac{\mathrm{d}\hat{\rho}_{sI}(t)}{\mathrm{d}t} = -\int_0^\infty \sum_{\alpha,\beta} C_{\alpha\beta}(\tau)\big[S_{\alpha I}(t)S_{\beta I}(t-\tau)\hat{\rho}_{sI}(t) - S_{\beta I}(t-\tau)\hat{\rho}_{sI}(t)S_{\alpha I}(t)\big] \\ + C_{\alpha\beta}(-\tau)\big[\hat{\rho}_{sI}(t)S_{\beta I}(t-\tau)S_{\alpha I}(t) - S_{\alpha I}(t)\hat{\rho}_{sI}(t)S_{\beta I}(t-\tau)\big]\,\mathrm{d}\tau\end{aligned}$$

Transforming back to the Schrödinger representation,

$$\frac{\mathrm{d}\hat{\rho}_s(t)}{\mathrm{d}t} = -i[\hat{H}_s, \hat{\rho}_s(t)] + e^{-i\hat{H}_s t}\left(\frac{\mathrm{d}\hat{\rho}_{sI}(t)}{\mathrm{d}t}\right)e^{i\hat{H}_s t}.$$

We will need the following manipulations while solving:

$$\begin{aligned}e^{-iH_s t}S_{\alpha I}(t)S_{\beta I}(t-\tau)\hat{\rho}_{sI}(t)e^{iH_s t} &= e^{-iH_s t}S_{\alpha I}(t)e^{iH_s t}e^{-iH_s t}S_{\beta I}(t-\tau)e^{iH_s t}e^{-iH_s t}\hat{\rho}_{sI}(t)e^{iH_s t} \\ &= S_\alpha e^{-iH_s t}S_\beta e^{iH_s t}\hat{\rho}_s\end{aligned}$$

Finally,

$$\frac{\mathrm{d}\hat{\rho}_s(t)}{\mathrm{d}t} = -i[\hat{H}_s, \hat{\rho}_s(t)] - \int_0^\infty \sum_{\alpha,\beta} C_{\alpha\beta}(\tau)\big[S_\alpha, S_{\beta I}(-\tau)\hat{\rho}_s(t)\big] + C_{\alpha\beta}(-\tau)\big[\hat{\rho}_s(t)S_{\beta I}(-\tau), S_\alpha\big]\,\mathrm{d}\tau$$

10.6.1 Evaluating the correlation function

Let us try to solve for the correlation function in the case of the pure dephasing model, where

$$\hat{H}_e = \sigma_z \sum_i c_i q_i$$

and

$$E(\tau) = \sum_i c_i \hat{q}_i(\tau) \qquad\qquad E(0) = \sum_i c_i \hat{q}_i$$

Note that we are still in the interaction representation. We have previously derived that

$$\hat{q}(\tau) = \sqrt{\frac{1}{2m\omega_i}}[a_i e^{-\omega_i \tau} + a_i^\dagger e^{i\omega_i \tau}]$$

So our final task is to evaluate

$$\left\langle \sum_i c_i[a_i e^{-\omega_i\tau} + a_i^\dagger e^{i\omega_i\tau}] \sum_j c_j \sqrt{\frac{1}{2m\omega_j}}[a_j + a_j^\dagger] \right\rangle_{\hat{\rho}_e}.$$

The i-th oscillator should be only correlated with the i-th oscillator. The expression above now becomes

$$\left\langle \sum_i c_i^2[a_i a_i e^{-\omega_i\tau} + a_i^\dagger a_i^\dagger e^{i\omega_i\tau} + a_i a_i^\dagger e^{-i\omega_i\tau} + a_i^\dagger a_i e^{i\omega\tau}] \right\rangle_{\hat{\rho}_e}.$$

Look at the i-th oscillator alone. Consider the following terms. First,

$$\begin{aligned}\operatorname{tr}\left[a_i a_i \sum_n |n\rangle\langle n| \frac{e^{-\beta H_i}}{Z}\right] &= \sum_n \langle n|a_i a_i|n\rangle \frac{e^{-\beta H_n}}{Z} \\ &= 0\end{aligned}$$

Similarly, we get that

$$\operatorname{tr}\left[a_i^\dagger a_i^\dagger \sum_n |n\rangle\langle n| \frac{e^{-\beta H_n}}{Z}\right] = 0.$$

The only non zero terms are thus

$$\begin{aligned}\operatorname{tr}\left[a_i a_i^\dagger \sum_n |n\rangle\langle n| \frac{e^{-\beta H_n}}{Z}\right] &= \sum_n \langle n|a_i a_i^\dagger|n\rangle \frac{e^{-\beta H_n}}{Z} \\ &= \sum_n \langle n|a_i^\dagger a_i + 1|n\rangle \frac{e^{-\beta H_n}}{Z} \\ &= \sum_n \frac{n e^{-\beta(n\hbar\omega_i + \frac{1}{2})}}{\sum_m e^{-\beta(m\hbar\omega_i+\frac{1}{2})}} + 1 \\ &= \frac{e^{\beta\hbar\omega_i}}{(e^{\beta\hbar\omega_i}-1)^2} \Big/ \frac{e^{\beta\hbar\omega_i}}{e^{\beta\hbar\omega_i}-1} + 1 \\ &= \frac{1}{e^{\beta\hbar\omega_i}-1} + 1 \\ &= \frac{1}{1-e^{-\beta\hbar\omega_i}}\end{aligned}$$

and

$$\begin{aligned}\operatorname{tr}\left[a_i^\dagger a_i \sum_n |n\rangle\langle n| \frac{e^{-\beta H_n}}{Z}\right] &= \sum_n \langle n|a_i a_i^\dagger + 1 - 1|n\rangle \frac{e^{-\beta H_n}}{Z} \\ &= \frac{1}{1-e^{-\beta\hbar\omega_i}} - 1 \\ &= \frac{1}{e^{\beta\hbar\omega_i}-1}.\end{aligned}$$

Thus in summary the correlation function is given by

$$\sum_i c_i^2 \left(\frac{e^{-i\omega_i\tau}}{1-e^{-\beta\hbar\omega_i}} + \frac{e^{i\omega_i\tau}}{e^{\beta\hbar\omega_i}-1}.\right)$$

References

[1] M. Rab, J. H. Cole, N. G. Parker, A. D. Greentree, L. C. L. Hollenberg, and A. M. Martin. Spatial coherent transport of interacting dilute bose gases. *Physical Review A*, 77(6), Jun 2008.