Lecture 21

Scattering

beam → target

detects

\[ P_b = \sum_n P_{bn} |\psi_{bn}\rangle \langle \psi_{bn}| \]

\[ P_t = \sum_n P_{tn} |\psi_{tn}\rangle \langle \psi_{tn}| \]

\( P_{bn}, P_{tn} \) classical probabilities

Problem: understand properties of interaction by looking at the statistical distribution of particles detected

average beam momentum

\[ \langle \vec{p} \rangle_b = \text{Tr}(\vec{P} P_b) \]
\[ \langle \bar{P} \rangle_+ = \text{Tr} (\bar{P} \rho_+) \]

In the lab frame \( \langle \hat{P} \rangle = 0 \), but we are not necessarily assuming \( \langle \bar{P} \rangle = 0 \).

We start by first focusing on a single quantum measurement

\[ |\psi_-(t)\rangle = \text{state of beam-target system at time } t \]

\[ |\psi_+(t)\rangle = \text{detected state at time } t \]

Both states are solutions of the Schrödinger equation

\[ i\hbar \frac{d}{dt} |\psi_-(t)\rangle = H |\psi_-(t)\rangle \]

\[ i\hbar \frac{d}{dt} |\psi_+(t)\rangle = H |\psi_+(t)\rangle \]
These have the solved form:

\[ |\psi_+ (t)\rangle = e^{-i\frac{\gamma t}{\hbar}} |\psi_+ (0)\rangle \]

The probability that this beam target state will be measured to be in the state \( |\psi_+ \rangle \) is

\[ P_{bt} = |\langle \psi_+ (t) | \psi_- (t) \rangle|^2 \]

since both states are solutions of the Schrödinger equation this probability is independent of time

\[ \langle \psi_+ (t) | \psi_- (t) \rangle = e^{-i\frac{\gamma t}{\hbar}} \langle \psi_+ (0) | e^{-i\frac{\gamma}{\hbar}} |\psi_- (0)\rangle \]

\[ \langle \psi_+ (t) | \psi_- (0) \rangle = \langle \psi_+ (0) | \psi_- (0) \rangle \]
The difficulty is that in general the state $|\Psi(t)\rangle$ are not known. However long before the collision $|\Psi_{-}(t)\rangle$ looks like a freely moving beam particle and a non interacting target particle at rest, similarly when the colliding particles are beyond the range of the interaction the system looks like 2 free particles headin towards the detector.
If \( T_- \) is a time long before the collision and \( T_+ \) is a time long after the collision we can express this condition as

\[
\| |\psi_-(T_-)\rangle - |\psi^o_-(T_-)\rangle\| = 0
\]

\[
\| |\psi_+(T_+)\rangle - |\psi^o_+(T_+)\rangle\| = 0
\]

where \( |\psi^o_\pm(t)\rangle \) are solutions of the Schrödinger equation without interactions. This means that the above can be written

\[
-i\hbar \left\{ \frac{d}{dt} - \frac{1}{\hbar^2} \mathbf{\nabla}^2 - V_0(t) \right\} |\psi(t)\rangle = -i\hbar \mathbf{\nabla}_\perp \cdot \mathbf{E}(t) |\psi(t)\rangle
\]

\[
\| \mathbf{E} \cdot |\psi_+(T_+)\rangle - \mathbf{E} \cdot |\psi^o_+(T_+)\rangle \| \approx 0
\]

\[
\| \mathbf{E} \cdot |\psi_-(T_-)\rangle - \mathbf{E} \cdot |\psi^o_-(T_-)\rangle \| \approx 0
\]
The minimum value of $T_\pm$ depends on properties of the states, but nothing changes if they are increased.

To eliminate the dependence on the structure of the state we can use

$$\lim_{t \to \pm \infty} \| e^{-iHt/\hbar} \| \psi_{\pm}(0) \| - e^{-iHt/\hbar} \psi_{\pm}(0) \| = 0$$

since $e^{-iHt/\hbar}$ is unitary

This can be replaced by

$$\lim_{t \to \pm \infty} \| e^{-iHt/\hbar} \| \psi_{\pm}(0) \| - e^{-iHt/\hbar} \| \psi_{\pm}(0) \| = 0$$

These are called the scattering asymptotic conditions.
The scattering asymptotic condition replace the initial conditions -

The states $|\Psi_{\pm}(t)\rangle$ represent states of non-interacting particles. We write these conditions as

$$\lim_{t \to \pm \infty} e^{\frac{iHt}{\hbar}} |\Psi_{\pm}(t)\rangle = |\Psi_{\pm}(\infty)\rangle$$

The operators

$$\hat{N}_{\pm} = \lim_{t \to \pm \infty} e^{\frac{iHt}{\hbar}} e^{\frac{iH_0 t}{\hbar}}$$

are called Møller wave operators.

It follows that the probability amplitude
can be expressed as

\[ \langle \Psi_+ (0) | \Psi_- (0) \rangle = \]

\[ \langle \Psi_0 (0) | \Omega_+ \Omega_- | \Psi_0 (0) \rangle = \]

\[ \langle \Psi_+ (0) | S | \Psi_- (0) \rangle \]

The operator

\[ S = \Omega_+ \Omega_- \]

is called the scattering operator.

**Theorem (Intertwining)**

\[ H \Omega_\pm = \Omega_\pm H_0 \]

**Proof**

\[ e^{-i \Omega_\pm / \hbar} \]

\[ e^{-i (S \Omega_\pm) / \hbar} e^{-i t H_0} \]

\[ \lim_{t \to \pm} e^{-i \Omega_\pm / \hbar} e^{-i t H_0} = \]
\[
\lim_{t \to \pm \infty} e^{-iH_0 t} e^{iH(t+s)/\hbar} = \Omega e^{iH_0 s/\hbar}
\]

Let \( t^\prime = t + s \). For fixed \( s \), \( t^\prime \to \pm \infty \) as \( t \to \pm \infty \). Therefore

\[
\Omega \pm e^{iH_0 s/\hbar}
\]

differentiating with respect to \( s \) and setting \( s = 0 \) gives

\[
iH \Omega \pm = \Omega \pm (iH_0) \quad \forall
\]

\[
H \Omega \pm = \Omega \pm H_0
\]

**Corollary**

\[
H_0 S = S H_0
\]

\[
H_0 S = H_0 \Omega_+ \Omega_- = \Omega^+_+ \Omega_- H_0 = S H_0
\]
Comment: This is a statement of energy conservation - this makes sense because the energy does not change when the particles move freely.

The condition $H_{-2+} = \mathcal{D}_{-2} \pm H_0$ follow because if the eigenvalues of $H$ and $H_0$ are not the same oscillation kill the state.

Note that

$H_0 |\Psi_\theta\rangle = E |\Psi_\theta\rangle$

Then

$H_{-2+} |\Psi_\theta\rangle = E \mathcal{D}_{-2} |\Psi_\theta\rangle$
so $\Sigma^\pm$ transform eigenstates of $H_0$ to eigenstates of $H$ with the same energy. We also have

$$\Sigma^\pm |\Psi_0(t)\rangle = \Sigma^\pm e^{-iHt/\hbar} |\Psi_0(t)\rangle$$

$$= e^{-iHt/\hbar} \Sigma^\pm |\Psi_0(t)\rangle$$

$$= |\Psi^\pm (t)\rangle$$

This implies

$$\Sigma^\pm |\Psi_0(t)\rangle = |\Psi^\pm (t)\rangle$$

Theorem

$$\Sigma^+_+ + \Sigma^-_+ = I$$

$$\lim_{t \to \infty} e^{iHT/\hbar} e^{-iH_0/\hbar} e^{iHT/\hbar} e^{-iH_0/\hbar} = I$$

$$\begin{array}{c}
\lim_{t \to \infty} e^{iHT/\hbar} e^{-iH_0/\hbar} e^{iHT/\hbar} e^{-iH_0/\hbar} \\
= I
\end{array}$$
Note if \( H \) has bound states with energy \( E < 0 \), then

\[
H \left| \Psi_b \right> = E_b \left| \Psi_b \right>
\]

\[
\langle \Psi_b | \Sigma_{\pm} = \int \langle \Psi_b | \Sigma_{\pm} | \varepsilon \rangle d\varepsilon \langle \varepsilon | \varepsilon \rangle 
\]

\[
\int \langle \Psi_b | \varepsilon \rangle d\varepsilon < \varepsilon \rangle
\]

This vanishes because \( H_0 \) only has eigenstates with positive energy while \( \left| \Psi_b \right> \) has negative energy.

\[
\left| \Psi_b \right> \left| \varepsilon \right>
\]

are eigenstates of \( H \) with different energies.
Theorem: The scattering operator is unitary

\[ S^+ S = S^+ \Omega_+ S^+ \Omega_- \]

\[ S^+ S = \Omega^+ \Omega = \lim_{t \to -\infty} \left( iH t, iH t, -14eC/\hbar, iH t/\hbar \right) \]

while \( S \) is unitary, \( \Omega \) may not be unitary.
\[ \langle \psi^0_+(t) | S | \psi^0_-(0) \rangle = \]

\[ \langle \psi^0_+(t) | S^+ + \Omega - 1 \psi^0_-(0) \rangle = \]

\[ \lim_{t \to \infty} \lim_{s \to \infty} \langle \psi^0_+(0) | e^{i H_0 t / \hbar} - i H t / \hbar \ e^{i H_0 s / \hbar} \langle \psi^0_-(0) \rangle = \]

\[ \lim_{t \to \infty} \langle \psi^0_+(0) | e^{i H_0 t / \hbar} - 2 i H t / \hbar \ e^{i H_0 t / \hbar} \langle \psi^0_-(0) \rangle = \]

Next write the limit as the integral of a derivative.

\[ = \langle \psi^0_+(0) | \psi_-(0) \rangle + \]

\[ \int_0^t \langle \psi^0_+(0) | d/dt (e^{i H_0 t / \hbar} - 2 i H t / \hbar \ e^{i H_0 t / \hbar}) \ | \psi_-(0) \rangle = \]

\[ = \langle \psi^0_+(0) | \psi_-(0) \rangle + \]

\[ \int_0^t \langle \psi^0_+(0) | \left\{ e^{i H_0 t / \hbar} ( - i (H - H_0) ) e^{i H_0 t / \hbar} \right\} \langle \psi_-(0) \rangle \]
\[ = \langle \psi_+^{o}(0) | \psi_-^{o}(0) \rangle \]

\[ (-i) - \frac{i}{\hbar} \int_0^t \langle \psi_+^{o}(t) | e^{-2iHt/\hbar} e^{iHt/\hbar} \psi_-^{o}(0) \rangle \, dt \]

In order to do the time integral expand \( \psi_{\pm}^{o}(t) \) in terms of a complete set of eigenstates of \( H_0 \)

\[ I = \int dE_1 E \langle E_1 \rangle \]

(There is an implied sum over other variables)

\[ = \langle \psi_+^{o}(0) | \psi_-^{o}(0) \rangle + \]

\[ \frac{i}{\hbar} \int_0^t dt \langle \psi_+^{o}(t) | E_1 \rangle \, dE_1 \left\{ \right. \]

\[ \langle E_1 | \psi_-^{o}(0) \rangle e^{-2 \left( H - \frac{E_1 + E_2}{2} \right) t/\hbar} \langle E_1 \rangle + \]

\[ \left. \langle E_2 | \psi_-^{o}(0) \rangle e^{-2 \left( H - \frac{E_1 + E_2}{2} \right) t/\hbar} \langle E_2 \rangle \right\} \]

\[ \langle E_2 | \psi_-^{o}(0) \rangle \, dE_1 \, dE_2 \]
For this to make sense the \( E_1 \) and \( E_2 \) integral must be evaluated before doing the \( t \) integral.

* If the integrals are done in the correct order including a factor \( e^t \) does not change the integrals provided \( \epsilon \) is small enough.

* With the \( \epsilon \) the order does not matter. This means that it is possible to do the \( t \) integrals first then taking \( \epsilon \) after doing the \( E_1, E_2 \) integrals.
\[ \langle \psi^+ (0) | \psi^- (0) \rangle + \frac{i}{\hbar} \int \langle \psi^+ (0) | E_1 \rangle \, dE_1 \]

\[ \langle E_1 | \left\{ V \frac{1}{\hbar^2 (H - E_1 + E_2 - \epsilon)} + \frac{1}{\hbar^2 (H - E_1 - E_2 - \epsilon)} \right\} \]

\[ dE_2 < E_2 \psi^0 > \]

Let \( \bar{E} = (E_1 + E_2) / 2 \)

\[ = \langle \psi^+ (0) | \psi^- (0) \rangle + \int \langle \psi^+ (0) | E_1 \rangle \, dE_1 \]

\[ \langle E_1 | \left\{ V \frac{1}{-2 (H - \bar{E} - E - \frac{i\hbar}{2})} + \frac{1}{-2 (H - \bar{E} + \frac{i\hbar}{2})} \right\} \]

\[ 1 \, dE_2 \, \langle E_2 | \psi^0 (0) \rangle \]

Next we use the sec

\[ \text{Resolvent Identity} \]

\[ \frac{1}{z-H} = \frac{1}{z-H_0} + \frac{1}{z-H_0} \frac{1}{z-H} \]

\[ = \frac{1}{z-H_0} + \frac{1}{z-H} \frac{1}{z-H_0} \]
where \( Z \) is any complex number where \( (Z-H)^{-1} \) and \( (Z-H_0)^{-1} \) exist.

The proof follows by multiplying

\[
(Z-H_0) \left[ \mathcal{L} (Z-H) \right] (Z-H) \left[ \mathcal{L} (Z-H_0) \right]
\]

where \( \mathcal{L} \) is the resolvent identity

\[
= \langle \psi_+ | \psi_- \rangle + \int \langle \psi_+ | \varepsilon | \psi_- \rangle \, d\varepsilon,
\]

\[
\frac{i}{2} \langle \varepsilon | \left\{ \psi_+ \left( \frac{1}{E-H+\varepsilon} + \frac{1}{E-H_0+\varepsilon} \right) \psi_- \rangle \hbar \rangle \langle \varepsilon_2 | \psi_+ \rangle \langle \psi_- | \psi_0 \rangle
\]

\( \varepsilon' = \frac{\hbar}{2} \varepsilon \)
\[
= \langle \psi_1^0 (0) | \psi_2^0 (0) \rangle + \int dE_1 dE_2 \langle \psi_1^0 (0) | E_1 \rangle \times \\
\langle E_2 | \frac{1}{E - E_1 + i\epsilon} V \left( \frac{1}{E - H_0 + i\epsilon} + \frac{1}{E-H+i\epsilon'} \right) V \left( \frac{1}{E - H_0 + i\epsilon'} + \frac{1}{E-H+i\epsilon} \right) \rangle \langle E_2 | \psi_2^0 (0) \rangle
\]

In the form the \( H_0 \)'s can be replaced by \( E_1 \neq E_2 \)

On the left,

\[
\frac{1}{E - E_1 + i\epsilon'} = \frac{1}{\frac{1}{2} (E_1 + E_2) - E_1 + i\epsilon} = \frac{2}{E_2 - E_1 + 2i\epsilon}
\]

On the right,

\[
\frac{1}{E - E_2 + i\epsilon} = \frac{1}{\frac{1}{2} (E_1 + E_2) - E_2 + i\epsilon} = \frac{2}{E_1 - E_2 + 2i\epsilon}
\]

Using these in the above,

\[
\langle \psi_1^0 (0) | \psi_2^0 (0) \rangle + \int dE_1 dE_2 \langle \psi_1^0 (0) | E_1 \rangle \times \\
\langle E_2 | V^* V (E - H_0 + 2i\epsilon) V | E_2 \rangle \times \\
\frac{2}{2} \left( \frac{1}{E_2 - E_1 + 2i\epsilon'} + \frac{1}{E_1 - E_2 + 2i\epsilon} \right) \\
- \frac{1}{E_2 - E_1 - 2i\epsilon}
\]
Note

\[
\frac{1}{E_2 - E_1 + 2i\epsilon} - \frac{1}{E_1 - E_2 - 2i\epsilon} =
\]

\[
-\frac{4i\epsilon}{(E_2 - E_1)^2 + 4\epsilon^2}
\]

In the limit \( \epsilon \to 0 \)

\[-2i \pi \delta(E_2 - E_1)\]

To show this consider

\[
\int \frac{-4i\epsilon}{(E_2 - E_1)^2 + 4\epsilon^2} \delta(E_1)\, dE_1 =
\]

\[-i \int \frac{1}{(\frac{E_2 - E_1}{2\epsilon})^2 + 1} \delta(E_1)\, dE_1\]

Let \( u = \frac{E_2 - E_1}{2\epsilon} \) \( du = \frac{dE_1}{2\epsilon} \)

\[-2i \int \frac{du}{u^2 + 1} \delta(E_2 + 2\epsilon u)\, du\]

As \( \epsilon \to 0 \) this becomes

\[-2i \delta(E_2) \int \frac{du}{u^2 + 1} = -2\pi i \int \delta(E_2 - E_1) \delta(E_1)\, d\epsilon\]
This gives an energy conserving \( \delta \) function \( \Rightarrow E_1 = E_2 = E \)
so the expression
\[
\langle \psi_+^{\circ}(0) | S | \psi_-^{\circ}(0) \rangle = \langle \psi_+^{\circ}(0) | \psi_-^{\circ}(0) \rangle
\]
\[
\int \langle \psi_+^{\circ}(0) | E \rangle \, dE \times \langle E \mid \psi_+^{\circ}(0) \rangle
\]
\[
\left[ -2\pi i \delta(E-E') \left[ V + V \frac{1}{E-H+i\epsilon} V \right] \right]
\]
\[
1E' \rangle \, dE' \langle E'\mid \psi_-^{\circ}(0) \rangle
\]
The operator
\[
\tau(E+i\epsilon) = V + V (E-H+i\epsilon)^{-1} V
\]
is called the transition operator
\[
S = I - 2\pi i \delta(E-E') \tau(E+i\epsilon)
\]