4 - The Time Evolution Operator and the S-matrix

Consider the Schrödinger equation which we write

$$i\frac{\partial}{\partial t}|\Psi,t\rangle_S = H|\Psi,t\rangle_S, \tag{44}$$

where H is the Hamiltonian and $|\Psi,t\rangle$ is the state at time t. The subscript S refers to the Schrödinger picture where operators are time-independent (except for explicit time-dependent terms) and states are time-dependent. Let us furthermore split the Hamiltonian into a free Hamiltonian (containing typically kinetic energy and mass terms) and an interacting part that contains the interactions of different particles, i.e. $H = H_F + H_{I,S}$. Here the notation $H_{I,S}$ means the interaction part of the Hamiltonian in the Schrödinger picture. Define the state

$$|\Psi,t\rangle_I = e^{iH_F t}|\Psi,t\rangle_S, \tag{45}$$

which is called the interaction picture state and has subscript I, and also define the interaction picture operators

$$O_I = e^{iH_F t} O_S e^{-iH_F t}, \tag{46}$$

where O_S is a Schrödinger picture operator (typically time-independent).

Exercise (1)**.**

Show that,

$$i\frac{\partial}{\partial t}|\Psi,t\rangle_I = H_I|\Psi,t\rangle_I, \tag{47}$$

where $H_I = e^{iH_F t} H_{I,S} e^{-iH_F t}$, and show that

$$\frac{d}{dt}O_I = -i[O_I, H_F],. \tag{48}$$

where you assume no explicit time-dependence in O_S. From now on H_I will denote the interaction part of the Hamiltonian in the interaction picture.

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Solution.

$$\begin{aligned}
i\frac{\partial}{\partial t}|\Psi,t\rangle_I &= i\frac{\partial}{\partial t}e^{iH_F t}|\Psi,t\rangle_S \\
&= i\frac{\partial}{\partial t}(e^{iH_F t})|\Psi,t\rangle_S + e^{iH_F t}(i\frac{\partial}{\partial t}|\Psi,t\rangle_S) \\
&= -H_F e^{iH_F t}|\Psi,t\rangle_S + e^{iH_F t}H|\Psi,t\rangle_S \\
&= -e^{iH_F t}H_F e^{-iH_F t}|\Psi,t\rangle_I + e^{iH_F t}He^{-iH_F t}|\Psi,t\rangle_I \\
&= e^{iH_F t}H_{I,S}e^{-iH_F t}|\Psi,t\rangle_I = H_I|\Psi,t\rangle_I
\end{aligned}$$

And now the second part,

$$
\begin{aligned}
\frac{d}{dt}O_I &= \frac{d}{dt}(e^{iH_Ft}O_Se^{-iH_Ft}) \\
&= iH_F(e^{iH_Ft}O_Se^{-iH_Ft}) + e^{iH_Ft}O_S(-iH_F)e^{-iH_Ft} \\
&= iH_FO_I - O_IiH_F = i[H_F, O_I].
\end{aligned}
$$

Exercise (2)**.**

Introduce the time evolution operator, $U(t,t_0)$, that evolves states from time t_0 to time t, i.e. $|\Psi,t\rangle_I = U(t,t_0)|\Psi,t_0\rangle_I$. Clearly $U(t_0,t_0) = 1$. Show that

$$
i\frac{\partial}{\partial t}U(t,t_0) = H_I(t)U(t,t_0). \tag{49}
$$

Note the explicit time-dependence on $H_I(t)$!

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Solution.

$$
|\Psi_t\rangle_I = U(t,t_0)|\Psi,t_0\rangle_I
$$

Show that

$$
i\frac{\partial}{\partial t}U(t,t_0) = H_I(t)U(t,t_0)
$$

Let $|\Psi,t_0\rangle_I$ be the interaction part of some state.

$$
\begin{aligned}
i\frac{\partial}{\partial t}(U(t,t_0)|\Psi,t_0\rangle_I) &= i\frac{\partial}{\partial t}(U(t,t_0)|\Psi,t_0\rangle)_I, \\
&= i\frac{\partial}{\partial t}|\Psi,t\rangle_I, \\
&= H_I|\Psi,t\rangle_I, \\
&= H_I(t)U(t,t_0)|\Psi,t_0\rangle_I
\end{aligned}
$$

Exercise (3)**.**

Show that

$$
U(t,t_0) = 1 - i\int_{t_0}^{t} dt_1 H_I(t_1)U(t_1,t_0), \tag{50}
$$

and

$$U(t,t_0) = 1 + (-i)\int_{t_0}^{t} dt_1 H_I(t_1) + (-i)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 H_I(t_1) H_I(t_2) + \ldots, \tag{51}$$

where $\ldots$ denote higher-order terms containing three or more factors of $H_I(t)$.

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Solution.

$$i\frac{\partial}{\partial t}U(t,t_0) = H_I(t)U(t,t_0)$$

Integrate on both sides

$$i\int_{t_0}^{t} \frac{\partial}{\partial t_1}U(t_1,t_0)dt_1 = \int_{t_0}^{t} H_I(t_1)U(t_1,t_0)dt_1$$

Multiply by i, and evaluate the left-hand side.

$$\begin{aligned}
i(U(t,t_0) - U(t_0,t_0)) &= \int_{t_0}^{t} H_I(t_1)U(t_1,t_0)dt_1, \\
(-1)(U(t,t_0) - 1) &= i\int_{t_0}^{t} H_I(t_1)U(t_1,t_0)dt_1, \\
-U(t,t_0) + 1 &= i\int_{t_0}^{t} H_I(t_1)U(t_1,t_0)dt_1, \\
U(t,t_0) &= 1 - i\int_{t_0}^{t} H_I(t_1)U(t_1,t_0)dt_1
\end{aligned}$$

Alright this seems reasonable. Let's try inserting the RHS in the differential equation and see where it gets us.

$$U(t,t_0) = 1 - i\int_{t_0}^{t} H_I(t_1)\left(1 - i\int_{t_0}^{t_1} H_I(t_2)U(t_2,t_0)dt_2\right)dt_1$$

By letting the outermost $H(t_1)$ integral distribute, we arrive at the expression we were looking for.

Exercise (4).

Now define the S-matrix for the process from initial state i to final state f, i.e. $i \to f$, by

$$S_{fi} = \lim_{t_0 \to -\infty} \lim_{t \to \infty} \langle f | U(t,t_0) | i \rangle. \tag{52}$$

Give a physical interpretation of this matrix element given what you know about $U(t,t_0)$ and relate it to how experiments are done. What have we assumed about the states $|f\rangle$ and $|i\rangle$? If you calculate S_{fi} in the Schrödinger picture will it be the same result?

Exercise (5).

Show that the first order contribution to S_{fi} can be written

$$S_{fi}^{(1)} = \delta_{fi} - i \int d^4x \langle f|\mathscr{H}|i\rangle, \tag{53}$$

where $H_I = \int d^3x \mathscr{H}$. $\mathscr{H}$ is called the Hamiltonian density. Since it contains only interaction terms, it differs from the Lagrangian density only by a sign (remember the basic idea that $L = T - V$ while $H = T + V$).

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Solution. Show that the first order contribution to S_{fi} can be written

$$S_{fi}^{(1)} = \delta_{fi} - i \int d^4x \langle f|\mathscr{H}|i\rangle$$

Where $H_I = \int d^3x \mathscr{H}$. Alright, let us take a look at S_{fi}

$$S_{fi} = \lim_{t_0 \to -\infty} \lim_{t \to \infty} \langle f|U(t,t_0)|i\rangle$$

Here f and i are initial and final states. Let's insert $U(t,t_0)$

$$S_{fi} = \lim_{t_0 \to -\infty} \lim_{t \to \infty} \left\langle f \middle| 1 - i \int_{t_0}^{t} H_I(t_1) U(t_1,t_0) dt_1 \middle| i \right\rangle$$

I could do this expansion an indefinite amount of times. I'll do it once more and then just throw away the remaining terms.

$$\begin{aligned} S_{fi} &\approx \lim_{t_0 \to -\infty} \lim_{t \to \infty} \left(\langle f|i\rangle - i \int_{t_0}^{t} \langle f| H_I(t_1) dt_1 |i\rangle \right), \\ &= \delta_{if} - i \int_{-\infty}^{\infty} \langle f| H_I(t_1) dt_1 |i\rangle, \\ &= \delta_{if} - i \int \int dt d^3x \langle f| \mathscr{H} |i\rangle, \\ &= \delta_{if} - i \int d^4x \langle f| \mathscr{H} |i\rangle \end{aligned}$$

If we assume that the interactions conserve energy and momentum, we have the commutation relation $[P^\mu, H] = 0$, where P^μ is the total energy and momentum operator. This operator acts on plane wave as $P^\mu|k\rangle = k^\mu|k\rangle$. It can also be used to generate finite translations in space and time by application of $e^{iP^\mu a_\mu}$, where a^μ is some space-time vector.

Exercise (6).

Show that $[P^\mu, H] = 0$ implies that $[e^{iP^\mu a_\mu}, H] = 0$.

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Solution. Show that $[P^\mu, H] = 0$ implies $[e^{iP^\mu a_\mu}, H] = 0$.

There are a couple of ways to show. One is to do an expansion into a power series. But I'm going to try to use exercise 1 instead.

$$\begin{aligned}
\frac{d}{dt} e^{iP_\mu a^\mu} &= \frac{d}{dt}(iP_\mu a^\mu) e^{iP_\mu a^\mu}, \\
&= ia^\mu e^{iP_\mu a^\mu} \frac{d}{dt} P_\mu, \\
&= -i[P^\mu, H] \cdot \left(ia_\mu e^{iP^\mu a_\mu} \right) = 0, \\
\Rightarrow 0 &= -i[e^{iP^\mu a^\mu}, H] = 0
\end{aligned}$$

Exercise (7).

The Hamiltonian density depends on space-time coordinates in general, $\mathscr{H}(x)$. Argue we can use translation operators to write $\mathscr{H}(x) = e^{iP^\mu x_\mu} \mathscr{H}(0) e^{-iP^\mu x_\mu}$ (Hint: Consider how $\mathscr{H}(x)$ looks when written in terms of quantum field operators and use the properties of the fields under translations in space and time).

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Solution. Let's recall $\mathscr{H}(x)$ in terms of field operators

$$\mathscr{H}(x,t) = \pi(x,t)^\dagger \pi(x,t) + \nabla\phi(x,t) \cdot \nabla\phi(x,t)^\dagger + m^2 \phi(x,t)\phi(x,t)$$

From exercise 3.12 we know that

$$\phi(x,t) = e^{iP^\mu x_\mu} \phi(0,0) e^{-iP^\mu x_\mu}$$

So we essentially need to show that this holds true for $\pi, \pi^\dagger, \nabla\phi, \nabla\phi^\dagger$ and $\phi^\dagger$, and then we will have shown the result.

Let's start with the daggered field operator

$$\phi^\dagger(x,t) = \left(e^{iP^\mu x_\mu} \phi(0,0) e^{-iP^\mu x_\mu} \right)^\dagger$$

Recall that the † reorders the terms and finds complex conjugate as well

$$\Rightarrow = e^{iP^\mu x_\mu} \phi(0,0)^\dagger e^{-iP^\mu x_\mu}$$

Since π is so similar to ϕ I will just assume that it holds for it as well.

Let's look at the gradient of the field operator

$$\begin{aligned}
\nabla\phi(x,t) &= \nabla \left(e^{iP^\mu x_\mu} \phi(0,0) e^{-iP^\mu x_\mu} \right), \\
&= \left(\nabla e^{iP^\mu x_\mu} \right) \phi(0,0) e^{-iP^\mu x_\mu} + e^{iP^\mu x_\mu} \phi(0,0) \nabla \left(e^{-iP^\mu x_\mu} \right)
\end{aligned}$$

The gradient just pulls down the 3-momentum $\mathbf{p}$ and i

$$= (i\mathbf{p})\left(e^{iP^\mu x_\mu}\phi(0,0)e^{-iP^\mu x_\mu}\right) + e^{iP^\mu x_\mu}\phi(0,0)(-i\mathbf{p})e^{-iP^\mu x_\mu}$$

Now we can commute $\phi(0,0)$ and $(-i\mathbf{p})$ if we pick up a commutator as well. The other terms cancel, and the sign is flipped

$$= ie^{iP^\mu x_\mu}[\phi(0,0),\mathbf{p}]e^{-iP^\mu x_\mu}$$

Let's evaluate this commutator, now we clearly want to look at equal times,

$$[\phi(0,0),\mathbf{p}] = -\left[\phi(0,0),\int d^3x\left\{\pi(x,0)^\dagger\nabla\phi(x,0)^\dagger + \nabla\phi(x,0)\pi(x,0)\right\}\right]$$

Now a bunch of these are zero the first terms is, and using the piano on the second term, we get a single non-zero term.

$$\begin{aligned}
&= -\int d^3x\,[\phi(0,0),\pi(x,0)]\,\nabla\phi(x,0),\\
&= -\int d^3x i\delta^3(x-0)\nabla\phi(x,0),\\
&= -i\nabla\phi(0,0)
\end{aligned}$$

We can insert this commutator.

$$\begin{aligned}
\nabla\phi(x,t) &= ie^{iP^\mu x_\mu}(-i\nabla\phi(0,0))e^{-iP^\mu x_\mu},\\
&= e^{iP^\mu x_\mu}\nabla\phi(0,0)e^{-iP^\mu x_\mu}
\end{aligned}$$

As a final note before we do the last calculation

$$\begin{aligned}
\phi(x,t)\phi(x,t)^\dagger &= e^{iP^\mu x_\mu}\phi(0,0)e^{-iP^\mu x_\mu}e^{iP^\mu x_\mu}\phi(0,0)^\dagger e^{-iP^\mu x_\mu},\\
&= e^{iP^\mu x_\mu}\phi(0,0)\phi(0,0)^\dagger e^{-iP^\mu x_\mu}
\end{aligned}$$

So now when we consider

$$\mathscr{H}(0) = \pi(0,0)^\dagger\pi(0,0) + \nabla\phi(0,0)\nabla\phi(0,0)^\dagger + m^2\phi(0,0)^\dagger\phi(0,0)$$

We see that

$$e^{iP^\mu x_\mu}\mathscr{H}(0)e^{-iP^\mu x_\mu} = \mathscr{H}(x,t)$$

Exercise (8)**.**

Show that this implies that we can isolate the space-time dependence of $S_{fi}^{(1)}$ through

$$\langle f|\mathscr{H}(x)|i\rangle = \langle f|\mathscr{H}(0)|i\rangle e^{i(p_f^\mu - p_i^\mu)x_\mu}, \tag{54}$$

where p_f and p_i are the total four-momenta of final and initial states respectively.

Show that we now obtain

$$S^{(1)}_{fi} = \delta_{fi} - i(2\pi)^4 \langle f|\mathscr{H}(0)|i\rangle \delta^4(p_f - p_i). \tag{55}$$

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Solution. Let's take a look at

$$\langle f|\mathscr{H}(x)|i\rangle = \left\langle f \left| e^{iP^\mu x_\mu} \mathscr{H}(0) e^{-iP^\mu x_\mu} \right| i \right\rangle$$

We should consider the operator acts on the state i.

$$e^{-iP^\mu x_\mu} |i\rangle$$

Now clearly $P_\mu|i\rangle = p_i|i\rangle$ it just gives the momentum. And we can consider coordinates as well $P^\mu_k|i\rangle = p^\mu_{i_k}|i\rangle$, $k = 1,2,3,4$. Let's write it out as a power series and a sum

$$\begin{aligned}
e^{-iP^\mu x_\mu}|i\rangle = \prod_k^4 e^{-iP_k x_k}|i\rangle &= \prod_k^4 \sum_n^\infty \frac{(-iP_k x_k)^n}{n!}|i\rangle, \\
&= \prod_k^4 \sum_n^\infty \frac{(-ix_k)^n (P_k)^n}{n!}|i\rangle, \\
&= \prod_k^4 \sum_n^\infty \frac{(-ix_k p_{i_k})^n}{n!}|i\rangle, \\
&= e^{-ip_i x_\mu}
\end{aligned}$$

We can do a similar trick for the left side,

$$\langle f|e^{iP^\mu x_\mu} = \left(e^{-iP^\mu x_\mu}|f\rangle\right)^\dagger = \langle f|\, e^{ip_f x_\mu}$$

Therefore,

$$\langle f|\mathscr{H}(x)|i\rangle = \langle f|\mathscr{H}(0)|i\rangle e^{i(p_f - p_i)x_\mu}$$

We can just plug this in,

$$S^{(1)}_{fi} = \delta_{fi} - i\int d^4x \langle f|\mathscr{H}(0)|i\rangle e^{i(p_f - p_i)x_\mu}$$

We can move the bracket outside the integral since we have isolated the space time dependence

$$\begin{aligned}
&= \delta_{fi} - i\int d^4x \left(e^{i(p_f - p_i)x_\mu}\right) \langle f|\mathscr{H}(0)|i\rangle, \\
&= \delta_{fi} + (2\pi)^4 \delta^4(p_f - p_i)\langle f|\mathscr{H}(0)|i\rangle
\end{aligned}$$

I get a sign error here, we can hopefully resolve this at some point

Exercise (9)**.**

Consider now the second order contribution to the S-matrix. Show that it can we written in the form

$$S_{fi}^{(2)} = (-i)^2 \int d^4x_1 \int d^4x_2 \theta(t_1 - t_2) \langle f | \mathscr{H}(x_1) \mathscr{H}(x_2) | i \rangle, \tag{56}$$

where $x_1^\mu = (t_1, \mathbf{x}_1)$ and $x_2^\mu = (t_2, \mathbf{x}_2)$, while $\theta(x)$ is the Heaviside step function which is $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x < 0$. Finally, show that we can write this in the form

$$S_{fi}^{(2)} = (-i)^2 (2\pi)^4 \delta^4(p_f - p_i) \int d^4x \theta(t) \langle f | \mathscr{H}(x) \mathscr{H}(0) | i \rangle, \tag{57}$$

where $x = x_1 - x_2$.

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Solution. The first rewrite is rather simple. Let's recall the second order term.

$$S_{fi}^{(2)} = \lim_{t_0 \to -\infty} \lim_{t \to +\infty} (-i)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int d^3x_1 \int d^3x_2 \langle f | \mathscr{H}(x_1) \mathscr{H}(x_2) | i \rangle$$

Where I have inserted the hamiltonian densities. We can evaluate the limits.

$$S_{fi}^{(2)} = (-i)^2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \int d^3x_1 \int d^3x_2 \langle f | \mathscr{H}(x_1) \mathscr{H}(x_2) | i \rangle$$

Where we can rewrite the innermost integral using a heaviside function

$$\int_{-\infty}^{t_1} dt_2 = \int_{-\infty}^{\infty} \theta(t_1 - t_2) dt_2, \quad \theta(t_1 - t_2) = \begin{cases} 0 & t_2 > t_1 \\ 1 & t_1 > t_2 \end{cases}$$

Inserting this and collecting the integrals we get

$$S_{fi}^{(2)} = (-i)^2 \int d^4x_1 \int d^4x_2 \theta(t_1 - t_2) \langle f | \mathscr{H}(x_1) \mathscr{H}(x_2) | i \rangle$$

At this point we should make a substitution

$$\begin{aligned} X &= x_2, \quad x = x_1 - x_2, \\ dX &= dx_2 \quad x_1 = x + x_2 = x + X, \\ dx_1 &= dx \end{aligned}$$

Also note that in this substitution $t_1 - t_2 \to t$.

$$S_{fi}^{(2)} = (-i)^2 \int d^4x \int d^4X \theta(t) \langle f | \mathscr{H}(x + X) \mathscr{H}(X) | i \rangle$$

At this point we can employ the relations we showed in 4.8. We shall expand the hamiltonian densities.

$$S_{fi}^{(2)} = (-i)^2 \int d^4x \int d^4X \theta(t) \left\langle f \left| e^{iP^\mu X_\mu} \mathscr{H}(x) e^{-iP^\mu X_\mu} e^{iP^\mu X_\mu} \mathscr{H}(0) e^{-iP^\mu X_\mu} \right| i \right\rangle$$

The middle terms cancel and we can pull out the exponents by letting them act on the states.

$$= (-i)^2 \int d^4x \int d^4X \theta(t) \langle f | \mathscr{H}(x) \mathscr{H}(0) | i \rangle e^{i(p_f - p_i)X}$$

We can pull out the bracket,

$$= (-i)^2 \int d^4x \langle f|\mathscr{H}(x)\mathscr{H}(0)|i\rangle \int d^4\overline{X}\theta(t)e^{i(p_f - p_i)X}$$

We can also pull out the heaviside step-function and evaluate the integral

$$= (-i)^2(2\pi)^4\delta^4(p_f - p_i)\int d^4x\langle f|\mathscr{H}(x)\mathscr{H}(0)|i\rangle$$