A Subtle Detail in LSZ Reduction

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1 Introduction

In this note we discuss a subtle detail in the proof of the LSZ reduction formula in many textbooks like Itzykson's [1], Srednicki's [2] and Schwartz's [3]. The problem is that we are playing with the time-order symbol T very uncarefully in an ill-defined way. There's also alternative way to the theorem naturally avoiding such issue, as shown in Peskin's [4] and Weinberg's [5].

We will use the $(+,-,-,-)$ metric throughout this note.

2 Review of LSZ Reduction Formula

First we give a very brief review of the reduction formula. To focus on our main issue about the time-ordered product, we would deal with a single scalar field with mass m only. We also forget things related to renormalization for now. Similarly in the following section, we will omit all the unrelated (yet important!) treatment in our discussion, just to make sure the reader won't get lost in those complex techniques of QFT.

The most important usage of LSZ reduction formula is to provide a conncetion between the scattering amplitudes and the correlation functions. More precisely, a scattering amplitude is the *residue* on the multiparticle mass shell of the corresponding correlation function, up to a Fourier transformation connecting momentum and coordinate spaces. We can write this as

$$\begin{aligned} \langle q_1, \cdots, q_{n'}; \mathrm{out} | p_1, \cdots, p_n; \mathrm{in} \rangle = \mathrm{i}^{n+n'} \int d^4x_1\, e^{-\mathrm{i}p_1 x_1} \left(\partial_1^2 + m^2\right) \cdots \int d^4x_1'\, e^{\mathrm{i}q_1 x_1'} \left(\partial_{1'}^2 + m^2\right) \\ \times \langle \Omega | \, \mathrm{T}\varphi(x_1) \cdots \varphi(x_1') \cdots | \Omega \rangle \ . \end{aligned} \tag{1}$$

In this form of the reduction formula, we automatically pick up only the residue of on the mass shell by multiplying $\partial^2 + m^2$.

To show that $\partial^2 + m^2$ indeed has all the correct signs in our mostly negative metric, we can rewrite our formula using integration by part as

$$\begin{aligned} &\int d^4x_1\, e^{-\mathrm{i}p_1 x_1} \cdots \int d^4x_1'\, e^{\mathrm{i}q_1 x_1'} \langle \Omega | \, \mathrm{T}\varphi(x_1) \cdots \varphi(x_1') \cdots | \Omega \rangle \\ \xrightarrow[q_j^2 \to m^2]{p_i^2 \to m^2} &\prod_{i=1}^{n} \frac{i}{p_i - m^2} \prod_{j=1}^{n'} \frac{i}{q_j - m^2} \langle q_1, \cdots, q_{n'}; \mathrm{out} | p_1, \cdots, p_n; \mathrm{in} \rangle \ . \end{aligned} \tag{2}$$

This is also a form where our interpretation about "scattering amplitudes being the residue of the correlation functions" becomes much clearer.

3 The Issue with Time-Ordered Symbol

One usual way to the formula is to using the following expressions of the creation (annihilation) operator for in and out state.

$$
\begin{aligned}
a^\dagger_{\mathbf{k}}(+\infty) - a^\dagger_{\mathbf{k}}(-\infty) &= \int_{-\infty}^{+\infty} dt\ \partial_0 a^\dagger_{\mathbf{k}}(t) \\
&= -\mathrm{i} \int_{-\infty}^{+\infty} dt\, \partial_0 \int d^3\mathbf{x}\, e^{-\mathrm{i}kx} \overleftrightarrow{\partial_0} \varphi(x) \\
&= -\mathrm{i} \int d^4x\, e^{-\mathrm{i}kx} (\partial_0^2 + \omega_{\mathbf{k}}^2) \varphi(x) \\
&= -\mathrm{i} \int d^4x\, e^{-\mathrm{i}kx} (\partial_0^2 + \mathbf{k}^2 + m^2) \varphi(x) \\
&= -\mathrm{i} \int d^4x\, e^{-\mathrm{i}kx} (\partial_0^2 - \nabla^2 + m^2) \varphi(x) \\
&= -\mathrm{i} \int d^4x\, e^{-\mathrm{i}kx} (\partial^2 + m^2) \varphi(x)\ . \qquad (3)
\end{aligned}
$$

Notice that here we have merge two steps into one: we identify $\mathbf{k}^2$ as an operator $-\nabla^2$ acting on e^{-ikx} and then integrate by part to make it act on $\varphi(x)$. A similar relation for the annihilation operator can be obtained by simply taking a complex conjugate.

Everything is fine so far. A useful remark (excerpted from Srednicki's textbook) is that the last expression vanishes for free fields by the equation of motion, as expected (since the creation and annihilation operator should be time-independent). Another comment (from my advisor Xianyu) is that, in the cannonical quantization scheme, even though the quantization is not realized in a Lorentz-invariant way, after one integration over time we arrive at some Lorentz-invariant expressions, which is a magic in Minkowski spacetime (while other fully symmetric spaces like dS have no such magic).

The doubtful treatment then is, we add one time-order symbol T to

$$
\langle q_1, \cdots, q_{n'}; \mathrm{out} | p_1, \cdots, p_n; \mathrm{in} \rangle = \langle \Omega |\, a_{\mathbf{q}_1}(+\infty) \cdots a^\dagger_{\mathbf{p}_1}(-\infty) \cdots | \Omega \rangle \qquad (4)
$$

which seems to have no effect, as the operators inside are already ordered correctly. Then we substitute (3) into it and perform the time ordering. Now all the creation operators are thrown to the left side and the annihilation operators to the right side, resulting zero since the states are simply vacuum states. The only surviving term is the one purely made of $\int d^4x\, e^{-\mathrm{i}kx}(\partial^2 + m^2)\varphi(x)$. Thus the proof is finished.

But the problem here is, the time-order symbol is defined clearly only if we specify the time variables to be ordered. We should *not* interpret the time-order symbol as simply putting everything in order when dealing with equations with different time variablebbs on the opposite sides. For example $A(t_1)B(t_2) = C(t_3)$ never implies $\mathrm{T}A(t_1)B(t_2) = \mathrm{T}C(t_3)$ when we interpret T too naively, since it has simply no effect on the RHS but does add a time-order θ function on the LHS. Thus we need a more careful treatment when adding the time-order symbol.

4 A Careful Treatment of the Time-Order

When adding the time-order symbol to (4), we have two direct interpretation but neither works out as we would naively expected. One interpretation is that we treat those $\pm\infty$ as time variables already fixed to certain values, in which case the time-order symbol means simply nothing as there's just no time variables to be ordered. The other interpretation is to treat them as independent variables which we set to $\pm\infty$ outside the time-order symbol. But if we do that, (3) is not valid since the time variables are already set to $\pm\infty$. Even though we could carefully calculate a new version of (3) with unfixed variables (with proper treatment of the boundary terms), the time order still acts on those original time variables, which never changed during our substitution. So the time-order symbol cannot place creation operators on the left side and annihilation operators on the right side in this case either.

We start from a very general identity to deal with the time derivative of a time-order symbol. To make sure the symbol is well defined, we write the time variables to be ordered as subscripts of T. Assuming that the time variables t_i are in order as $t_1 > \cdots > t_n$, we have

$$
\begin{aligned}
&\frac{d}{dt}\mathrm{T}_{t_1\cdots t_n t}A_1(t_1)\cdots A_n(t_n)B(t)\\
&=\frac{d}{dt}\sum_{i=0}^{n}\theta(t-t_{i+1})\theta(t_i-t)A_1(t_1)\cdots A_i(t_i)B(t)A_{i+1}(t_{i+1})\cdots A_n(t_n)\\
&=\sum_{i=0}^{n}\theta(t-t_{i+1})\theta(t_i-t)A_1(t_1)\cdots A_i(t_i)\frac{dB(t)}{dt}A_{i+1}(t_{i+1})\cdots A_n(t_n)\\
&\quad+\sum_{i=0}^{n}\left(\delta(t-t_{i+1})\theta(t_i-t)-\theta(t-t_{i+1})\delta(t-t_i)\right)A_1(t_1)\cdots A_i(t_i)B(t)A_{i+1}(t_{i+1})\cdots A_n(t_n)\\
&=\mathrm{T}_{t_1\cdots t_n t}A_1(t_1)\cdots A_n(t_n)\frac{dB(t)}{dt}\\
&\quad+\sum_{i=0}^{n}\left(\delta(t-t_{i+1})-\delta(t-t_i)\right)A_1(t_1)\cdots A_i(t_i)B(t)A_{i+1}(t_{i+1})\cdots A_n(t_n)\\
&=\mathrm{T}_{t_1\cdots t_n t}A_1(t_1)\cdots A_n(t_n)\frac{dB(t)}{dt}\\
&\quad+\sum_{i=1}^{n}\delta(t-t_i)A_1(t_1)\cdots A_{i-1}(t_{i-1})\left[B(t_i),A_i(t_i)\right]A_{i+1}(t_{i+1})\cdots A_n(t_n)\ .
\end{aligned}
\tag{5}
$$

For simplicity, we have let the summation index i run from 0 to n. Every time we encounter the non-existing time variables t_0, t_{n+1}, it simply means that the corresponding θ function is not included (thus the terms with δ function as its derivative is discarded).

We can now get rid of the assumption of the order of $t_1, \cdots, t_n$, as we can always put them in the correct order first and then apply the result above. We arrive at a general formula

$$
\begin{aligned}
&\frac{d}{dt}\mathrm{T}_{t_1\cdots t_n t}A_1(t_1)\cdots A_n(t_n)B(t)\\
&=\mathrm{T}_{t_1\cdots t_n t}A_1(t_1)\cdots A_n(t_n)\frac{dB(t)}{dt}\\
&\quad+\sum_{i=1}^{n}\delta(t-t_i)\mathrm{T}_{t_1\cdots t_n}A_1(t_1)\cdots A_{i-1}(t_{i-1})\left[B(t_i),A_i(t_i)\right]A_{i+1}(t_{i+1})\cdots A_n(t_n)\ .
\end{aligned}
\tag{6}
$$

The derivative formula will be used throughout our proof of the LSZ reduction formula. First, it gives a correct version of our insertion of (3). A more general version of (3) would be

$$
\partial_0 a^\dagger_{\mathbf{k}}(t) = -\mathrm{i}\int d^3x\, e^{-\mathrm{i}kx}(\partial^2+m^2)\varphi(x)\ . \tag{7}
$$

This can be derived in a very similar way to (3).

To insert it into the scattering amplitude, we need the integration of (6) over time.

$$
\begin{aligned}
&B(+\infty)\mathrm{T}_{t_1\cdots t_n}A_1(t_1)\cdots A_n(t_n)-\mathrm{T}_{t_1\cdots t_n}A_1(t_1)\cdots A_n(t_n)B(-\infty)\\
&=\int_{-\infty}^{+\infty}dt\,\mathrm{T}_{t_1\cdots t_n t}A_1(t_1)\cdots A_n(t_n)\frac{dB(t)}{dt}\\
&\quad+\sum_{i=1}^{n}\mathrm{T}_{t_1\cdots t_n}A_1(t_1)\cdots A_{i-1}(t_{i-1})\left[B(t_i),A_i(t_i)\right]A_{i+1}(t_{i+1})\cdots A_n(t_n)\ .
\end{aligned}
\tag{8}
$$

We would take $A_i(t_i)$ to be the field operators and $B(t)$ to be the creation (annihilation) operator. Thus we would encounter their commutation realtion. Using the cannonical commutation relation

$$
[\varphi(t,\mathbf{x}),\varphi(t,\mathbf{x}')]=0,\ \ [\varphi(t,\mathbf{x}),\dot\varphi(t,\mathbf{x}')]=\mathrm{i}\delta^{(3)}(\mathbf{x}-\mathbf{x}')
$$

we can calculate the equal-time commutation relation as

$$
\begin{aligned}
\left[\varphi(x), a_{\mathbf{k}}^{\dagger}(t)\right] &= \left[\varphi(x), -\mathrm{i}\int d^3x'\, e^{-\mathrm{i}\omega_{\mathbf{k}}t+\mathrm{i}kx'}\overleftrightarrow{\partial_0}\varphi(x,\mathbf{x}')\right] \\
&= -\mathrm{i}\int d^3x' \left[\varphi(x), e^{-\mathrm{i}\omega_{\mathbf{k}}t+\mathrm{i}kx'}\dot{\varphi}(t,\mathbf{x}') + \mathrm{i}\omega_{\mathbf{k}}e^{-\mathrm{i}\omega_{\mathbf{k}}t+\mathrm{i}kx'}\varphi(x,\mathbf{x}')\right] \\
&= e^{-\mathrm{i}kx} \ .
\end{aligned} \tag{9}
$$

There's still one more thing to do. After the insertion we would get something like $\mathrm{T}\varphi(x)\partial_y^2\varphi(y)$. We need to move the derivative operator outside the time-order symbol. This can also be dealt with using (6).

$$
\begin{aligned}
&\mathrm{T}_{t_1\cdots t_n t}\varphi(x_1)\cdots\varphi(x_n)\ddot{\varphi}(x) \\
=\ &\frac{d}{dt}\left(\mathrm{T}_{t_1\cdots t_n t}\varphi(x_1)\cdots\varphi(x_n)\dot{\varphi}(x)\right) \\
&\quad + \mathrm{i}\sum_{i=1}^{n}\delta^{(4)}(x-x_i)\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_{i-1})\varphi(x_{i+1})\cdots\varphi(x_n) \\
=\ &\frac{d^2}{dt^2}\left(\mathrm{T}_{t_1\cdots t_n t}\varphi(x_1)\cdots\varphi(x_n)\varphi(x)\right) \\
&\quad + \mathrm{i}\sum_{i=1}^{n}\delta^{(4)}(x-x_i)\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_{i-1})\varphi(x_{i+1})\cdots\varphi(x_n) \ .
\end{aligned} \tag{10}
$$

Now we can combine all our results (7), (8), (9) and (10). We find a strict version of (3) as

$$
\begin{aligned}
&a_{\mathbf{k}}^{\dagger}(+\infty)\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_n) - \mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_n)a_{\mathbf{k}}^{\dagger}(-\infty) \\
=\ &\int_{-\infty}^{+\infty}dt\,\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_n)\frac{d}{dt}a_{\mathbf{k}}^{\dagger}(t) + \sum_{i=1}^{n}\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_{i-1})\left[a_{\mathbf{k}}^{\dagger}(t_i),\varphi(x_i)\right]\varphi(x_{i+1})\cdots\varphi(x_n) \\
=\ &-\mathrm{i}\int d^4x\,e^{-\mathrm{i}kx}\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_n)(\partial^2+m^2)\varphi(x) - \sum_{i=1}^{n}e^{-\mathrm{i}kx_i}\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_{i-1})\varphi(x_{i+1})\cdots\varphi(x_n) \\
=\ &-\mathrm{i}\int d^4x\,e^{-\mathrm{i}kx}(\partial^2+m^2)\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_n)\varphi(x) \\
&\quad + \sum_{i=1}^{n}\int d^4x\,e^{-\mathrm{i}kx}\delta^{(4)}(x-x_i)\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_{i-1})\varphi(x_{i+1})\cdots\varphi(x_n) \\
&\quad - \sum_{i=1}^{n}e^{-\mathrm{i}kx_i}\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_{i-1})\varphi(x_{i+1})\cdots\varphi(x_n) \\
=\ &-\mathrm{i}\int d^4x\,e^{-\mathrm{i}kx}(\partial^2+m^2)\mathrm{T}_{t_1\cdots t_n}\varphi(x_1)\cdots\varphi(x_n)\varphi(x) \ .
\end{aligned} \tag{11}
$$

This is just we wanted! We see that abusing the time-order symbol gives correct answer only because the terms from (8) and (10) cancel. We may interpret this as that, (8) sends the time derivative into the time-order symbol while (10) takes it out again. But a careful treatment as above should always be considered.

5 Another Approach to LSZ

There are, however, another approach to the reduction formula, which naturally avoid those issues with the time-order symbol. Another advantage of such method is that it can be generalized to field with non-zero spin more easily (but we are not going to discuss such generalization in this note).

The key difference is that, in the method above, we started from the scattering amplitude and tried to "reduce" it to the correlation function. In this alternative method, we start from the correlation function instead. We identify the residue of the correlation function as the scattering amplitude. Since we have the time-order symbol at the very beginning, we can always manually pick up the latest or the earliest field operator and directly take it outside

T. Notice that in the final form of (2) we have no ∂ operators, so the issues about the time derivative is also automatically avoided.

Here we only present a sketch of the method. We consider the object on the LHS of (2)

$$\int d^4x_1\, e^{-\mathrm{i}p_1x_1}\cdots\int d^4x_1'\, e^{\mathrm{i}q_1x_1'}\,\langle\Omega|\,\mathrm{T}\varphi(x_1)\cdots\varphi(x_1')\cdots|\Omega\rangle\ .$$

This is just the Fourier transform of a correlation function. We try to find its singularities in the energy variables ${p_i}_0, {q_j}_0$. Since they are presented here in a similar form, we treat them together as $k=-p_i, q_j$.

The momentum k appears only in an analytical function $e^{\mathrm{i}kx}$, so all its singularities should come from the unbounded region $t\to-\infty$ and $t\to+\infty$. Thus we can take φx outside the time-ordered product. It turns out that, we have a pole at $k_0\to-E_{\mathbf{k}}$ from the early time contribution as

$$\int d^4x\, e^{+\mathrm{i}kx}\,\langle\Omega|\,\mathrm{T}\varphi(x_1)\cdots\varphi(x_1')\cdots|\Omega\rangle \xrightarrow{k_0\to-E_{\mathbf{k}}} \frac{\mathrm{i}}{k^2-m^2}\,\langle\Omega|\,\mathrm{T}\varphi(x_1)\cdots\varphi(x_1')\cdots|\mathbf{k};\mathrm{in}\rangle\ , \tag{12}$$

and a pole at $k_0\to+E_{\mathbf{k}}$ from the late time contribution as

$$\int d^4x\, e^{+\mathrm{i}kx}\,\langle\Omega|\,\mathrm{T}\varphi(x_1)\cdots\varphi(x_1')\cdots|\Omega\rangle \xrightarrow{k_0\to+E_{\mathbf{k}}} \frac{\mathrm{i}}{k^2-m^2}\,\langle\mathbf{k};\mathrm{out}|\,\mathrm{T}\varphi(x_1)\cdots\varphi(x_1')\cdots|\Omega\rangle\ , \tag{13}$$

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