Lehmann–Symanzik–Zimmermann (LSZ) Reduction Formula

Earlier in class (see my notes) I explained the two-point correlation functions and showed how their poles are related to the physical masses of particles and the strengths of bare fields. The LSZ reduction formula focuses on the $n > 2$ correlation functions

$$\mathcal{F}_n(x_1, \ldots, x_n) \stackrel{\text{def}}{=} \langle\Omega|\,\mathbf{T}\hat{\Phi}(x_1)\cdots\hat{\Phi}(x_n)\,|\Omega\rangle \tag{1}$$

— where the quantum fields $\hat{\Phi}(x)$ are in the Heisenberg picture of quantum mechanics — and relates the poles of their Fourier transforms

$$\mathcal{F}_n(p_1, \ldots, p_n) = \int\! d^4x_1\, e^{ip_1x_1} \cdots \int\! d^4x_n\, e^{ip_nx_n} \times \mathcal{F}_n(x_1, \ldots, x_n), \tag{2}$$

to the S–matrix elements between the physical asymptotic states. The poles happen when any of the n momenta p_i approaches the mass shell, $p_i^2 \to M^2_{\text{phys}}$, and the most interesting pole is the simultaneous pole when all n momenta go on-shell. Specifically, let

$$p_1^0 \to +E(\mathbf{p}_1) = +\sqrt{\mathbf{p}_1 + M^2}, \quad \ldots, \quad p_k^0 \to +E(\mathbf{p}_k) \tag{3}$$

for some $k < n$, but

$$p_{k+1}^0 \to -E(\mathbf{p}_{k+1}), \quad \ldots, \quad p_n^0 \to -E(\mathbf{p}_n). \tag{4}$$

In this limit, Lehmann–Symanzik–Zimmermann formula (published in 1955) gives us

$$\mathcal{F}_n(p_1, \ldots, p_n) \xrightarrow[\text{on shell}]{} \prod_{i=1}^{n} \frac{i\sqrt{Z}}{p_i^2 - M^2 + i\epsilon} \times \langle \text{out} : -p_{k+1}, \ldots, -p_n|\,\hat{S}\,|\text{in} : p_1, \ldots, p_k\rangle\,. \tag{5}$$

The field-strength factors $\sqrt{Z}$ in this formula stem from the $\mathcal{F}_n$ in eq. (1) being the correlation of the bare fields. If we re-define it as the correlation function of the renormalized fields — or equivalently, use the counterterm perturbation theory to calculate the correlation function, — then we would have $\mathcal{F}_n^{\text{renormalized}} = Z^{-n/2}\mathcal{F}_n^{\text{bare}}$ and consequently

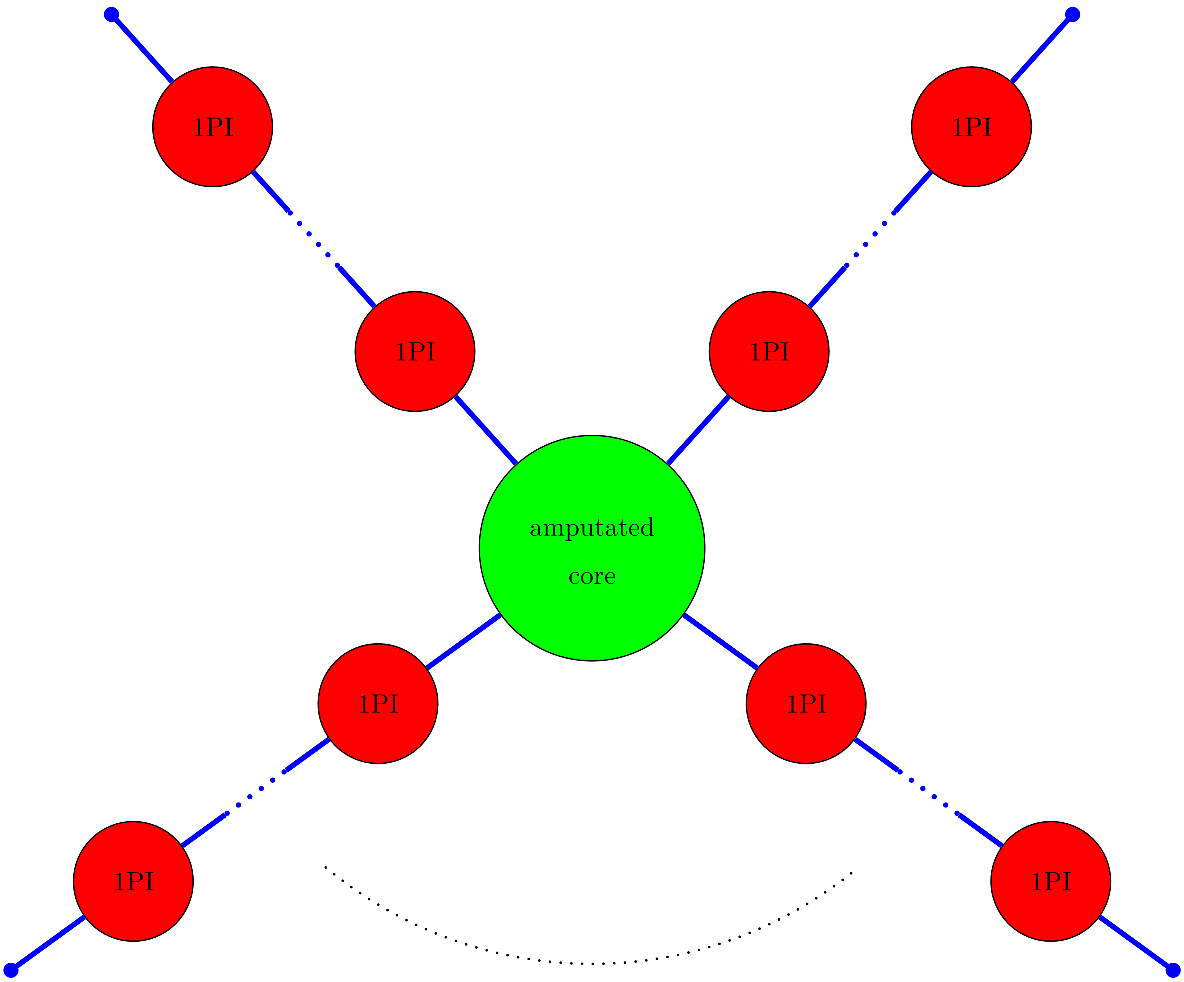
$$\mathcal{F}_n^{\text{renormalized}}(p_1, \ldots, p_n) \xrightarrow[\text{on shell}]{} \prod_{i=1}^{n} \frac{i}{p_i^2 - M^2 + i\epsilon} \times \langle \text{out} : -p_{k+1}, \ldots, -p_n|\,\hat{S}\,|\text{in} : p_1, \ldots, p_k\rangle\,. \tag{6}$$

Perturbation Theory for the Correlation Functions

Before deriving the LSZ reduction formula, let me show how the poles at $p_i^2 \to M^2$ arise from formal resummation of the perturbation theory. For simplicity, let's focus on the connected correlation functions, which in perturbation theory obtain as

$$\mathcal{F}_n^{\text{conn}}(p_1, \ldots, p_n) \;=\; \sum \begin{pmatrix} \text{all connected diagrams} \\ \text{with } n \text{ external vertices} \end{pmatrix}. \qquad (7)$$

Topologically, a general diagram of this kind has an amputated core, plus any number of external leg bubbles on any of the n external legs, thus



(8)

Each external leg bubble here is one-particle irreducible (1PI) — if we cut any propagator internal to the bubble, it stays connected. As to the amputated core, if we cut any propagator internal to the core, it may stay connected or break into two disconnected parts, but if it breaks then each part must remain connected to at least two external legs.

A general diagram (8) contributing to the connected n-point function may have:

- Any kind of amputated core with n external legs.
- Any number $N_i = 0, 1, 2, \ldots$ of leg bubbles in each of the n legs.
- And any such bubble may be any kind of 1PI subgraph with 2 external legs.

⋆ Most importantly, we may chose any amputated core we like and any leg bubbles we like completely independently from each other.

Consequently, when we formally sum over all connected Feynman diagrams with n external vertices, the sum factorizes into a product of a sum over the cores and a sum over the bubbles in each leg,

$$\mathcal{F}_n^{\text{conn}}(p_1, \ldots, p_n) \;=\; \sum \binom{\text{connected}}{\text{diagrams}} \;=\; \sum \binom{\text{amputated}}{\text{cores}} \times \prod_{i=1}^{n} \binom{\text{external}}{\text{leg factors}}. \tag{9}$$

where each external leg factors includes the blue propagators and the leg bubbles, and should be summed over all numbers of bubbles of any kinds. In general, for N_i bubbles we have $N_i + 1$ blue propagators with fixed momentum p_i, thus

$$\begin{aligned}
\binom{\text{external}}{\text{leg factor}}_i \;&=\; \sum_{N_i=0}^{\infty} \left(\frac{i}{p_i^2 - m_b^2 + i\epsilon}\right)^{N_i+1} \times \left[\sum \binom{\text{single}}{\text{bubbles}}\right]^{N_i} \\
&=\; \sum_{N_i=0}^{\infty} \left(\frac{i}{p_i^2 - m_b^2 + i\epsilon}\right)^{N_i+1} \times \left[-i\Sigma(p_i^2)\right]^{N_i} \\
&=\; \frac{i}{p_i^2 - m_b^2 - \Sigma(p^2) + i\epsilon} \;=\; \mathcal{F}_2(p^2),
\end{aligned} \tag{10}$$

exactly as in the two-point correlation function. Therefore,

$$\mathcal{F}_n^{\text{conn}}(p_1, \ldots, p_n) \;=\; \prod_{i=1}^{n} \mathcal{F}_2(p_i^2) \times \sum \binom{\text{amputated}}{\text{cores}}. \tag{11}$$

This formula explains where the poles in the correlation functions come from: When any of the momenta p_i goes on-shell, $p_i^2 \to M_{\rm phys}^2$, the corresponding $\mathcal{F}_2(p_i^2)$ has a pole,

$$\mathcal{F}_2(p^2) \;=\; \frac{iZ}{p_i^2 - M^2 + i\epsilon} \;+\; \text{finite}, \tag{12}$$

which translates into the pole of the whole product (11). When all of the n momenta go on shell at the same time, all n of the $\mathcal{F}_2(p_i^2)$ factors develop poles, thus

$$\mathcal{F}_n^{\rm conn}(p_1,\ldots,p_n) \;\longrightarrow\; \prod_{i=1}^{n} \frac{iZ}{p_i^2 - M^2 + i\epsilon} \times \sum \begin{pmatrix} \text{amputated} \\ \text{cores} \end{pmatrix}. \tag{13}$$

Note the combined residue of this n-fold pole,

$$\text{Residue}\left[\mathcal{F}_n^{\rm conn}(p_1,\ldots,p_n)\right]_{\text{all } p_i^2\to M^2} \;=\; (iZ)^n \times \sum \begin{pmatrix} \text{amputated} \\ \text{cores} \end{pmatrix}. \tag{14}$$

Thus far, we have explained the poles of the Lehmann–Symanzik–Zimmermann formula (5). In a moment, we should compare the residues. But first let's cluster-expand the LHS of the LSZ formula into connected correlation functions while the S-matrix element on the RHS likewise expands into connected and disconnected pieces. For example, for $n = 4$ we have

$$\begin{aligned} \mathcal{F}_4(p_1,p_2,p_3,p_4) \;=\;& \mathcal{F}_4^{\rm conn}(p_1,p_2,p_3,p_4) \\ &+\; \mathcal{F}_2(p_1,p_2)\times\mathcal{F}_2(p_3,p_4) \;+\; \mathcal{F}_2(p_1,p_3)\times\mathcal{F}_2(p_2,p_4) \\ &+\; \mathcal{F}_2(p_1,p_4)\times\mathcal{F}_2(p_2,p_3), \end{aligned} \tag{15}$$

and at the same time

$$\begin{aligned} \langle -p_3,-p_4|\,\hat S\,|p_1,p_2\rangle \;=\;& (2\pi)^4\delta^{(4)}(p_1+p_2+p_3+p_4)\times\langle -p_3,-p_4|\,i\widehat{\mathcal{M}}\,|p_3,p_4\rangle \\ &+\; \langle -p_2|\,\hat S\,|p_1\rangle\times\langle -p_4|\,\hat S\,|p_3\rangle \;+\; \langle -p_3|\,\hat S\,|p_1\rangle\times\langle -p_4|\,\hat S\,|p_2\rangle \\ &+\; \langle -p_4|\,\hat S\,|p_1\rangle\times\langle -p_3|\,\hat S\,|p_2\rangle\,. \end{aligned} \tag{16}$$

In terms of the LSZ formula for $n = 4$, we get 4 terms — 1 connected and 3 disconnected — on each side of the equation. The corresponding disconnected terms on the left-hand and the right hand sides match each other by the LSZ formula for $n = 2$, so the connected terms should also match each other,

$$\mathcal{F}_4^{\rm conn}(p_1,p_2,p_3,p_4) \xrightarrow[\text{on shell}]{} \prod_{i=1}^{4}\left(\frac{i\sqrt{Z}}{p_i^2-M^2+i\epsilon}\right)\times(2\pi)^4\delta^{(4)}(p_{\rm net})\times\langle -p_3,-p_4|\,i\widehat{\mathcal{M}}\,|p_1,p_2\rangle\,, \tag{17}$$

Likewise, for $n > 4$

$$\begin{aligned}\mathcal{F}_n^{\rm conn}(p_1,\ldots,p_4) \xrightarrow[\text{on shell}]{} \prod_{i=1}^{n}\left(\frac{i\sqrt{Z}}{p_i^2-M^2+i\epsilon}\right) &\times(2\pi)^4\delta^{(4)}(p_{\rm net})\\ &\times\langle -p_{k+1},\ldots,-p_n|\,i\widehat{\mathcal{M}}\,|p_1,\ldots,p_k\rangle\end{aligned} \tag{18}$$

for $p_1^0,\ldots,p_k^0 > 0$ while $p_{k+1}^0,\ldots,p_n^0 < 0$.

Now let's compare the residue of the combined pole here,

$$\begin{aligned}\text{Residue}\left[\mathcal{F}_n^{\rm conn}(p_1,\ldots,p_n)\right]_{\text{on shell}} \;=\; &(i\sqrt{Z})^n\times(2\pi)^4\delta^{(4)}(p_{\rm net})\\ &\times\langle -p_{k+1},\ldots,-p_n|\,i\widehat{\mathcal{M}}\,|p_1,\ldots,p_k\rangle\,,\end{aligned} \tag{19}$$

to the residue (14) of the same connected correlation function which obtains from the Feynman rules. Matching the two expressions, we see that the LSZ formula implies

$$(2\pi)^4\delta^{(4)}(p_{\rm net})\times\langle -p_{k+1},\ldots,-p_n|\,i\widehat{\mathcal{M}}\,|p_1,\ldots,p_k\rangle \;=\; Z^{n/2}\times\sum\begin{pmatrix}\text{amputated}\\ \text{cores}\end{pmatrix}. \tag{20}$$

And this is why we calculate the scattering amplitudes using only the amputated Feynman diagrams!

The factor $Z^{n/2}$ in eq. (20) follows from using the correlation functions for bare fields and hence the bare perturbation theory for the amputated diagrams. In the counterterm perturbation theory, this factor goes away and we are left with

$$(2\pi)^4\delta^{(4)}(p_{\rm net})\times i\mathcal{M}(\text{on shell }p_1,\ldots,p_n) \;=\; \sum\begin{pmatrix}\text{amputated cores}\\ \text{with } n \text{ external lines}\end{pmatrix}. \tag{21}$$

Deriving the LSZ Reduction Formula

Now that we know what is the LSZ reduction formula good for, let's prove it. Let's start by focusing on a single momentum, say p_1, and look for the quantum origin of the poles when that momentum goes on shell, $p_1^0 \to \pm E(\mathbf{p}_1)$. To simplify our notations, we keep the $(x_2, \ldots, x_n)$ coordinates of the n-point correlation function in the coordinate basis, only the x_1 gets Fourier transformed to the momentum basis, thus

$$\mathcal{F}_n(p_1; x_2, \ldots, x_n) \;=\; \int d^4x_1\, e^{-ip_1x_1} \times \mathcal{F}_n(x_1, x_2, \ldots, x_n). \tag{22}$$

Let's split the time integral here over $t_1 = x_1^0$ into 3 integration ranges: Range (i) from $-\infty$ to some very early but finite time T_1; range (II) from T_1 to some very late but finite time T_2; and range (III) from T_2 to $+\infty$. Thus,

$$\mathcal{F}_n(p_1; x_2, \ldots, x_n) \;=\; \sum_{i=1}^{3} \int\limits_{\text{range}\#i} dt_1\, e^{-ix_1^0p_1^0} \times \int d^3\mathbf{x}_1\, e^{-i\mathbf{x}_1\mathbf{p}_1} \times \mathcal{F}_n(x_1, x_2, \ldots, x_n). \tag{23}$$

Note that in the coordinate space, the $\mathcal{F}_n(x_1, x_2, \ldots, x_n)$ is an analytic function of the x_1^μ. Consequently, integrating the $\mathcal{F}_n \times$phase over a finite range#2 of time cannot possibly produce a pole — all such integrals are analytic and finite. Instead, the poles at $p_1^0 = \pm E(\mathbf{p}_1)$ must come from integrating over the semi-infinite time ranges #1 and #3. So let's take a closer look at these time ranges.

For the first time range $x_1^0 < T_1$, the x_1 point is earlier than all the other $n-1$ points $x_2, \ldots, x_n$, hence

$$\mathbf{T}\big(\hat{\Phi}(x_1)\cdots\Phi(x_n)\big) \;=\; \mathbf{T}\big(\hat{\Phi}(x_2)\cdots\Phi(x_n)\big) \times \hat{\Phi}(x_1) \tag{24}$$

and therefore

$$\begin{aligned}\mathcal{F}_n(x_1, x_2, \ldots, x_n) \;&=\; \langle\Omega|\,\mathbf{T}\big(\hat{\Phi}(x_2)\cdots\Phi(x_n)\big) \times \hat{\Phi}(x_1)\,|\Omega\rangle \\ &=\; \sum_{|\Psi\rangle} \langle\Omega|\,\mathbf{T}\big(\hat{\Phi}(x_2)\cdots\Phi(x_n)\big)\,|\Psi\rangle \times \langle\Psi|\,\hat{\Phi}(x_1)\,|\Omega\rangle\,,\end{aligned} \tag{25}$$

where the sum is over all quantum states Ψ. Similar to what we did in an earlier class for the two-point functions (see my notes, pages 9–11), we restrict the sum to the quantum states which can be created by the field $\hat{\Phi}$ from the vacuum $|\Omega\rangle$, and then we label such states as $|\psi, q\rangle$ where q^μ is the net momentum of the state while ψ denotes the rest of its quantum numbers, discrete or continuous. Consequently,

$$\sum_{|\Psi\rangle} = \sum_\psi \int \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{1}{2E(\mathbf{q};\psi)} \tag{26}$$

for

$$q^0 = +E(\mathbf{q},\psi) = +\sqrt{\mathbf{q}^2 + M^2(\psi)}. \tag{27}$$

Also, the x_1 and the q dependence of the matrix element $\langle\psi, q|\,\hat{\Phi}(x_1)\,|\Omega\rangle$ obtain as simply

$$\langle\psi, q|\,\hat{\Phi}(x_1)\,|\Omega\rangle = e^{+iqx_1} \times \langle\psi|\,\hat{\Phi}\,|\Omega\rangle\,. \tag{28}$$

Plugging these formulae into eq. (25) and hence into the range#1 contribution to the $\mathcal{F}_n(p_1; x_2, \ldots, x_n)$, we arrive at

$$\begin{pmatrix}\text{range\#1}\\ \text{contribution}\end{pmatrix} = \int\limits_{-\infty}^{T_1} dt_1 \int d^3\mathbf{x}_1\, e^{-ix_1p_1} \sum_\psi \int \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{1}{2E(\mathbf{q};\psi)}\, \langle\Omega|\,\mathbf{T}\big(\hat{\Phi}(x_2)\cdots\Phi(x_n)\big)\,|\psi, q\rangle \\ \times \langle\psi|\,\hat{\Phi}\,|\Omega\rangle \times e^{+iqx_1}. \tag{29}$$

Now let's integrate over the x_1 before integrating over $\mathbf{q}$ and summing over ψ. The only x_1-dependent factors here are the $e^{-ip_1x_1} \times e^{+iqx_1}$, so the space integral

$$\int d^3\mathbf{x}_1\, e^{+i\mathbf{p}_1\cdot\mathbf{x}_1} \times e^{-i\mathbf{q}\cdot\mathbf{x}_1} = (2\pi)^3\delta^{(3)}(\mathbf{q} - \mathbf{p}_1) \tag{30}$$

sets $\mathbf{q} = \mathbf{p}_1$, and hence $q^0 = +E(\mathbf{q},\psi) = +E(\mathbf{p}_1,\psi)$. Consequently, the time integral over the range#1 becomes

$$\begin{aligned}\int\limits_{-\infty}^{T_1} dt_1\, e^{-it_1p_1^0} \times e^{+it_1q^0} &= \int\limits_{-\infty}^{T_1} dt_1\, \exp\big(-it_1(p_1^0 - E(\mathbf{p}_1))\big)\\ &\to \int\limits_{-\infty}^{T_1} dt_1\, \exp\big(t_1(\epsilon - ip_1^0 + iE(\mathbf{p}_1))\big) \qquad \langle\!\langle\, \text{for } \epsilon \to +0 \,\rangle\!\rangle\\ &= \frac{e^{T_1(\epsilon - ip_1^0 + iE(\mathbf{p}_1))}}{\epsilon - ip_1^0 + E(\mathbf{p}_1)} \underset{\epsilon\to 0}{\longrightarrow} \frac{i\,e^{-iT_1(p_1^0 - E(\mathbf{p}_1))}}{p_1^0 - E(\mathbf{p}_1) + i\epsilon}\,.\end{aligned} \tag{31}$$

Consequently, the big integral (29) reduces to

$$\begin{pmatrix}\text{range\#1}\\ \text{contribution}\end{pmatrix} = \sum_\psi \frac{1}{2E(\mathbf{p}_1,\psi)} \times \frac{ie^{-iT_1(p_1^0-E(\mathbf{p}_1))}}{p_1^0-E(\mathbf{p}_1)+i\epsilon} \times \langle\Omega|\,\mathbf{T}\big(\hat\Phi(x_2)\cdots\Phi(x_n)\big)\,|\psi,\mathbf{p}\rangle \times \langle\psi|\,\hat\Phi\,|\Omega\rangle \tag{32}$$

Note that for a discrete state ψ there is a pole at $p^0 = +E(\mathbf{p},\psi) = +\sqrt{\mathbf{p}^2+M(\psi)^2}$. In particular, the one-particle state of physical mass M contributes the pole

$$\frac{ie^{-iT_1(p_1^0-E(\mathbf{p}_1))}}{2E(\mathbf{p}_1)(p_1^0-E(\mathbf{p}_1)+i\epsilon)} \times \langle\Omega|\,\mathbf{T}\big(\hat\Phi(x_2)\cdots\Phi(x_n)\big)\,|1:\mathbf{p}\rangle \times \sqrt{Z} \tag{33}$$

where the $\sqrt{Z}$ factor comes from $\langle 1|\,\hat\Phi\,|\Omega\rangle = \sqrt{Z}$. Moreover, near the pole

$$\frac{ie^{-iT_1(p_1^0-E(\mathbf{p}_1))}}{2E(\mathbf{p}_1)(p_1^0-E(\mathbf{p}_1)+i\epsilon)} = \frac{i}{(p_1^0)^2-E^2(\mathbf{p}_1)+i\epsilon} + \text{finite} = \frac{i}{p_1^2-M^2_{\text{phys}}+i\epsilon} + \text{finite}. \tag{34}$$

so we may rewrite the pole in the usual relativistic form.

So here is the bottom line: for p_1^μ going to the positive-energy mass shell, the correlation function $\mathcal{F}_n(p_1;x_2,\ldots,x_n)$ has a pole $i/(p_1^2-M^2+i\epsilon)$ with residue

$$\text{residue} = \sqrt{Z} \times \langle\Omega|\,\mathbf{T}\big(\hat\Phi(x_2)\cdots\Phi(x_n)\big)\,|1:p_1\rangle\,. \tag{35}$$

This pole comes from the first range of the time integration, $-\infty < x_1^0 < T_1$.

The third range of time integration, $T_2 < x_1^0 < +\infty$, can be handled in the similar manner. To save time, let me skip the gory details of the calculation and simply give you the bottom line. This time, the pole is for p_1 going to the negative-energy mass shell, $p_1^0 \to -E(\mathbf{p}_1,M)$, and its residue is

$$\text{residue} = \sqrt{Z} \times \langle 1:(-p_1)|\,\mathbf{T}\big(\hat\Phi(x_2)\cdots\Phi(x_n)\big)\,|\Omega\rangle\,. \tag{36}$$

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Thus far, we have focused on the pole for a single momentum p_1 going on shell. Now let's Fourier transform to coordinates x_1 and x_2 to the momenta p_1 and p_2,

$$\mathcal{F}_n(p_1,p_2;x_3,\ldots x_n) \;=\; \int\!d^4x_1\,e^{-ip_1x_1}\int\!d^4x_2\,e^{-ip_2x_2}\times\mathcal{F}_n(x_1,x_2,x_3,\ldots,x_n), \tag{37}$$

and then take both momenta p_1 and p_2 on-shell at the same time, say $p_1^0 \to +E(\mathbf{p}_1, M)$ and $p_2^0 \to +E(\mathbf{p}_2, M)$. Similar to what we had for a single momentum, this time we get a combined pole

$$\frac{i}{p_1^2 - M^2 + i\epsilon} \times \frac{i}{p_2^2 - M^2 + i\epsilon} \tag{38}$$

which emerges from the time integrals $\int dt_1$ and $\int dt_2$ over the asymptotic past range, $t_1, t_2 \to -\infty$. For two fields $\hat{\Phi}(x_1)$ and $\hat{\Phi}(x_2)$ at the asymptotic past points, we have

$$\langle\Omega|\,\mathbf{T}\hat{\Phi}(x_1)\cdots\hat{\Phi}(x_n)\,|\Omega\rangle \;=\; \sum_{\Psi}\langle\Omega|\,\mathbf{T}\hat{\Phi}(x_3)\cdots\hat{\Phi}(x_n)\,|\Psi\rangle\times\langle\Psi|\,\mathbf{T}\hat{\Phi}(x_1)\hat{\Phi}(x_2)\,|\Omega\rangle\,, \tag{39}$$

and the pole (38) comes from $|\Psi\rangle = |\text{in}(p_1, p_2)\rangle$ — the asymptotic incoming state of two particles. Strictly speaking, we should treat these two particles as being in the wave-packet states with small δp rather tan having definite momenta $\mathbf{p}_1$ and $\mathbf{p}_2$. This way, each wave packet has a finite coordinate-space size $1/2\delta p$, so in the asymptotic past when the two particles were very far from each other, their respective wave packets did not overlap, and the particles did not interact with each other until they approached each other at a later time. Therefore, in the asymptotic past $x_1^0, x_2^0 \to -\infty$ we have

$$\begin{aligned}\langle\text{in}(q_1,q_2)|\,\mathbf{T}\hat{\Phi}(x_1)\hat{\Phi}(x_2)\,|\Omega\rangle \;&=\; \langle\text{in}(q_1)|\,\hat{\Phi}(x_1)\,|\Omega\rangle\times\langle\text{in}(q_2)|\,\hat{\Phi}(x_2)\,|\Omega\rangle \;+\; (q_1\leftrightarrow q_2)\\ &=\; Z\times\text{wavepacket}_{q_1}(x_1)\times\text{wavepacket}_{q_2}(x_2) \;+\; (q_1\leftrightarrow q_2)\\ &\approx\; Z\times e^{iq_1x_1}\times e^{iq_2x_2} \;+\; (q_1\leftrightarrow q_2).\end{aligned} \tag{40}$$

Plugging this formula into eq. (39) and performing the Fourier transform (37) similarly to what we did for a single coordinate, we find that when both momenta p_1 and p_2 approach the positive-energy mass shell, the correlation function develops a double pole

$$\begin{aligned}\mathcal{F}_n(p_1,p_2;x_3\,\ldots,x_n) \;\xrightarrow[p_1,p_2\to\text{mass shell}]{}\; &\frac{i\sqrt{Z}}{p_1^2-M^2+i\epsilon}\times\frac{i\sqrt{Z}}{p_2^2-M^2+i\epsilon}\\ &\times\langle\Omega|\,\mathbf{T}\hat{\Phi}(x_3)\cdots\hat{\Phi}(x_n)\,|\text{in}(p_1,p_2)\rangle\,.\end{aligned} \tag{41}$$

Now, let's Fourier transform the remaining coordinates $x_3, \ldots, x_n$ to momenta $p_3, \ldots, p_n$

and the take all these momenta to the negative-energy mass shell, each $p_i \to -E(\mathbf{p}_i, M)$. This time, the poles come from integrating each time variable $t_3, \ldots, t_n$ over the asymptotic future range and

$$\langle\Omega|\,\mathbf{T}\hat{\Phi}(x_3)\cdots\hat{\Phi}(x_n)\ \supset \langle\text{out}(-q_3,\ldots,-q_n)|\,. \tag{42}$$

Specifically,

$$\begin{aligned}\langle\Omega|\,\mathbf{T}\hat{\Phi}(x_3)\cdots\hat{\Phi}(x_n)\,|\text{out}(-q_3,\ldots,-q_n)\rangle\ &=\ Z^{(n-2)/2}\times e^{-iq_3x_2}\cdots e^{-iq_nx_x}\\ &\qquad+\ \text{particle permutations,}\end{aligned} \tag{43}$$

hence after the Fourier transform

$$\begin{aligned}\langle\Omega|\,\mathbf{T}\hat{\Phi}(p_3)\cdots\hat{\Phi}(p_n)\,|\text{in}(p_1,p_2)\rangle\ &\xrightarrow[p_3,\ldots,p_n\to\text{mass shell}]{}\ \prod_{i=3}^{n}\left(\frac{i\sqrt{Z}}{p_i^2-M^2+i\epsilon}\right)\times\\ &\qquad\times\langle\text{out}(-p_3,\ldots,-p_n)|\text{in}(p_1,p_2)\rangle\,,\end{aligned} \tag{44}$$

where the poles — and their residues — arise exactly as we saw for a single $p^0 \to -E(\mathbf{p})$.

Finally, plugging eq. (44) into eq. (41), we arrive at

$$\mathcal{F}_n(p_1,\ldots,p_n)\ \xrightarrow[\text{all }p_i\to\text{mass shell}]{}\ \prod_{i=1}^{n}\left(\frac{i\sqrt{Z}}{p_i^2-M^2+i\epsilon}\right)\times\langle\text{out}(-p_3,\ldots,-p_n)\,|\,\text{in}(p_1,p_2)\rangle\,. \tag{45}$$

Note that all of the above analysis was done in the Heisenberg picture of the quantum mechanics, so the asymptotic incoming and outgoing states in eq. (45) are the Heisenberg-picture states. Translating them into the interaction picture turns the Dirac bracket of the $|\text{in}\rangle$ and $\langle\text{out}|$ states into the S-matrix element,

$$\langle\text{out}(-p_3,\ldots,-p_n)\,|\,\text{in}(p_1,p_2)\rangle_H\ =\ \langle\text{out}(-p_3,\ldots,-p_n)|\,\hat{S}\,|\text{in}(p_1,p_2)\rangle_I\ . \tag{46}$$

Consequently, eq. (45) becomes the Lehmann–Symanzik–Zimmermann formula

$$\mathcal{F}_n(p_1,\ldots,p_n)\ \xrightarrow[\text{all }p_i\to\text{mass shell}]{}\ \prod_{i=1}^{n}\left(\frac{i\sqrt{Z}}{p_i^2-M^2+i\epsilon}\right)\times\langle\text{out}(-p_3,\ldots,-p_n)|\,\hat{S}\,|\text{in}(p_1,p_2)\rangle\,. \tag{5}$$

Quod erat demonstrandum.