Finite Volume QFT
&
QCD Spectroscopy

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Correlation Functions & Lattice QCD

In previous lectures, we have learned about how to describe reactions with non-perturbative scattering theory, and also how to compute low-energy hadronic observables from non-perturbative QCD, namely lattice QCD.

In these lectures, we will connect the static energy spectrum of hadrons in a box to scattering systems via a non-perturbative mapping, the so-called Lüscher formalism.

Let us first review some aspects of Lattice QCD calculations. Lattice QCD is a numerical technique to stochastically estimate QCD correlation functions. To accomplish this, QCD is formulated in a discrete, Euclidean spacetime which is bounded in a finite volume subject to some boundary conditions. Note that both the Euclidean & finite volume nature of spacetime forbids any notion of computing scattering dynamics directly from lattice QCD, since Euclidean spacetimes do not have real time evolutions & finite volumes do not allow free asymptotic states.

However, we can circumvent these issues by examining the behaviour of the scaling of finite volume corrections to corresponding infinite volume correlation functions. Since the LSZ formalism relates QFT correlation functions to scattering amplitudes, these corrections allow one to relate finite-volume energies to scatterings. Essentially,

$$C_L(P) = C_\infty(P) + \delta C_L(P)$$

Finite-volume correlator (LQCD)

Infinite-volume correlator (LSZ ⇒ Scattering)

Correction that connects FV & IV

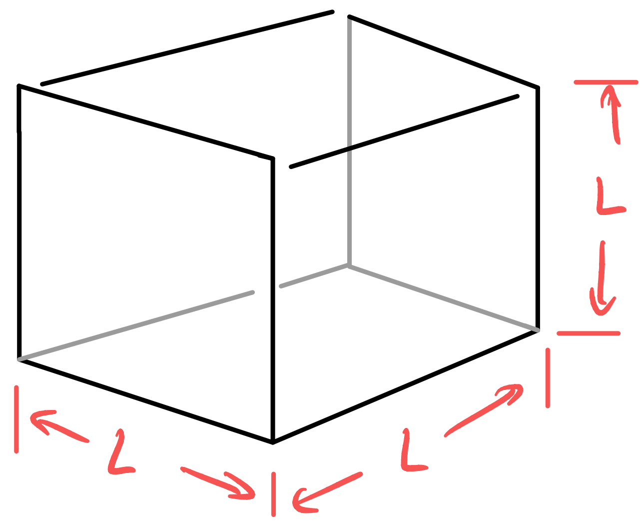
Our objectives are as follows:

- Examine the spectral rep. of 2-point correlators
- Determine the scaling relation for stable hadrons
- Compute the FV corrections to free two-particle correlators
- Study weakly interacting systems & deriving the Lüscher quantization condition
- Extracting resonances from LQCD

Preliminaries

We work in a continuous 3+1 Minkowski spacetime, $\text{diag}\, g = (+1,-1,-1,-1)$, which is confined in a cubic volume L^3 & infinite temporal extent, $T \to \infty$. The spatial volume is subject to periodic boundary conditions (PBCs)

$x_j = x_j + L\,\hat{e}_j \quad , j = 1,2,3 .$



- The spectrum of a confined system is discrete, E_n, $n \in \mathbb{N}_0$, & since the Hamiltonian is Hermitian, $\mathcal{H}^\dagger = \mathcal{H}$,

A eigenstate $|E_n, L\rangle$ has real energies, $E_n \in \mathbb{R}$

$$\boxed{\mathcal{H}|E_n, L\rangle = E_n |E_n, L\rangle}$$

The energies are independent of the spacetime signature,

$$t \to -i\tau \quad \Rightarrow \quad e^{-iE_n t} \to e^{-E_n \tau}$$

Euclidean time

So, we will work in Minkowski time

- We assume spacetime lattice discretization errors are negligible, thus work with continuous spacetime.

- Most practical spectral calculations use anisotropic lattices, $T \gg L$, so we again assume that finite T effects are negligible, thus $T \to \infty$.

- Spatial PBCs impose quantization conditions on the momentum. Consider a field operator $\mathcal{O}$. PBCs enforce

$$\mathcal{O}(t,\vec{x}) = \mathcal{O}(t,\vec{x}+L\hat{e})$$

Introducing the Fourier transform,

$$\mathcal{O}(t,\vec{x}) = \int \frac{d^3\vec{p}}{(2\pi)^3}\, e^{i\vec{p}\cdot\vec{x}}\, \tilde{\mathcal{O}}(t,\vec{p}),$$

we find

$$\int \frac{d^3\vec{p}}{(2\pi)^3}\, e^{i\vec{p}\cdot\vec{x}}\, \tilde{\mathcal{O}}(t,\vec{p}) = \int \frac{d^3\vec{p}}{(2\pi)^3}\, e^{i\vec{p}\cdot(\vec{x}+L\hat{e})}\, \tilde{\mathcal{O}}(t,\vec{p})$$

$$\Rightarrow e^{i\vec{p}\cdot L\hat{e}} = 1 \quad \Rightarrow \quad \boxed{\vec{p} = \frac{2\pi}{L}\vec{n}, \quad \vec{n}\in\mathbb{Z}^3}$$

Note the Fourier transform pair conventions

$$\boxed{\begin{aligned} \tilde{f}(p) &= \mathcal{F}[f(x)] = \int_{-\infty}^{\infty} dx\, e^{-ipx} f(x) \\ f(x) &= \mathcal{F}^{-1}[\tilde{f}(p)] = \frac{1}{L}\sum_p e^{ipx}\tilde{f}(p) \end{aligned}}$$

Infinite volume		Finite Volume
$\int \frac{dp}{2\pi}$	$\longleftrightarrow$	$\frac{1}{L}\sum_p$
$2\pi\,\delta(p'-p)$	$\longleftrightarrow$	$L\,\delta_{p'p}$

A key concept we will use in relating IV & FV physics is the Poisson Summation formula, which we write in the form

$$\boxed{\frac{1}{L^3}\sum_{\vec{p}} f(\vec{p}) = \sum_{\vec{n}} \int \frac{d^3\vec{p}}{(2\pi)^3}\, e^{iL\vec{n}\cdot\vec{p}} f(\vec{p})}$$

The PSF is the key we need in relating FV & IV quantities. Let's define the sum-integral operation

$$\frac{1}{L^3} \sumint_{\vec{p}} f(\vec{p}) \equiv \left[\frac{1}{L^3} \sum_{\vec{p} \in \frac{2\pi}{L}\mathbb{Z}^3} - \int \frac{d^3\vec{p}}{(2\pi)^3} \right] f(\vec{p})$$

By the PSF, we have

$$\left[\frac{1}{L^3} \sum_{\vec{p}} - \int \frac{d^3\vec{p}}{(2\pi)^3} \right] f(\vec{p}) = \sum_{\vec{n} \neq \vec{0}} \int \frac{d^3\vec{p}}{(2\pi)^3} \, e^{i\vec{p}\cdot\vec{n}L} f(\vec{p})$$

Suppose $f(\vec{p})$ is a smooth function in $\vec{p}$ (physical)

$$f(\vec{p}) = \sqrt{4\pi} \sum_{\ell=0}^{\infty} \sum_{m_\ell=-\ell}^{\ell} Y_{\ell m_\ell}(\hat{p}) \, f_{\ell m_\ell}(p)$$

↑ spherical harmonics

Recall plane-wave expansion

$$e^{i\vec{p}\cdot\vec{n}L} = 4\pi \sum_{\ell=0}^{\infty} i^\ell j_\ell(npL) \sum_{m_\ell=-\ell}^{\ell} Y_{\ell m_\ell}(\hat{n}) \, Y^*_{\ell m_\ell}(\hat{p})$$

↑ spherical Bessel functions

Inserting expansions into sum-integral, & converting the measure to spherical coordinates,

$$\frac{1}{L^3}\,\sum\!\!\!\!\!\!\!\int_{\vec{p}} f(\vec{p}) = \sum_{\vec{n}\neq\vec{0}} \int d^2\hat{p} \int_0^\infty \frac{dp\,p^2}{(2\pi)^3}\, e^{i\vec{p}\cdot\vec{n}L} f(\vec{p})$$

$$= \sum_{\vec{n}\neq\vec{0}} \frac{(4\pi)^{3/2}}{(2\pi)^3} \sum_{l',m_{l'}} \sum_{l,m_l} i^{l'} \int_0^\infty dp\,p^2\, j_{l'}(pnL)\, f_{lm_l}(p)$$

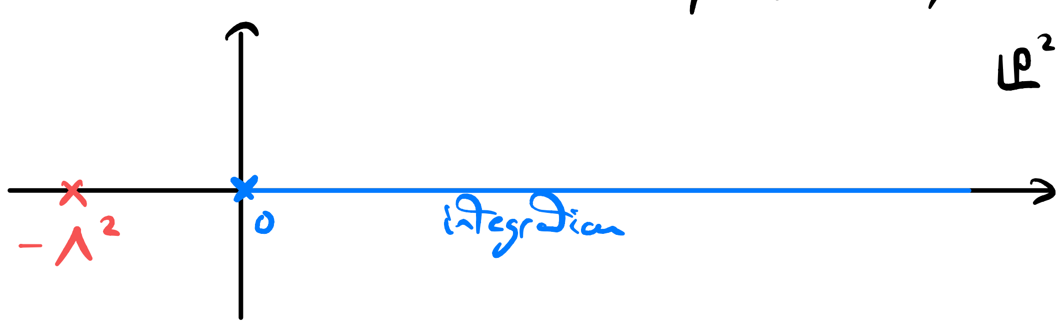
$$\times\; Y_{lm_l}(\hat{n}) \underbrace{\int d^2\hat{p}\; Y^*_{l'm_{l'}}(\hat{p})\, Y_{lm_l}(\hat{p})}_{\delta_{l'l}\,\delta_{m_{l'}m_l}}$$

$$= \sum_{\vec{n}\neq\vec{0}} \pi^{-3/2} \sum_{l,m_l} i^l\, Y_{lm_l}(\hat{n}) \int_0^\infty dp\,p^2\, j_l(pnL)\, f_{lm_l}(p)$$

Consider $l=0$ mode only, $j_0(pnL) = \dfrac{\sin pnL}{pnL}$

$$\Rightarrow \frac{1}{L^3}\,\sum\!\!\!\!\!\!\!\int_{\vec{p}} f(\vec{p}) = \frac{1}{2\pi^2} \sum_{\vec{n}\neq\vec{0}} \frac{1}{nL} \int_0^\infty dp\; p\sin(pnL)\, f_{00}(p)$$

Consider a function like $f_{00}(p) = \dfrac{1}{p^2+\Lambda^2}$, $\Lambda > 0$



then,

$$I = \int_0^\infty dp \; p \sin(pnL) \; \frac{1}{p^2+\Lambda^2}$$

← integrand even under $p \to -p$

$$= \frac{1}{2}\int_{-\infty}^{\infty} dp \; \frac{p \sin(pnL)}{p^2+\Lambda^2} \;=\; \frac{1}{2}\,\mathrm{Im}\int_{-\infty}^{\infty} dp \; \frac{p}{p^2+\Lambda^2}\, e^{ipnL}$$

$\sin x = \mathrm{Im}\, e^{ix}$

Consider Cauchy theorem: $\oint_\gamma dz \; f(z) = 0$

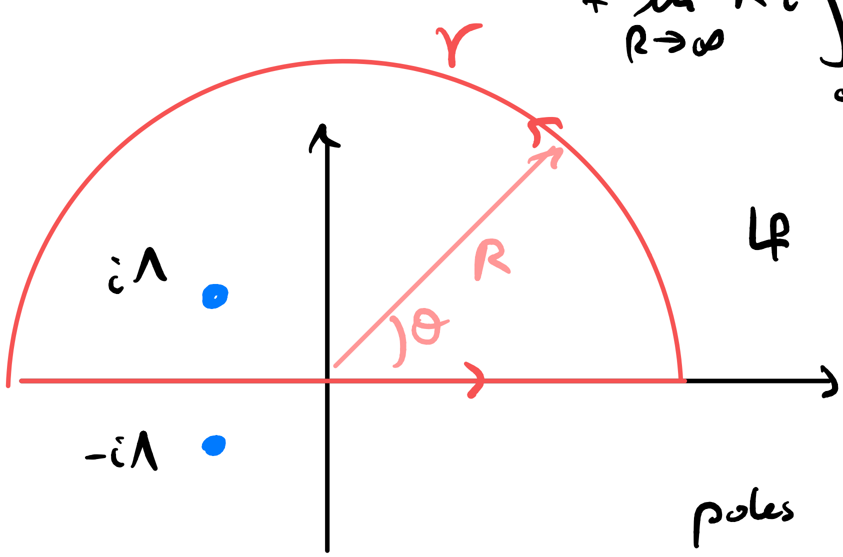
if $f(z)$ analytic in domain bounded by γ

$$\oint_\gamma dp \; \frac{p}{p^2+\Lambda^2}\, e^{ipnL} = \int_{-\infty}^{\infty} dp \; \frac{p}{p^2+\Lambda^2}\, e^{ipnL}$$

$$+ \lim_{R\to\infty} R i \int_0^\pi d\theta \; e^{i\theta} \, \frac{Re^{i\theta}}{R^2 e^{i2\theta} + \Lambda^2} \, e^{ipnL}$$

$p = Re^{i\theta}$ ↓

Vanishes as $R \to \infty$



poles at

$$p^2+\Lambda^2 = (p+i\Lambda)(p-i\Lambda) = 0$$

By residue theorem,

$$\oint_{\gamma} dp \, \frac{p}{p^2+\Lambda^2} e^{ipnL} = 2\pi i \, \mathrm{Res}[p = i\Lambda]$$
$$= 2\pi i \left(\frac{p}{p+i\Lambda} e^{ipnL} \right) \Big|_{p=i\Lambda}$$
$$= 2\pi i \left(\frac{i\Lambda}{2i\Lambda} e^{-n\Lambda L} \right)$$
$$= \pi i \, e^{-n\Lambda L}$$

So, we find the integral I is

$$I = \frac{1}{2} \mathrm{Im} \int_{-\infty}^{\infty} dp \, \frac{p}{p^2+\Lambda^2} e^{ipnL}$$
$$= \frac{1}{2} \mathrm{Im} \left(\pi i \, e^{-n\Lambda L} \right) = \frac{\pi}{2} e^{-n\Lambda L}$$

Therefore, sum-integral difference (for our example) is

$$\frac{1}{L^3} \oint_{\vec{p}} f(\vec{p}) = \frac{1}{2\pi^2} \sum_{\vec{n} \neq \vec{0}} \frac{1}{nL} I$$
$$= \frac{1}{4\pi} \sum_{\vec{n} \neq \vec{0}} \frac{1}{nL} e^{-n\Lambda L}$$

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exponentially suppressed scaling in box volume L

This illustrates an important property we will exploit.

Let $\frac{1}{L^3}\sum_{\vec{p}} f(\vec{p})$ be the FV quantity of interest.

then,

$$\frac{1}{L^3}\sum_{\vec{p}} f(\vec{p}) = \int \frac{d^3\vec{p}}{(2\pi)^3} f(\vec{p}) + \underbrace{\frac{1}{L^3}\sum\!\!\!\!\!\!\int_{\vec{p}} f(\vec{p})}_{\text{this is FV correction to IV term}}$$

if $f(\vec{p})$ is smooth, then by PSF

$$\boxed{\frac{1}{L^3}\sum\!\!\!\!\!\!\int_{\vec{p}} f(\vec{p}) \sim e^{-mL}}$$

m = lightest mass scale in theory

i.e., $m = m_\pi$ in QCD.

If $f(\vec{p})$ has some non-analytic behavior, e.g., poles/cuts, then this need not be so, & in general the correction scales like $1/L^3$.

A comment about regularization. Recall in QFTs, one often needs to introduce a regularization scheme to tame UV divergences. This is true for FV quantities as well, e.g.,

$$\frac{1}{L^3}\sum_{\vec{p}}{}' f(\vec{p}) \to \frac{1}{L^3}\sum_{\vec{p}}{}' f^R(\vec{p})$$

some regularization scheme
e.g., Pauli-Villars

Looking at the correction, i.e., the sum-integral difference

$$\frac{1}{L^3}\mathop{\sum\!\!\!\!\!\!\int}_{\vec{p}}{}' f^R(\vec{p}) = \frac{1}{L^3}\sum_{\vec{p}}{}' f^R(\vec{p}) - \int\frac{d^3\vec{p}}{(2\pi)^3} f^R(\vec{p})$$

$$= \sum_{\vec{n}\neq\vec{0}}\int\frac{d^3\vec{p}}{(2\pi)^3} e^{i\vec{p}\cdot\vec{n}L} f^R(\vec{p})$$

But, notice that as $\vec{p}\to\infty$

$$\frac{1}{L^3}\sum_{\vec{p}}{}' f^R(\vec{p}) - \int\frac{d^3\vec{p}}{(2\pi)^3} f^R(\vec{p}) \sim \Lambda - \Lambda \to 0$$

cutoffs characterizing divergence

$\Rightarrow$ the FV correction is independent of the regularization scheme!

Spectral Decomposition

The primary objects of interest in LQCD calculations are correlation functions, or correlators. Here we focus on 2-point correlators,

$x = (t, \vec{x})$

$$C_L(x) = \langle \mathcal{T}\, \mathcal{O}(x)\, \mathcal{O}^\dagger(0) \rangle$$

finite volume

some scalar operator (simplicity)

time-ordering operator

Consider Fourier transform,

$$C_L(P) = \int_L d^4x\, e^{iP\cdot x}\, C_L(x)$$

$P = (E, \vec{P})$

$$= \int_L d^4x\, e^{iP\cdot x} \langle \mathcal{T}\, \mathcal{O}(x)\, \mathcal{O}^\dagger(0) \rangle$$

Let us first consider $t > 0$ time ordering

$$\mathcal{T}\, \mathcal{O}(x)\, \mathcal{O}^\dagger(0) = \underline{\mathcal{O}(x)\, \mathcal{O}^\dagger(0)\, \theta(t)} + \mathcal{O}^\dagger(0)\, \mathcal{O}(x)\, \theta(-t)$$

So,

$$C_L(P) = \int_0^\infty dt \int_L d^3\vec{x}\, e^{iP\cdot x} \langle \mathcal{O}(x)\, \mathcal{O}^\dagger(0) \rangle \; + \; (t < 0)$$

Next, we insert a complete set of energy eigenstates

$$\mathcal{H} | E_n, \vec{P}, L \rangle = E_n(\vec{P}, L) | E_n, \vec{P}, L \rangle$$

So, with normalization $\langle E_{n'}, \vec{P}', L | E_n, \vec{P}, L \rangle = \delta_{n'n} \delta_{\vec{P}'\vec{P}}$ the resolution of identity is

$$\mathbb{1} = \sum_n \sum_{\vec{P}} | E_n, \vec{P}, L \rangle \langle E_n, \vec{P}, L |$$

We will suppress all other quantum numbers.

So, find

$$C_L(P) = \sum_n \sum_{\vec{P}'} \int_0^\infty dt \int_L d^3\vec{x}\ e^{iP\cdot x} \langle 0 | \mathcal{O}(x) | E_n, \vec{P}', L \rangle \langle E_n, \vec{P}', L | \mathcal{O}^\dagger(0) | 0 \rangle$$

Under spacetime translations, $\mathcal{O}(x) = e^{i\hat{P}\cdot x} \mathcal{O}(0) e^{-i\hat{P}\cdot x}$

with $\hat{P} = (\hat{H}, \hat{\vec{P}})$

To ensure convergence in $t \to \infty$, we let $\hat{H} \to \hat{H} - i\epsilon$ with $\epsilon \to 0^+$ implicit. Then,

$$e^{-i\hat{P}\cdot x} | E_n, \vec{P}', L \rangle = e^{-i(E_n - i\epsilon)t} e^{i\vec{P}'\cdot\vec{x}} | E_n, \vec{P}', L \rangle$$

We find,

$$C_L(P) = \sum_n \sum_{\vec{p}'} \int_0^\infty dt\, e^{i(E-E_n+i\epsilon)t} \times \int_L d^3\vec{x}\, e^{-i(\vec{P}-\vec{P}')\cdot\vec{x}} \, |Z_n(\vec{P}',L)|^2 + (t<0)$$

where $Z_n(\vec{P},L) \equiv \langle 0 | \mathcal{O}(0) | E_n, \vec{P}, L \rangle$

Now, $\int_L d^3\vec{x}\, e^{-i(\vec{P}-\vec{P}')\cdot\vec{x}} = L^3 \delta_{\vec{P}\vec{P}'}$

& $$\int_0^\infty dt\, e^{i(E-E_n+i\epsilon)t} = \left.\frac{e^{i(E-E_n+i\epsilon)t}}{i(E-E_n+i\epsilon)}\right|_0^\infty$$

$$= \frac{i}{E-E_n+i\epsilon}$$

So, we find

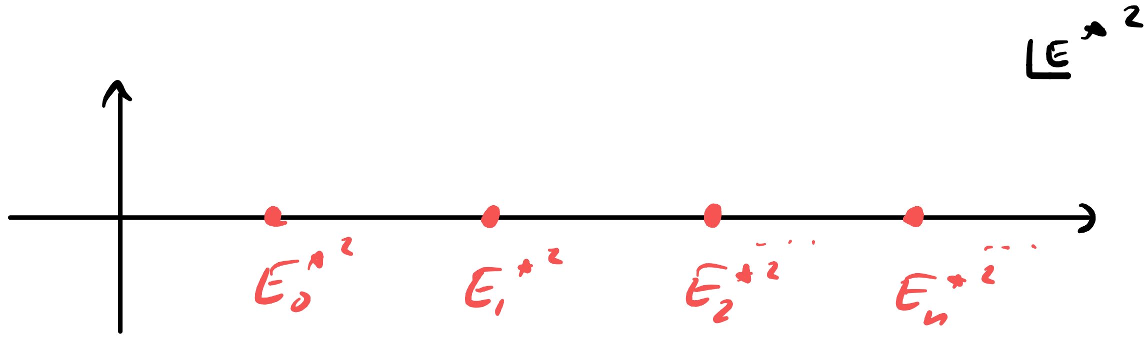
$$\boxed{C_L(P) = L^3 \sum_n \frac{i}{E-E_n+i\epsilon} |Z_n(\vec{P},L)|^2 + (t<0)}$$

Considering the t<0 term gives a pole of the form $E+E_n-i\epsilon$

$$\Rightarrow \boxed{C_L(P) = \sum_n 2E_n L^3 \frac{i}{E^2-E_n^2+i\epsilon} |Z_n(\vec{P},L)|^2}$$

So, the analytic structure of FV correlators is a sequence of poles in E^2 (or E). Recall the center-of-momentum (CM) frame, $\vec{P}^* = \vec{0}$

$$\Rightarrow \qquad E^{*2} = E^2 - \vec{P}^2 = P^2$$



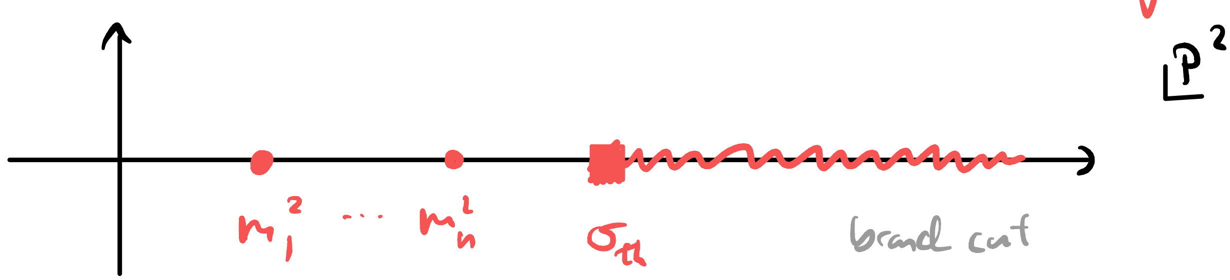
For IV correlators, we can follow the same idea, & derive the Källén-Lehmann spectral representation,

$$C_{\infty}(P) = \int d^4x \, e^{iP\cdot x} \langle T \, \mathcal{O}(x) \, \mathcal{O}^\dagger(0) \rangle$$

$$= \sum_{j=0}^{n} \frac{i Z_j}{P^2 - m_j^2} + \int_{\sigma_{th}}^{\infty} \frac{d\sigma}{2\pi} \frac{\rho(\sigma)}{P^2 - \sigma + i\epsilon}$$

possible stable/bound states

scattering continuum



The analytic structure is different for IV correlators & FV correlators. The FV correction is

$$C_L(P) = C_\infty(P) + \delta C_L(P)$$

poles cuts poles & cuts

By LSZ theorem, can get access to amplitudes $i\mathcal{M}$ in C_∞. From lattice QCD, get access to E_n. Here, can relate $E_n \Leftrightarrow i\mathcal{M}$ via FV correction $\delta C_L(P)$. To do so, we will use an all-orders approach in QFT to construct a diagrammatic representation for these objects. We will show that the results are general, independent on any particular QFT.

Single Particles

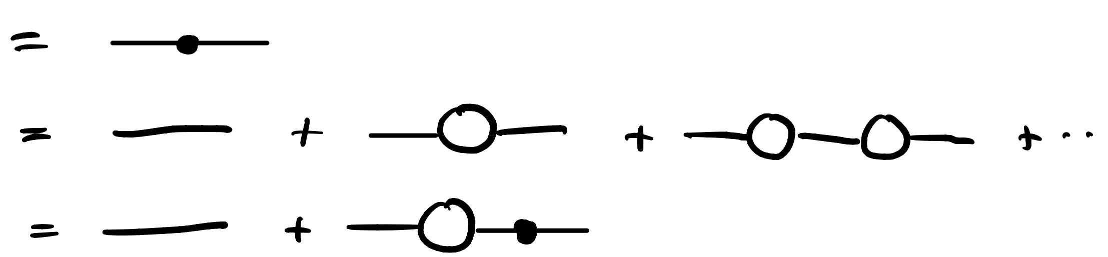
We will first examine FV corrections to single particle states. To be concrete, consider real scalar φ^4 theory,

mass parameter (Not physical)

$$\mathcal{L} = \frac{1}{2}\partial_\mu\varphi\,\partial^\mu\varphi - \frac{1}{2}m^2\varphi^2 - \frac{\lambda}{4!}\varphi^4$$

Our results are generally QFT independent, but we use a particular one, or a generalized EFT, as a catalyst.

Recall the Feynman diagram expansion for the fully dressed propagator. First, ∞-volume

$C_\infty(P) =$ 

self-energy $i\Pi(P^2)$ (1PI)

Can show,

$$C_\infty(P) = \frac{i}{P^2 - m^2 + \Pi(P^2)}$$

The physical mass is given by

$$C_\infty(p^2) = \frac{i}{p^2 - m_{phys}^2 + i\epsilon} + i\,S(p^2)$$

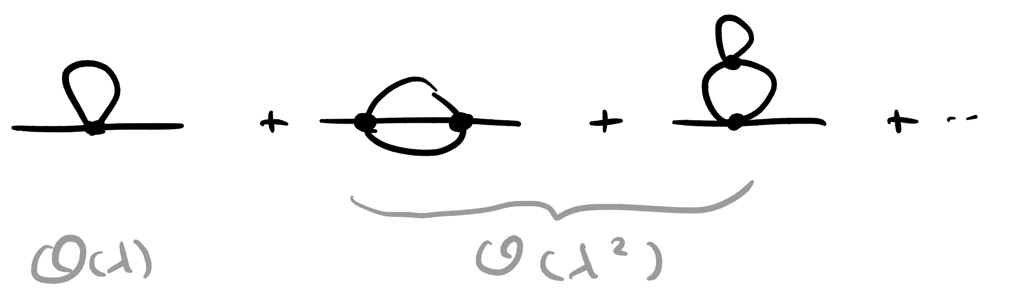
↑ regular about $p^2 = m^2$

with

$$\boxed{m_{phys}^2 - m^2 + \Pi(m_{phys}^2) = 0}$$

The self energy is of the form,

$i\Pi(p^2) =$



At $\mathcal{O}(\lambda)$,

$$i\Pi(p^2) = -i\lambda \int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2 - m^2 + i\epsilon} + \mathcal{O}(\lambda^2)$$

↳ divergent, needs some regulator

example: Pauli-Villars, ... then renormalize, blah blah ...

$$\frac{1}{k^2 - m^2 + i\epsilon} \longrightarrow \frac{1}{k^2 - m^2 + i\epsilon} + \sum_j \frac{a_j}{k^2 - \Lambda_j^2 + i\epsilon}$$

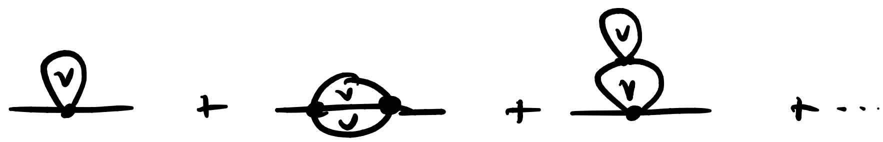
w/ a_j to be determined & $\Lambda_j \to \infty$ at end

↳ to keep degree of divergence low

Repeating the same exercise in the FV, we find

$$C_L(P) = \frac{i}{P^2 - m^2 + \Pi_L(P^2)}$$

with $i\Pi_L(P^2) =$



$\uparrow$ FV loops

$$= -i\lambda \frac{1}{L^3} \sum_{\vec{k}} \int_{-\infty}^{\infty} \frac{dk^0}{2\pi} \frac{i}{k^2 - m^2 + i\epsilon} + \mathcal{O}(\lambda^2)$$

The FV pole position is $P^2 = m_L^2$ (NOT necessarily m_{phys}^2!)

$$\boxed{m_L^2 - m^2 + \Pi_L(m_L^2) = 0} \qquad \boxed{m_L = E^*_{n=0}(L)}$$

Now, take $m_L^2 - m_{phys}^2$,

$$\delta m_L^2 = m_L^2 - m_{phys}^2 = -\left[\Pi_L(m_L^2) - \Pi(m_{phys}^2)\right]$$

Let us assume $\frac{\delta m_L^2}{m_L} \ll 1 \Rightarrow \Pi_L(m_L^2) \simeq \Pi_L(m_{phys}^2)$

So,

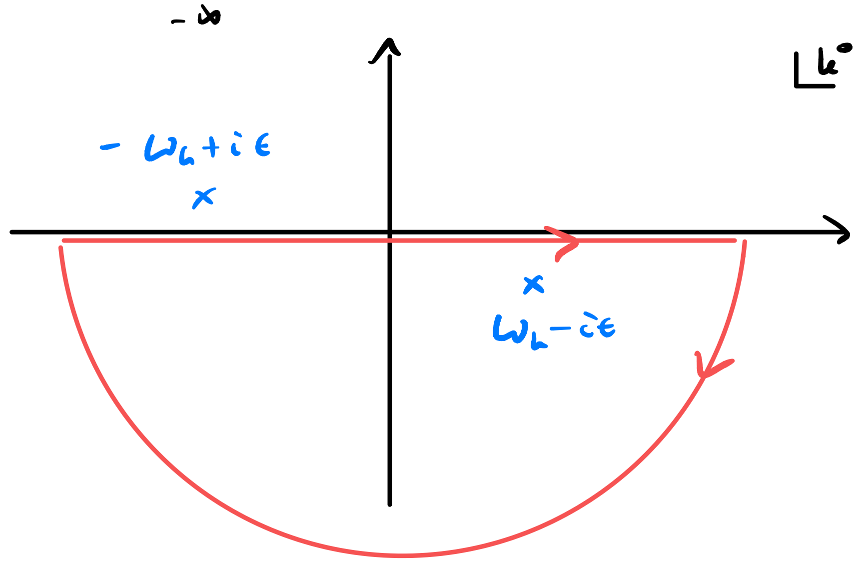
$$\delta m_L^2 = -\left[\Pi_L(m_{phys}^2) - \Pi(m_{phys}^2)\right]$$

$$= +i\lambda\left[\frac{1}{L^3}\sum_{\vec k} - \int\frac{d^3\vec k}{(2\pi)^3}\right]\int_{-\infty}^{\infty}\frac{dk^0}{2\pi}\,\frac{i}{k^2-m^2+i\epsilon}$$

going to implicitly assume regularization & renormalization program

Let's first do temporal integral

$$\int_{-\infty}^{\infty}\frac{dk^0}{2\pi}\,\frac{i}{k^2-m^2+i\epsilon} = \int_{-\infty}^{\infty}\frac{dk^0}{2\pi}\,\frac{i}{(k^0-\omega_k+i\epsilon)(k^0+\omega_k-i\epsilon)} = \frac{1}{2\omega_k}$$



$$\omega_k = \sqrt{m^2+\vec k^2}$$

$$\Rightarrow \quad \delta m_L^2 = i\lambda\left[\frac{1}{L^3}\sum_{\vec k} - \int\frac{d^3\vec k}{(2\pi)^3}\right]\frac{1}{2\sqrt{m^2+\vec k^2}}$$

smooth function in integration region!

Can show, via PSF, that

$$\delta m_L^2 = \frac{\lambda}{2(2\pi m L)^{3/2}}\,e^{-mL} + \mathcal{O}(e^{-\sqrt{2}mL})$$

So, we find that

$$\boxed{m_L^2 = m_{phys}^2 + \mathcal{O}(e^{-m_{phys} L})}$$

In QCD, the lightest mass scale is the pion, m_π

So, the FV correction to a hadron mass m_h is

$$\boxed{E^*_{n=0}(L) = m_h + \mathcal{O}(e^{-m_\pi L})}$$

In practical calculations, want to keep L sufficiently large to suppress these effects, e.g., $m_\pi L \sim 4$ gives $\sim 1\%$ correction, which we hope to ignore.

The energy of the lowest state in a generic moving frame is simply

$$E_0(\vec{P}, L) = \sqrt{m_h^2 + \vec{P}^2} + \mathcal{O}(e^{-m_\pi L})$$

$$= \sqrt{m_h^2 + \left(\frac{2\pi \vec{n}}{L}\right)^2} + \mathcal{O}(e^{-m_\pi L})$$

Two Particle Systems

In Describing excited states, we must address that most hadrons are resonances of scattering processes. Thus, to rigorously describe excited states, we must access the scattering amplitude with LQCD.

Let us first consider non-interacting two particles

Non-Interacting Two-Particle Spectrum

Let's again consider real scalar φ^4 theory. We construct a local operator as

$$\mathcal{O}(x) = \xi \int_L d^4y \int_L d^4z \, A(y,z) \, \varphi(x+y) \, \varphi(x+z)$$

symmetry factor, $\xi = \frac{1}{2!}$

some local function associated w/ wave function of 2-particle state created by $\mathcal{O}(x)$

So,

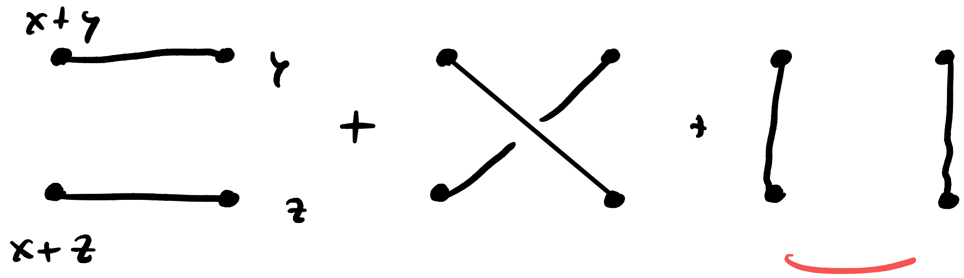
$$C_L(P) = \int_L d^4x \, e^{iP\cdot x} \langle T \, \mathcal{O}(x) \mathcal{O}^\dagger(0) \rangle$$

$$= \xi^2 \int_L d^4x \, e^{iP\cdot x} \int_L d^4y' \int_L d^4z' \int_L d^4y \int_L d^4z \, A(y',z') A(y,z)$$

$$\times \langle T \, \varphi(x+y') \varphi(x+z) \varphi(y) \varphi(z) \rangle$$

Diagrammatically,

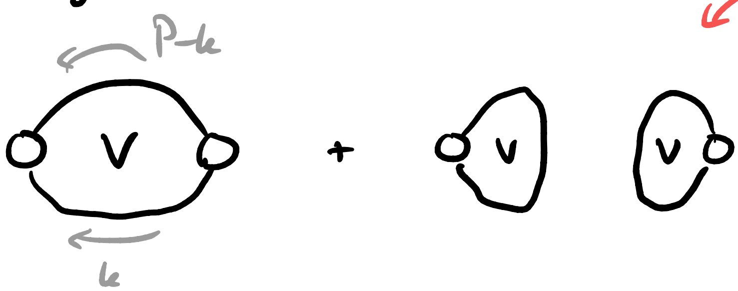
$$\langle T\,\varphi(x+y')\,\varphi(x+z)\,\varphi(y)\,\varphi(z)\rangle$$

$=$ 

So, we write "generalized Feynman rules"

Disconnected

Does not contribute (Drop)

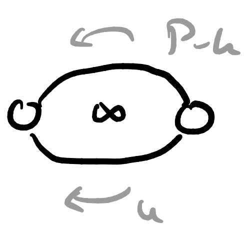
$C_L(P) =$ 

$$= i\,\frac{1}{L^3}\sum_{\vec{k}}\int_{-\infty}^{\infty}\frac{dk^0}{2\pi}\,A(k,P)\,\frac{i}{k^2-m^2+i\epsilon}\,\frac{i}{(P-k)^2-m^2+i\epsilon}\,A^*(k,P)$$

with

$$A(k,P) = \int_L d^4y\int_L d^4z\; e^{ik\cdot y}\,e^{i(P-k)\cdot z}\,A(y,z)$$

The corresponding IV correlator is

$C_\infty(P) =$ 

$$= i\int\frac{d^4k}{(2\pi)^4}\,A(k,P)\,\frac{i}{k^2-m^2+i\epsilon}\,\frac{i}{(P-k)^2-m^2+i\epsilon}\,A^*(k,P)$$

Let's examine the spectrum via FV correction

$$\delta C_L(P) = C_L(P) - C_\infty(P)$$

$$= i\left[\frac{1}{L^3}\sum_{\vec{k}} - \int\frac{d^3\vec{k}}{(2\pi)^4}\right]\int_{-\infty}^{\infty}\frac{dk^0}{2\pi}\, A(k,P)\,\frac{i}{k^2-m^2+i\epsilon}\,\frac{i}{(P-k)^2-m^2+i\epsilon}\,A^*(k,P)$$

We will again assume some UV regulator & assume $A(k,P)$ is sufficiently smooth in k, i.e., non-singular.

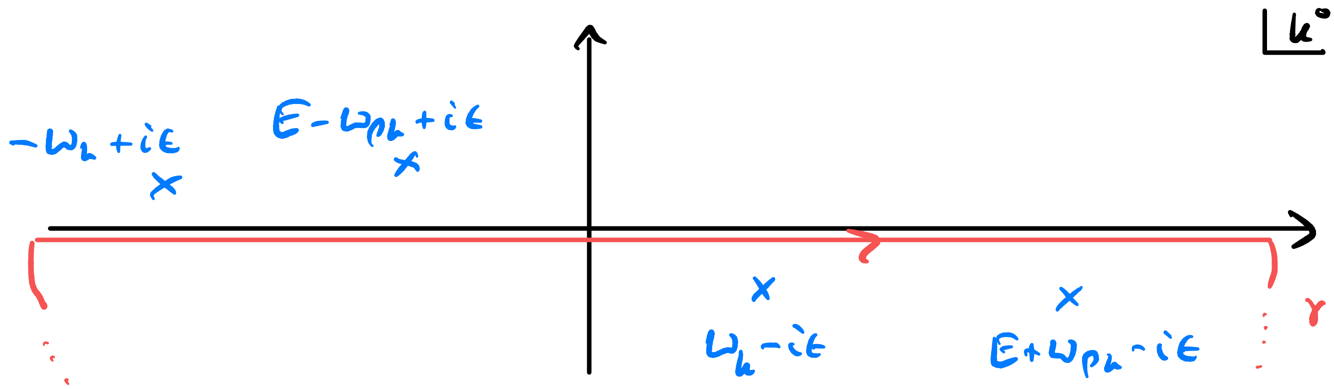
Let's perform k^0 integral. Poles at

$$(k^2-m^2+i\epsilon)((P-k)^2-m^2+i\epsilon) = 0$$

$$\Rightarrow (k^0-\omega_k+i\epsilon)(k^0+\omega_k-i\epsilon)(E-k^0-\omega_{P_k}+i\epsilon)(E-k^0+\omega_{P_k}-i\epsilon)$$

w/ $\omega_k = \sqrt{m^2+\vec{k}^2}$

$\omega_{P_k} = \sqrt{m^2+|\vec{P}-\vec{k}|^2}$



Assuming integrand is well-behaved at $k \to \infty$,
we have

$$\int_{-\infty}^{\infty} dk^0 \, f(k^0) = \oint_{\gamma} dk^0 \, f(k^0) = \sum_n{}' \, \mathrm{Res}\left[f(k^0) ; \, k^0 = k^0_n \right]$$

We pick up two poles, finding

$$\delta C_L(P) = \xi \left[\frac{1}{L^3} \sum_{\vec{k}}{}' - \int \frac{d^3\vec{k}}{(2\pi)^3} \right] A(\omega_k, \vec{k}, P) \frac{i}{2\omega_k \left((E-\omega_k)^2 - \omega_{Pk}^2 + i\epsilon \right)} A^*(\omega_k, \vec{k}, P)$$

$$+ \text{ term w/ } k^0 = E + \omega_{Pk} - i\epsilon$$

For physical energies, $P^2 > 0$, $E^* > 2m$
we find (exercise) that the second term does not
have any singularities in physical E^* region

$\Rightarrow$ FV correction is of $\mathcal{O}(e^{-mL})$

Further,

$$\frac{1}{(E-\omega_k)^2 - \omega_{Pk}^2 + i\epsilon} = \frac{1}{2\omega_{Pk}(E - \omega_k - \omega_{Pk} + i\epsilon)}$$

singular in E^*

$$+ \frac{1}{2\omega_{Pk}(E - \omega_k + \omega_{Pk} - i\epsilon)}$$

non-singular in E^*

So, we have

$$\delta C_L(P) = i \left[\frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^3\vec{k}}{(2\pi)^3} \right] \frac{\mathcal{A}(\omega_k, \vec{k}, P) \; i \; \mathcal{A}^*(\omega_k, \vec{k}, P)}{2\omega_k 2\omega_{Pk} (E - \omega_k - \omega_{Pk} + i\epsilon)}$$

$$+ \mathcal{O}(e^{-mL})$$

Now, introduce partial waves for $\mathcal{A}(\omega_k, \vec{k}, P)$. How?
So far, fixed 1 & 2 particles on mass-shell. Fixing the second gives (in pair CM frame)

$$\vec{k}^* = q^* \hat{k}^*$$

where $q^* = \frac{1}{2} \sqrt{E^{*2} - 4m^2}$, $E^* = \sqrt{P^2}$

this point is equivalent to where $E = \omega_k + \omega_{Pk}$
So, expand about this point

$$\mathcal{A}(\vec{k}^*, P) = \mathcal{A}(q^* \hat{k}^*, P) + \left[\mathcal{A}(\vec{k}^*, P) - \mathcal{A}(q^* \hat{k}^*, P) \right]$$

$$= \mathcal{A}(q^* \hat{k}^*, P) + (k^{*2} - q^{*2}) \frac{\partial}{\partial k^{*2}} \mathcal{A}(k^*, P) \Big|_{k^{*2} = q^{*2}}$$

$$+ \mathcal{O}((k^{*2} - q^{*2})^2)$$

$$\equiv \mathcal{A}(q^* \hat{k}^*, P) + \delta \mathcal{A}(k^*, P)$$

Terms w/ one or more $\delta\mathcal{A}(k^*, P)$ are suppressed as e^{-mL} like before since there is no singularity

$$\Rightarrow \delta C_L(P) = \xi \left[\frac{1}{L^3}\sum_{\vec{k}} - \int \frac{d^3 k}{(2\pi)^3} \right] \frac{\mathcal{A}(q^* \hat{k}^*, P)\, i\, \mathcal{A}^*(q^* \hat{k}^*, P)}{2\omega_k 2\omega_{pk}(E - \omega_k - \omega_{pk} + i\epsilon)}$$

$$+ \mathcal{O}(e^{-mL})$$

Can now PW expand

$$\mathcal{A}(q^* \hat{k}^*, P) = \sqrt{4\pi} \sum_{\ell, m_\ell} \mathcal{A}_{\ell m_\ell}(P)\, Y^*_{\ell m_\ell}(\hat{k}^*) \left(\frac{k^*}{q^*}\right)^\ell$$

Barrier factors to regulate artificial singularity of $Y_{\ell m}$ induced by expansion

So,

$$\boxed{\delta C_L(P) \equiv \sum_{\ell', m_{\ell'}} \sum_{\ell, m_\ell} \mathcal{A}_{\ell' m_{\ell'}}(P)\, i F_{\ell' m_{\ell'}, \ell m_\ell}(P, L)\, \mathcal{A}_{\ell m_\ell}(P) \quad + \mathcal{O}(e^{-mL})}$$

where F is purely geometric & kinematic

$$\boxed{F_{\ell' m_{\ell'}, \ell m_\ell}(P, L) \equiv \xi \left[\frac{1}{L^3}\sum_{\vec{k}} - \int \frac{d^3 k}{(2\pi)^3} \right] \left(\frac{k^*}{q^*}\right)^{\ell'} \frac{Y^*_{\ell' m_{\ell'}}(\hat{k}^*)\, Y_{\ell m_\ell}(\hat{k}^*)}{2\omega_k 2\omega_{pk}(E - \omega_k - \omega_{pk} + i\epsilon)} \left(\frac{k^*}{q^*}\right)^\ell}$$

The summand/Integrand has a pole that is physically associated with on-shell 2-particle states. We cannot use PSF as before, so the FV correction scales like $1/L^3$.

The FV function $F(P,L)$ characterizes the distortions induced by the periodic volume. It contains information on both the FV energies & IV continuum. To see this, first consider the imaginary part of $F(P,L)$, this comes only from the integral term,

$$\mathrm{Im}\, F_{\ell' m_\ell', \ell m_\ell}(P,L) = \xi \int \frac{d\vec{k}}{(2\pi)^3} \frac{Y^*_{\ell' m_\ell'}(\hat{k}^*)\, Y_{\ell m_\ell}(\hat{k}^*)}{2\omega_{pk}\, 2\omega_k} \delta(E-\omega_k-\omega_{pk})$$

Going to CM Frame, we find

$$\mathrm{Im}\, F_{\ell' m_\ell', \ell m_\ell}(P,L) = \frac{\xi q^*}{8\pi E^*} \delta_{\ell'\ell}\, \delta_{m_\ell' m_\ell}$$

$$= \rho\, \delta_{\ell'\ell}\, \delta_{m_\ell' m_\ell}$$ two-body phase-space

The real part contains information about the FV poles, which exist if $C_L^{-1}(P) = \delta C_L^{-1}(P) = 0$

$$\Rightarrow \boxed{\det\left[F^{-1}(P,L)\right] = 0}$$

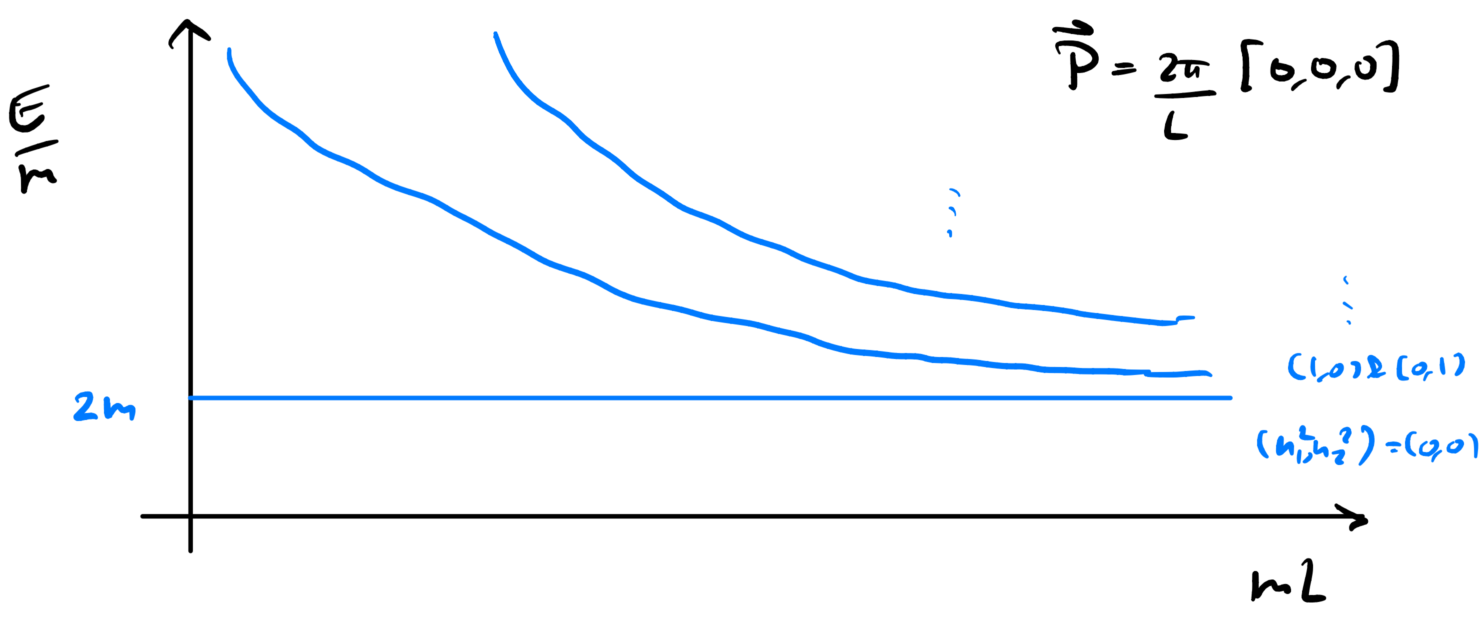
matrix in (ℓ, m_ℓ)-space

The solution of this gives

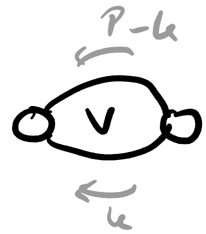
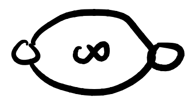
$$\boxed{\begin{aligned} E &= \omega_k + \omega_{Pk} \\ &= \sqrt{m^2 + \vec{k}^2} + \sqrt{m^2 + (\vec{P} - \vec{k})^2} \\ &= \sqrt{m^2 + \frac{4\pi^2}{L^2}\vec{n}_1^2} + \sqrt{m^2 + \frac{4\pi^2}{L^2}\vec{n}_2^2} \end{aligned}}$$

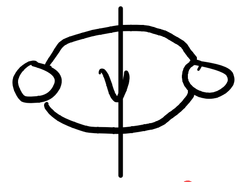
where $\vec{n}_1, \vec{n}_2 \in \mathbb{Z}^3$

This is exactly the FV spectrum of 2 free particles



Diagrammatically, we denote δC_L as

$\delta C_L(P) =$  $-$  $\leftarrow P$

$\equiv$ 

↖ FV "cut"

$\Rightarrow$ intermediate states on-shell

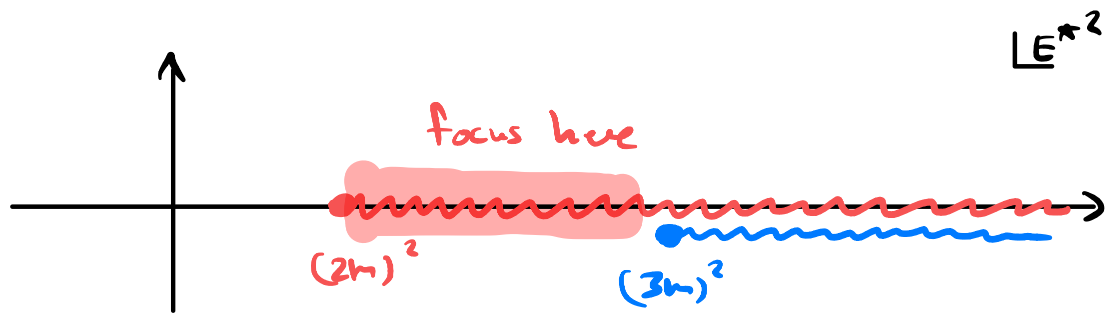
$$= A^*(P) \cdot iF(P,L) \cdot A^*(P)$$

↑

Matrices in (ℓ, m_ℓ)-space

Interacting Two-Particles

Let us now turn on interactions, focusing on φ^4 theory. Then we want to use our tools to determine scattering amplitudes. Let us focus on the elastic $2\to2$ scattering amplitude $i\mathcal{M}$, & restrict our energy range of interest to the elastic region. In doing so, we systematically have full control over the analytic structure without approximation



From S-matrix unitarity, we know that

$$\mathcal{M}_{\ell' m_{\ell'}, \ell m_\ell}(E^*) = \delta_{\ell'\ell}\,\delta_{m_{\ell'} m_\ell}\,\mathcal{M}_\ell(E^*)$$

rotational invariance

and

$$\boxed{\mathcal{M}_\ell = \mathcal{K}_\ell \frac{1}{1 - ip\mathcal{K}_\ell}}$$

$2\to2$ $\mathcal{K}$-matrix

The K-matrix contains all short-distance interactions not constrained by unitarity. Can relate to phase shifts via

$$\mathcal{K}_\ell^{-1} = \rho \cot \delta_\ell$$

So, also know $\quad \mathcal{M}_\ell = \frac{1}{\rho} \frac{1}{\cot\delta_\ell - i} = \frac{1}{\rho} e^{i\delta_\ell} \sin\delta_\ell$

Here I use typical relativistic normalization,

$$\langle \vec{p}\,' | \vec{p} \rangle = (2\pi)^3 \, 2\omega_p \, \delta^{(3)}(\vec{p}\,' - \vec{p})$$

So that $\quad \rho = \frac{\xi q^*}{8\pi E^*}$

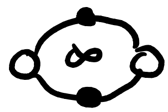
For a weakly interacting system near threshold, Effective range parametrization is useful. Consider S-wave scattering

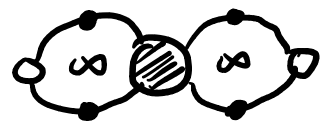
$$q^* \cot \delta_{\ell=0} = -\frac{1}{a_0} + \mathcal{O}(q^{*2})$$

near threshold, Find

$$\mathcal{M}_{\ell=0} = -\frac{16\pi}{\xi} m a_0 + \mathcal{O}(q^*)$$

Within QFT, the amplitude is given by applying LSZ to correlators. To all orders, we can write the correlator as

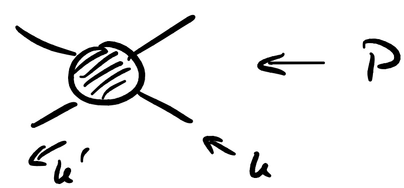
$C_\infty(P) =$ 

$+$ 

fully dressed propagator

off-shell $2\to2$ amplitude

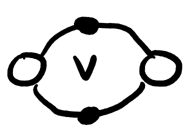
The amplitude is $i\mathcal{M} = \lim_{\text{on-shell}} i\mathcal{M}(k',k;P)$

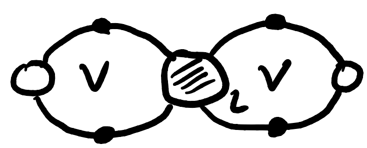
$= \lim_{\text{on-shell}}$ 

The fully dressed propagator is defined w/ unit residue, $i\Delta(k) = \dfrac{i}{k^2-m^2+i\epsilon} + iS(k^2)$

non-singular @ $k^2=m^2$

The analogous FV correlator is

$C_L(P) =$ 

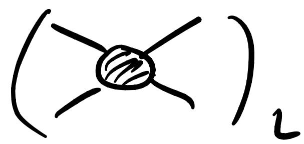
$+$ 

here, recall that $m_L - m_\infty = \mathcal{O}(e^{-mL})$

$\Rightarrow$ ()$_L$ = ()$_\infty$ $+ \mathcal{O}(e^{-mL})$

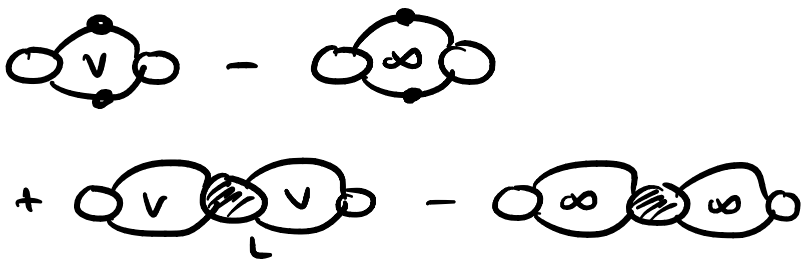
drop

We have introduced $i\mathcal{M}_L$ as the FV analogue of the off-shell amplitude.

$$i\mathcal{M}_L =$$ 

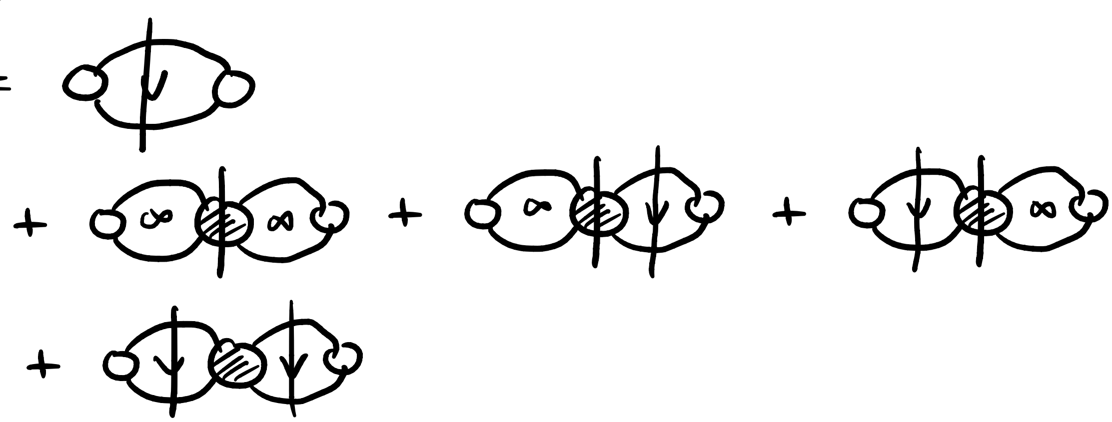
Let's examine the structure of the FV correction,

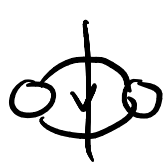
$$\delta C_L(P) = C_L(P) - C_\infty(P)$$

$=$ 

$=$ add & subtract useful zeroes

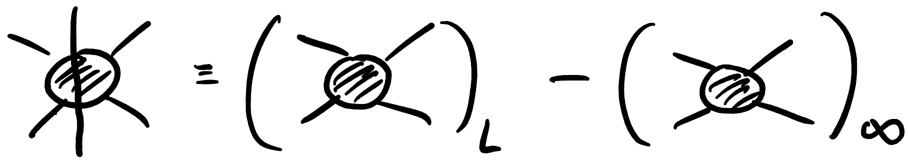
$\vdots$

$=$ 

here,  $= A(P) \cdot iF(P,L) \cdot A^*(P,L)$ as before,

this only has non-interacting poles

We have introduced the FV correction to the "amplitude",



$$\Rightarrow \quad i\delta\mathcal{M}_L \equiv i\mathcal{M}_L - i\mathcal{M}$$

Clearly, this is key to getting relationship between FV & IV objects.

Let's first look at weak coupling expansion,

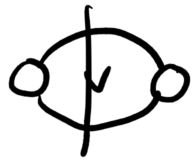
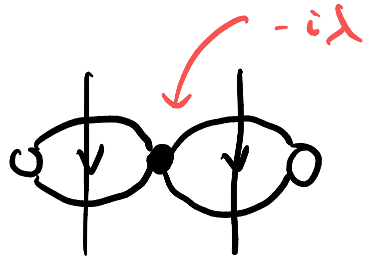
$$i\mathcal{M} = -i\lambda + \mathcal{O}(\lambda^2)$$

but, $i\mathcal{M}_L = -i\lambda + \mathcal{O}(\lambda^2)$ too, so

$$\delta\mathcal{M}_L = 0 + \mathcal{O}(\lambda^2)$$

$\Rightarrow$ This gives no info on interacting energies.
To see this, consider poles of δC_L

So, δC_L goes like

$\delta C_L(P) =$  $+$ 

$+ \mathcal{O}(\lambda^2)$

$$= A(P) \cdot iF(P,L) \cdot A^*(P)$$

$$+ A(P) \cdot iF(P,L) \cdot [-i\lambda] \cdot iF(P,L) \cdot A^*(P) + \mathcal{O}(\lambda^2)$$

where,

$$\mathcal{M}_{l'm_l', l m_l} = \delta_{l'l}\, \delta_{m_l' m_l}\, \frac{1}{2}\int_{-1}^{1} d\cos\theta \; P_l(\cos\theta) \left[-i\lambda + \mathcal{O}(\lambda^2)\right]$$

$$= -i\lambda\, \delta_{l0}\, \delta_{m_l 0} + \mathcal{O}(\lambda^2)$$

So, infinite-dimensional matrix is truncated at S-wave,

$$\delta C_L(P) \simeq A(P)\, iF_s(P,L) \left[1 + \lambda F_s(P,L) \right] A^*(P) + \mathcal{O}(\lambda^2)$$

with

$$F_s(P,L) \equiv F_{0000}(P,L) = \xi \left[\frac{1}{L^3} - \int \frac{d^3k}{(2\pi)^3} \right] \frac{1}{2\omega_k 2\omega_{Pk} (E - \omega_k - \omega_{Pk} + i\epsilon)}$$

Poles in C_L are same as poles in δC_L.

Recall that $F(P,L)$ gave free states

But, we run into an issue. Consider systems at rest, $\vec{P} = \vec{0}$

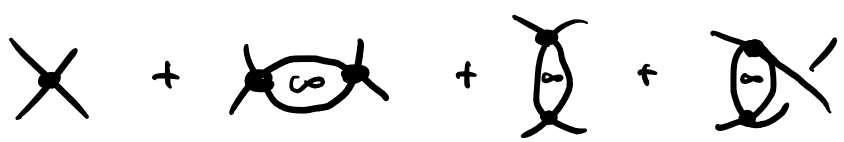
Poles in δC_L are at $$\frac{1}{1+\lambda F(E,L)} = 0$$

$$\Rightarrow \left[1 + \lambda \xi \frac{1}{L^3} \frac{1}{4m^2(E-2m)} + \sum_{\vec{k}\neq\vec{0}} \text{terms}\right]^{-1} = 0$$

This, again, only has poles at free energies!
A truncated expansion does not yield information on interacting energies, due to the fact that $E-2m = \mathcal{O}(\lambda)$, & we have neglected terms in the expansion.

Let us consider amplitude at $\mathcal{O}(\lambda^2)$,

$$i\mathcal{M} = -i\lambda + (-i\lambda)^2 \xi \int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2-m^2+i\epsilon} \frac{i}{(P-k)^2-m^2+i\epsilon} + (t,u) + \mathcal{O}(\lambda^3)$$

$=$  $+ \mathcal{O}(\lambda^3)$

FV "amplitude"

$$i\mathcal{M}_L = -i\lambda - \lambda^2 \xi \frac{1}{L^3} \sum_{\vec{k}} \int \frac{dk^0}{2\pi} \frac{i}{k^2-m^2+i\epsilon} \frac{i}{(P-k)^2-m^2+i\epsilon} + (t,u) + \mathcal{O}(\lambda^3)$$

Examine $\delta \mathcal{M}_L$,

$$\delta \mathcal{M}_L = -\lambda^2 \, i \left[\frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^3 \vec{k}}{(2\pi)^3} \right] \int_{-\infty}^{\infty} \frac{dk^0}{2\pi} \frac{i}{k^2 - m^2 + i\epsilon} \frac{i}{(P-k)^2 - m^2 + i\epsilon}$$

$$+ (t, u) + \mathcal{O}(\lambda^3)$$

The t- & u-channel terms have no singularities for $2m \leq E^* < 3m$. Conclude

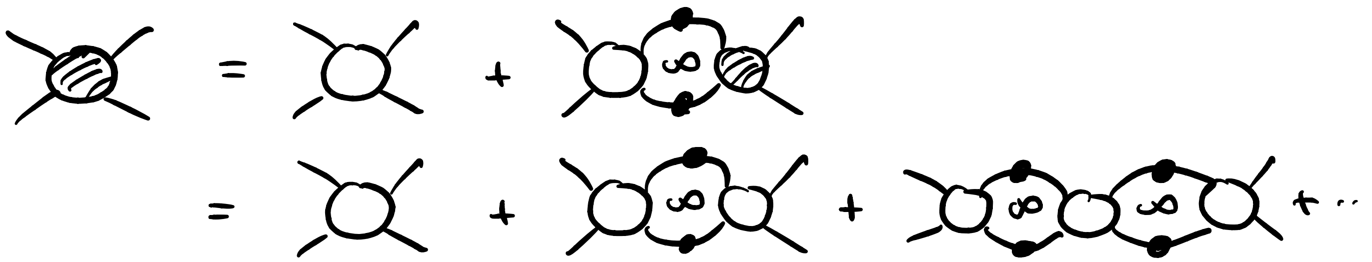
$$\delta \mathcal{M}_L \Big|_{t,u} \sim \mathcal{O}(e^{-mL})$$

Further, the s-channel term is exactly like what we considered for the F-function,

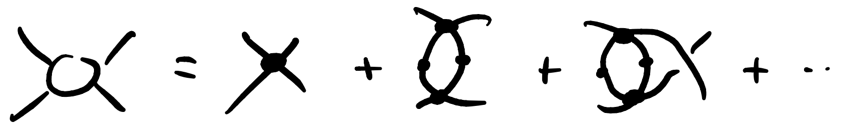
$$\Rightarrow \quad \delta \mathcal{M}_L = -\lambda^2 \, i F_s(P, L) + \mathcal{O}(e^{-mL}, \lambda^3)$$

As we have seen, it is enough to look at poles of $\delta \mathcal{M}_L$. But, again, find only non-interacting poles. What is going on? Pole structures emerge only when summing the infinite series of interactions.

Consider the Dyson-Schwinger eq. for $i\mathcal{M}$,



2PI Bethe-Salpeter kernel



This is an integral eqn. for $i\mathcal{M}$,

$$i\mathcal{M}(p',p) = iB(p',p) + \int \frac{d^4k}{(2\pi)^4}\, iB(p',k)\, i\Delta(k)\, i\Delta(P-k)\, i\mathcal{M}(k,p)$$

Similar expressions exists for $i\mathcal{M}_L$.

Suppose we truncate $iB = -i\lambda + \mathcal{O}(\lambda^2)$,

but sum the infinite s-channel series. We find for $\delta\mathcal{M}_L$,

$$\delta\mathcal{M}_L = -i\lambda \sum_{n=0}^{\infty} \left[F_s(P,L)\, \lambda \right]^n$$

$$= -i\lambda \frac{1}{1 - \lambda F_s(P,L)}$$

Now, poles of $\delta\mathcal{M}_L$ are at

$$1 - \lambda F_s(P, L) = 0$$

Let $\vec{P} = \vec{0}$, & consider near threshold state,

$$1 - \lambda \xi \frac{1}{4m^2} \frac{1}{L^3} \frac{1}{(E_0 - 2m)} + (\vec{l} \neq \vec{0}) = 0$$

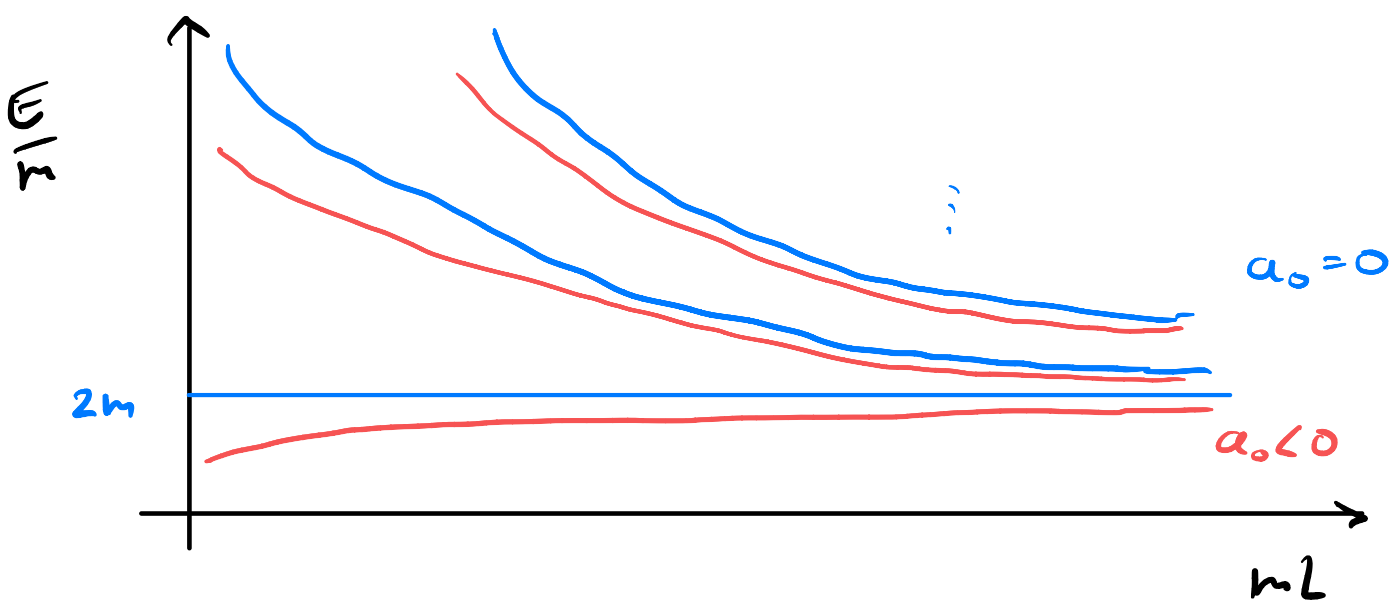
$$\Rightarrow \quad E_0 - 2m = \frac{\lambda \xi}{4m^2 L^3} + \mathcal{O}(\lambda^2)$$

But, $\mathcal{M} = -\lambda = -\frac{16\pi m a_0}{\xi}$ at threshold

So,

$$\boxed{E_0 - 2m = \frac{4\pi a_0}{m L^3} + \mathcal{O}(a_0^2)}$$

The presence of interactions shifts the energy levels!



We can expand this argument to all orders in λ, & arrive at a non-perturbative relation between the scattering amplitude & FV spectrum.
The result is

$$\boxed{\begin{aligned} \delta\mathcal{M}_L &= i\mathcal{M}(P)\cdot\sum_{n=0}^{\infty}\left[iF(P,L)\cdot i\mathcal{M}(P)\right]^n \\ &= i\mathcal{M}(P)\cdot\frac{1}{1+F(P,L)\cdot\mathcal{M}(P)} \end{aligned}}$$

matrix in (ℓ, m_ℓ) space

So, poles exists when

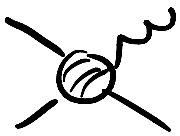
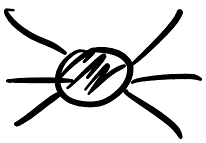
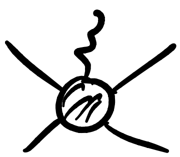
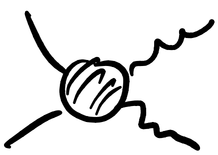
$$\boxed{\det\left[1+F(P,L)\cdot\mathcal{M}(P)\right]=0}$$

in (ℓ, m_ℓ)-space

This is the Lüscher quantization condition. It links the IV scattering amplitude & FV spectrum. It has been used to access scattering amplitudes & resonance physics from LQCD.

Outlook

We have only just touched on the basics of accessing amplitudes via LQCD. Current state of the art includes:

-  radiative transitions
-  $3 \to 3$ processes
-  resonance form-factors
-  Two-photon transitions