Lecture III: QCD in a finite volume

To be covered in today's lecture:

- ☐ 2→2 elastic scattering and Luescher's formula

  original papers: Luescher 1986, 1991

  - o Introduction and qualitative picture
  - o A derivation based on field theory

    arXiv:0507006   arXiv: 1409.1966
  - o Extension to multi-channel 2→2 scattering arXiv: 1204.1110
    arXiv: 1409.1966
  - o Bound states in a finite volume

    arXiv: 1108.5371   arXiv: 1107.1272
    arXiv: 1309.3556
  - o Other extensions and applications

    See arXiv: 1409.1966, arXiv: 1812.11899 and arXiv: 1706.06223 for reviews.

$2 \to 2$ elastic scattering and Luescher's formalism

Introduction and qualitative picture

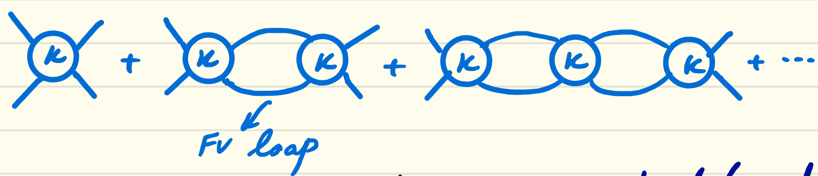
Now we can open up the discussion of an even more powerful method that allows accessing observables beyond those in the single-hadron sector. Since Lattice QCD calculations are performed in an Euclidean spacetime, one needs to analytically continue to the Minkowski to map to physical observables. In principle, such a continuation of an Euclidean theory to the Minkowski theory is gauranteed to produce the right theory if one has a property called reflection positivity, see Osterwalder, Schrader. However, Lattice-QCD correlation functions are evaluated at a discrete set of points and such a functional analytic continuation is not possible. For single-hadron energies, one already has access to these quantities in Euclidean correlation function as these are insensitive to the time signature of spacetime. For multi-hadron observables the situation is different since in order to define observables, namely S-matrix elements in this sectors one must define asymptotic states, such that at distant past and future, the corresponding wavepackets are non-overlaping and interactions occur at an intermediate time. So clearly such observables are sensitive to the time signature. There is in fact a no-go theorem, stated and proved by Maiani-Testa, that the elastic scattering amplitude of two hadrons can not be accessed from Euclidean correlation functions unless at kinematic thresholds. So what saves us here? It turned out that this statement is only true in infinite volume. Martin Luescher (and previously in a quantum mechanical setting Huang and Yang, 1957) showed that the FV spectrum of two hadrons can lead us to constructing the infinite-volume $2 \to 2$ elastic scattering amplitude in that channel. This is a strong statement and it arises from the fact that the same interactions that lead to scattering in an infinite volume, lead also to a shift in the energy of two hadrons in a FV compared with non-interacting hadrons in a volume. In this lecture, we discuss under what conditions such a relation can be found, provide a derivation, and mention a few extensions and applications of the method. In the end, I will comment on prospect of this program and ongoing directions in reseach in this area.

○ A derivation based on field theory

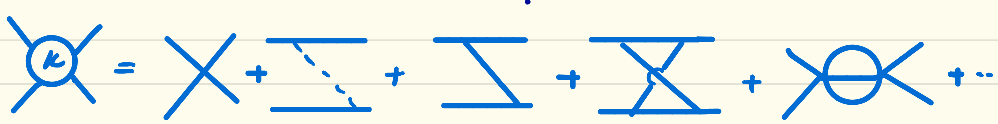
Once again, we consider a generic Low-energy effective theory in which hadrons are the degrees of freedom, but beside this, we make no other assumptions or truncation in the EFT expansion. Our goal is to identify the FV corrections to the energy of two hadrons that go as powers of $1/L$.

The two-hadron system is assumed to have a total energy that is not sufficient to produce a third on-shell hadron. We again consider a cubic volume with PBCs, but the same strategy can be applied to derive similar relations for other FV geometries or BCs, see e.g., Refs. arXiv:0311035, arXiv:1311.7686.

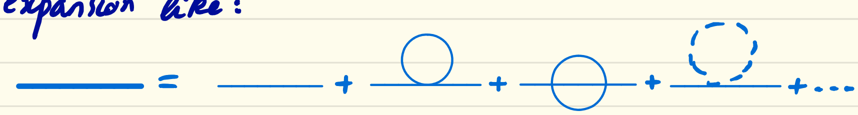
Let us now define a FV "amplitude" in this hadronic theory with one caveat. The notion of amplitude in a FV theory doesn't make sense since there is no asymptotic states, however what we are interested here are the FV energies which are the poles of FV correlation function, and these poles are the same in the amplitude that we are about to construct here. Now consider:

$-i\mathcal{M}^V =$ 

where K is a $2 \to 2$ Bethe-Salpeter kernel defined as:



Baiscally, this include every $2 \to 2$ irreducible diagram allowed in the theory except for those that include "s-channel" loops, those that look like , since we have already accounted for these loops explicitly in the expansion of $\mathcal{M}^V$ above. The reason for this distinction becomes clear shortly. The other ingredient of these diagrams is the fully dressed propagator, which in a given theory may have an expansion like:



where the thin lines are the bare propagator of the hadron and dassed lines are other hadrons that can possibly interact with the hadron of interest. With these building blocks, let us first make the following comments:

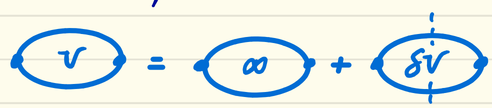
i) Below three-particle inelastic thresholds, the $2\to 2$ kernel κ is close to its infinite-volume counterpart up to exponential corrections in mL where m is the mass of the lightest hadron relevant to the given process. This is because off-shell states can not reach the boundaries of volume and give rize to large volume effects. So we have:

$$\kappa^L = \kappa^\infty + O(e^{-mL})$$

ii) The fully dressed propagator inside the s-channel loops can be replaced with their infinite-volume counterpart too using the same argument as before. Note that the s-channel loops already involve two hadrons which can propagate to the boundaries. So here:

$$D^L = D^\infty + O(e^{-mL})$$

iii) So now it is obvious that in this arrangement of the contributions to the amplitude, the only large (power-law) FV corrections arise from the s-channel loops, since there are only two particles propagating, and both can be put on-shell given the kinematic. In general, if you have a sum in which the summand is a nonsingular function of the variable that is being summed over, the sum can be approximated with a corresponding integral up to exponential corrections. So now for the s-channel loops, one has:

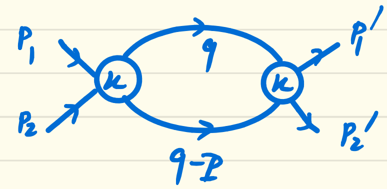


where δV denoted purely FV function contributing to the loop. It arises from the condition that both the particles running in the loop go on-shell, and hence the function itself is evaluated on-shell. These functions will be the subject of the rest of the discussions.

Explicitly, a generic s-channel loop, including generic momentum-dependent kernels K on left and right, can be written as:

$$iG^V(\vec{p},\vec{p}\,') \equiv \frac{\xi}{L^3}\sum_{\vec{q}\in\frac{2\pi n}{L}}\int\frac{dq^0}{(2\pi)}\frac{K(\vec{p},\vec{q})\,K(\vec{q},\vec{p}\,')}{[(q-P)^2-m_1^2+i\epsilon][q^2-m_2^2+i\epsilon]}$$

where: $P = \underbrace{P_1+P_2}_{\text{initial momenta}} = \underbrace{P_1'+P_2'}_{\text{Final momenta}}$



In an elastic scattering: $P_1^0+P_2^0 = P_1^{0\prime}+P_2^{0\prime}$,

hence: $|\vec{P}| = |\vec{P}\,'|$ where $\vec{p}$ and $\vec{p}\,'$ are the initial and final relative momenta in the system. Note also that we have assumed different masses for the two hadrons in the loop, for example this could correspond to πK scattering. ξ is a symmetry factor and is equal to $1/2$ if the two hadrons are identical and is 1 otherwise. Note that these relations are in the lab frame. In the CM frame the energy E^* is related to the total energy and momentum in the lab frame through: $E^* = \sqrt{E^2 - \vec{P}^2}$, and the relativistic γ factor is: $\gamma = E/E^*$.

Exercise 10: Show that the relative momentum of two on-shell hadrons in the CM frame is:

$$p^* = \frac{1}{2}\left[E^{*2} - 2(m_1^2 + m_2^2) + \frac{(m_1^2 - m_2^2)^2}{E^{*2}}\right]^{1/2}$$

Note that by on-shell condition, we mean when both hadrons inside the s-channel loops are on-shell, or explicitly when:

$$(q-P)^2 = m_1^2, \quad q^2 = m_2^2$$

when this happens, because of the conservation of energy in elastic processes, $|\vec{q}^*|$ value will be equal to $|\vec{p}^*|$ and $|\vec{p}'^*|$. This however doesn't fix the directionality. It is therefore convenient to decompose G^V as well as all functions in partial waves corresponding to the incoming and outgoing momenta in the function. Explicitly, one find that:

$$[\delta G^V]_{\ell m,\ell' m'} = [G^V - G^\infty]_{\ell m,\ell' m'} = -i\mathcal{K}_{\ell m,\ell_1 m_1}\,\delta\mathcal{G}^V_{\ell_1 m_1,\ell_2 m_2}\,\mathcal{K}_{\ell_2 m_2,\ell' m'}$$

where:
$$\delta\mathcal{G}^V_{\ell_1 m_1,\ell_2 m_2} = i\frac{p^*\xi}{8\pi E^*}\Big[\delta_{\ell_1,\ell_2}\delta_{m_1,m_2} + i\frac{4\pi}{p^*}\sum_{\ell,m}\frac{\sqrt{4\pi}}{p^{*\ell}}\times$$
$$c^{\vec{P}}_{\ell m}(p^{*2})\int d\Omega\, Y^*_{\ell_1 m_1} Y^*_{\ell m} Y_{\ell_2 m_2}\Big]$$

Here:
$$c^{\vec{P}}_{\ell m}(p^{*2}) = \frac{1}{\gamma}\Big[\frac{1}{L^3}\sum_{\vec{k}} - \mathcal{P}\int\frac{d^3k}{(2\pi)^3}\Big]\frac{\sqrt{4\pi}\,Y_{\ell m}(\hat{k}^*)\,k^{*\ell}}{k^{*2}-p^{*2}}$$

where $\mathcal{P}$ denotes the principal value of integral. Also:
$$\vec{k}^* = \gamma^{-1}(\vec{k}_{\parallel} - \alpha\vec{P}) + \vec{k}_{\perp}$$

where: $\alpha = \frac{1}{2}\Big[1+\frac{m_1^2-m_2^2}{E^{*2}}\Big]$, and $\vec{k}_{\parallel}$ and $\vec{k}_{\perp}$ are components of $\vec{k}$ that are parallel (prependicular) to vector $\vec{k}$ which is summed over.

Exercise 11: Derive the relation above from $\delta\mathcal{G}^V_{\ell_1 m_1,\ell_2 m_2}$ Starting from the integral form of G^V in the previous page. You can consult Ref. arXiv:0507006, but you must show all the details of the derivation.

BONUS

Now we are ready to find the so-called quantization conditions the relation between the discritized finite-volume energies of two hadrons and the $2\to 2$ elastic scattering amplitude. We start with $-i\mathcal{M}^V$ expansion in terms of G^V and $\mathcal{K}$:

$$i\mathcal{M}^V = (-i\mathcal{K}) + (-i\mathcal{K})\, iG^V\, (-i\mathcal{K}) + \cdots$$

$$= (-i\mathcal{K}) + (-i\mathcal{K})\, (iG^\infty + i\delta G^V)(-i\mathcal{K}) + \cdots$$

$$= \underbrace{(-i\mathcal{K}) + (-i\mathcal{K})\, iG^\infty\, (-i\mathcal{K}) + \cdots}_{i\mathcal{M}^\infty} +$$

$$\underbrace{(-i\mathcal{K} + (-i\mathcal{K})\, iG^\infty\, (-i\mathcal{K}) + \cdots)}_{i\mathcal{M}^\infty}\, i\delta G^V \underbrace{(-i\mathcal{K} + (-i\mathcal{K})\, iG^\infty\, (-i\mathcal{K}) + \cdots)}_{i\mathcal{M}^\infty} +$$

$$(i\mathcal{M}^\infty)\, i\delta G^V\, (i\mathcal{M}^\infty)\, i\delta G^V\, (i\mathcal{M}^\infty) + \cdots$$

$$= \frac{i\mathcal{M}^\infty}{1 + \delta G^V \mathcal{M}^\infty} = \frac{i}{(\mathcal{M}^\infty)^{-1} + \delta G^V}.$$

Note that all these relations must be realized in terms of matrices in the space of relevant partial waves that was just described. We are extremely close to the relation we want. Note that in a finite volume, $\mathcal{M}^V$ diverges at a set of discrete FV energies, E_n^*. Therefrore:

$$\det\left[\mathcal{M}^\infty(E_n^*)^{-1} + \delta G^V(E_n^*)\right] = 0$$

This is the relation between the infinite-volume scattering amplitude $\mathcal{M}^\infty$ and the finite-volume energies, E_n, often called Luescher's formula, although Luescher's formula was derived at the time for spinless equal-mass hadrons at rest.

Exercise 12: Assume that scattering in all partial waves but the S-wave ($\ell=0$) is negligable. Also assume that $m_1 = m_2$. Prove that the Luescher formula simplifies to:

$$p^* \cot \delta_s(p^*) = 4\pi C_{00}^{\vec{P}}(p^{*2})$$

Note that the $2\to 2$ elastic scattering amplitude can be decomposed as:

$$\mathcal{M}^{\infty}_{\ell_1 m_1, \ell_2 m_2} = \delta_{\ell_1,\ell_2}\,\delta_{m_1,m_2}\,\frac{8\pi E^*}{\xi p^*}\,\frac{e^{2i\delta_\ell(p^*)}-1}{2i}$$

o Extension to multi-channel $2\to 2$ scattering

Let's assume that there are two $2\to 2$ scattering channels, A, B, that can mix into each other. For example, a $\pi\pi$ channel can also mix with a $K\bar{K}$ channel under strong interactions. In these situations, the scattering amplitude can be promoted to a matrix in the space of these flavor channels:

$$i\mathcal{M}^{\infty} = \begin{pmatrix} i\mathcal{M}^{\infty}_{A\to A} & i\mathcal{M}^{\infty}_{A\to B} \\ i\mathcal{M}^{\infty}_{B\to A} & i\mathcal{M}^{\infty}_{B\to B} \end{pmatrix}$$

The diagonal components of this matrix can be decomposed to partial waves and be characterized by a set of scattering phase shifts. The off-diagonal elements are characterized by a mixing angle. As with the phase shifts, mixing angles can also be energy dependent.

As far as the $\delta\mathcal{G}^V$ matrix goes, it obviously does not mix the two channels:

$$\delta\mathcal{G}^V = \begin{pmatrix} \delta\mathcal{G}^V_{A\to A} & 0 \\ 0 & \delta\mathcal{G}^V_{B\to B} \end{pmatrix}$$

Note that within each $\delta\mathcal{G}^V_{A\to A}$ or $\delta\mathcal{G}^V_{B\to B}$, another kind of mixing occurs, but between various partial waves. This is because the finite cubic volume breaks rotational invariance down to cubic (octahedral) group, which means angular momentum is no longer a good quantum number. So if you are interested in beyond low energies where $\ell=0$ is the dominant contribution, you often need to deal with the det condition and simultaneously constrain more than one partial-wave phase shift.

Back to the two-channel $2\to2$ elastic scattering, it is now easy to see that the quantization condition must be generalized as follows:

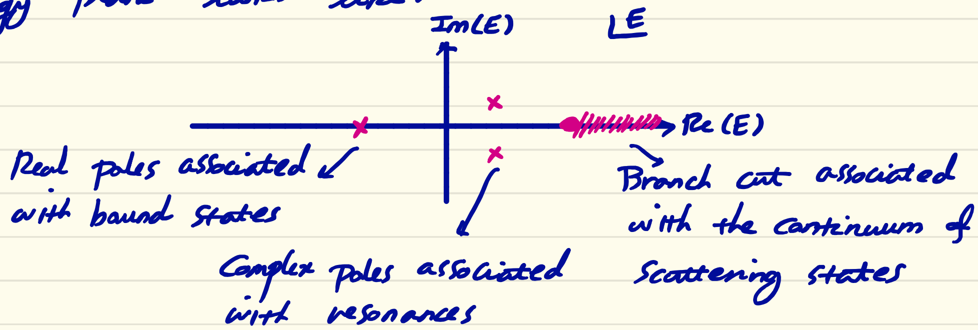
$$\det_{\text{channels}} \det_{\ell}\left[\mathcal{M}^{\infty}(E_n^*)^{-1} + \delta G^{V}(E_n^*)\right] = 0$$

where the first determinant is over the flavor-channel space and the second determinant is over the partial-wave space. This relation can be trivially generalized to any number of coupled $2 \to 2$ flavor channels!

Before ending this section, let us recall that even in the case of a single flavor channel, the scattering amplitude $i\mathcal{M}^{\infty}$ may not be diagonal in the partial-wave space. For example, in the two-nucleon systems in the spin-triplet $S=1$ channel, at any given total angular momentum J, two partial waves can mix into each other. In the deuteron channel for example, which has $J=1$, the s-wave and d-wave mix. The above quantization condition still allows us to determine this mixing angle from FV energies of two nucleons in this channel.

o Bound states and resonances from finite-volume formalism

Bound states are poles of the scattering amplitude below threshhold. For 2-2 scattering, the amplitude in the complex energy plane looks like:



In a finite volume, we only get real-valued discretized poles, so how do we get such a rich analytic structure for the amplitude? The answer is simple. We feed real-valued FV energies into the Luescher's quantization condition, and we obtain $i\mathcal{M}^{\infty}$ at those associated energies. We would then find reasonable parametrizations of the amplitudes as a function of energy that fit the amplitude at those energies we found. By analytically continuing those amplitudes, i.e., $E \to$ complex E, we can then constrain the analytic structures (find bound state poles, resonances, etc.). This is therefore similar to experiment: we get the value of phase shifts at a set of energies, and rely on various parametrizations to extend our knowledge.

Finally, we note that Luescher's quantization condition allows us to find a relation between the infinite-volume and finite-volume bound-state energies. Consider a non-relativistic two-body system with non-relativistic energy: $E^* = \frac{\vec{k}^{*2}}{m}$, where $\vec{k}$ is the relative momentum in the cm frame. For a bound state, $E^* \equiv -B < 0$. We define a binding momentum $\kappa^2 \equiv -k^{*2} > 0$, such that: $B = \frac{\kappa^2}{m} \Rightarrow \kappa = \sqrt{mB}$, where m is the mass of each of the two hadron (assuming the two have equal mass). Then, one can show:

$$\kappa^V = \kappa + \frac{Z^2}{L}\left[6e^{-\kappa L} + \frac{12}{\sqrt{2}}e^{-\sqrt{2}\kappa L} + \frac{8}{\sqrt{3}}e^{-\sqrt{3}\kappa L}\right] + O\left(\frac{e^{-2\kappa L}}{L}\right)$$

So FV corrections to binding momentum (energy) are exponentially suppressed in κL, rather than power-law suppressed. This result should not be surprising. A bound state has a localized wave-function $\propto e^{-\kappa r}$, hence cannot be affected by the boundary.

Exercise 13: Derive the relation above between κ^V and κ by considering the s-wave limit of the Luescher's quantization condition in the previous exercise.
Hint: Take advantage of Poisson resummation

formula to write the sum in $c_{00}^{(\vec{d})}$ as an infinite-volume integral and another sum/integral. These integrals can be analytically evaluated considering that the integrands have imaginary poles given the bound-state condition. You can consult arXiv: 1108.5371.

O Other extensions and applications

Extending the Luescher's formalism to other processes is an active field of research. One can generalize it to $2 \to 3$, $3 \to 3$ processes, although the formalism is more involved. One can also consider a process induced by other forces (e.g. electroweak process), but the initial / final states still interact via the strong force (e.g. $K \to \pi\pi$ decay, pp fusion, deuteron disintegration, neutrino less double beta decay, etc.). One can also come up with FV formalisms that give access to the amplitude in such processes from lattice-QCD computations of both multi-hadron energies and three and four point functions in a finite volume.

These formalism have been successfully applied in modern-day lattice-QCD computations to learn properties of hadrons and nuclei. There also remain some open questions. Can we formulate charge-particles scattering and decay in a model-independen, Luescher-like' form? What about four and higher body processes? Can we apply post-Luescher methods, such as that proposed in arXiv: 1903.11735 realistically? What are FV corrections to light-like quantities? What about FV corrections in Hamiltonian-simulation methods? Again, this is an active field of reseach, so get involved if interested!