Lecture notes on multi-nucleon physics from lattice QCD

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Module I: QFT in a finite volume

Lecture I: QED in a finite volume

To be covered in today's lecture:

- ☐ General motivation for FV QFT
- ☐ QED in a FV: formulation with PBCs and associated pathologies
  arXiv:1810.05923 arXiv:0804.2044
  arXiv:1406.4088 arXiv:1402.6741
- ☐ Solutions:
  - ○ QED_{TL} : $\tilde{A}_\mu(q=0)=0$
    arXiv:1810.05923 arXiv:0804.2044
  - ○ QED_L : $\tilde{A}_\mu(t,\vec{q}=0)=0$
    arXiv:1810.05923 arXiv:1406.4088
  - ○ QED_{C*} : PBCs → C^*BCs
    arXiv:1509.01636
  - ○ QED_m : $m_\gamma \neq 0$
    arXiv:1507.08916
- ☐ Computing observables with QED_L
  - ○ A charged sphere
    arXiv:1402.6741
  - ○ Mass of hadrons
    arXiv:1810.05923
  - ○ Muon magnetic moment
    arXiv:1402.6741
- ☐ prospects of LQCD+QED calculations

☐ General motivation for FV QFT

Any lattice gauge theory study is performed in a finite volume with a set of boundary conditions on the fields. An important question is then how large the volume effects are and how can one correct for them. It turned out that there are two distict situations when it comes to volume effects in a lattice QCD calculation:

i) Volume effects are contaminating the values of observables and they must be either identified and subtracted away analytically, or by the use of an extrapolation to the infinite volume limit with multiple calculations performed numerically at a range of volumes. This is often the case in the single-hadron sector or in special cases in multi-hadron observables such as binding energies.

ii) The infinite-volume limit of observables is of no use! Here, in fact the volume dependence of observables allow the determination of certain dynamical quantities such as scattering and transition amplitudes in the multi-hadron sector. So understanding the FV QFT is not just for the sake of correcting small corrections in quantities of interest, but instead to also enable otherwise impossible determinations from lattice QCD.

As a result, it is important to learn how QFT behaves in a finite volume with given BCs, whether to enable precise determination of hadronic quantities, or to extend the range of applicability of LQCD to multi-hadron physics. This module contains three lectures to cover this important aspect of LQCD studies in high-energy and nuclear physics. The first lecture introduces features of quantum electrodynamics (QED) in a FV, and shows how to mitigate a severe IR problem and how to compute the volume dependence of observables in the single-hadron sector. The following two lectures covers FV QCD and moves on to the FV formalisms for few-body observables

In all subsequent lectures, I will be assuming a continuum QFT. The strategies on how to mitigate discretization effects and how to take the continuum limit of a lattice QCD calculation are/will be covered in other lectures.

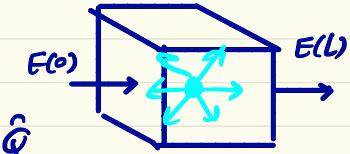
☐ QED in a FV: formulation with PBCs and associated pathologies

Consider a cubic volume of spatial length L with periodic boundary conditions (PBCs) on the fields, which is the common BCs in lattice calculations. It turned out that QED enclosed in such a volume with such BCs is quite problematic. There are a few way to see this issue, all of which sharing the same origin:

i) Gauss' law is incompatible with QED in a FV with PBCs. Charged particles can not be enclosed in such a volume!

Proof: This is not hard to see.

According to Gauss' law:



$$\int_V \nabla\cdot\vec{E}\,d^3x = \int_{\partial V} \underset{\substack{\downarrow\\ =0 \text{ with PBCs}}}{\vec{E}\cdot\hat{n}\,d^2x} = \underset{\substack{\downarrow\\ \neq 0}}{e\hat{Q}}$$

This incompatibility arises from the photon zero mode.

To see this consider QED action

$$S_{QED} = \int_T dt \int_V d^3x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + e\hat{Q}\bar{\psi}\gamma_\mu A^\mu \psi \right]$$

Classical equations of motion (EOM) arise from $\delta S_{QED} = 0$, which gives:

$$\delta S_{QED} = \int dt \int_V d^3x \left[-\frac{1}{2} \delta F_{\mu\nu} F^{\mu\nu} + e\hat{Q}\bar{\psi}\gamma_\mu \psi \, \delta A^\mu \right]$$

$$= \frac{1}{TL^3} \sum_k \int dt \, d^3x \, e^{-ik\cdot x} \delta\tilde{A}_\mu(k) \left[-\partial_\nu F^{\mu\nu}(x,t) + \overset{e\hat{Q}\bar{\psi}\gamma^\mu\psi}{\nearrow} j^\mu(x,t) \right] = 0$$

Therefore Guass' law arise from $k=0$ term of the sum, corresponding to the zero mode of the photon. This must not be surprising. Only with a force that is infinite range, the information on the surface of a volume far at infinity can result in the knowledge of the existence of a charge sitting at origin, hence the Guass' law.

ii) Laplacian is not invertible on a finite volume with PBCs:

Proof: Consider the QED action this time in the Feynman gauge and without matter field. In infinite volume:

$$S[A_\mu] = \int d^4x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} (\partial_\mu A^\mu)^2 \right]$$

$$= -\frac{1}{2}\int d^4x\, A_\mu(x)\,\partial^2 A^\mu(x)$$

In momentum space, this becomes:

$$S[A_\mu] = \frac{1}{2}\int \frac{d^4k}{(2\pi)^4}\, k^2 \sum_\mu [\tilde{A}_\mu(k)]^2$$

where the Fourier modes $\tilde{A}$ are defined as:

$$\tilde{A}_\mu(k) = \int d^4x\, e^{-ik\cdot x} A_\mu(x)$$

So we see that the photon propagator must be:

$$D_{\mu\nu}(x-y) = -(\partial^2)^{-1}\delta(x-y)\,\delta_{\mu\nu} = \int \frac{d^4k}{(2\pi)^4}\, \frac{\delta_{\mu\nu}}{k^2}\, e^{ik\cdot(x-y)}$$

Should we worry about $k=0$ term above? The answer is no! The zero mode constitutes a set of measure zero, hence the integral above is finite.

Now consider the FV counterpart of above. With periodic BCs on an hypercube of spatial extent L and temporal extent T, the momentum modes are discretized as: $k_\mu = \frac{2\pi n_\mu}{L}$, $n_\mu \in \mathbb{Z}^4$, and the Fourie decomposition of A_μ becomes:

$$\tilde{A}_\mu(k) = \int_{\mathbb{T}^4 \equiv L^3\times T} d^4x\, A_\mu(x)\, e^{-ikx}, \quad A_\mu(x) = \frac{1}{TL^3}\sum_{k\in\hat{\mathbb{T}}^4} \tilde{A}_\mu(k)\, e^{ik\cdot x}$$

With this, the action of the theory now is:

$$S[A_\mu] = \frac{1}{2TL^3} \sum_k k^2 \sum_\mu [\tilde{A}_\mu(k)]^2$$

And the propagator is: $D_{\mu\nu}(x-y) = \frac{1}{TL^4} \sum_{k \in \mathbb{T}^4} \frac{\delta_{\mu\nu}}{k^2} e^{ik\cdot(x-y)}$.

Now this form is clearly problematic. $k=0$ term is a singular term in the sum, causing the propagator to become ill-defined.

A deeper look into this problem reveals that this issue is quite similar to the issue of gauge redundancy in QED in infinite volume. There again the photon propagator was ill-defined and a Fadeev-Popov gauge fixing scenario removed the undesired singularity. The question is what is the gauge redundancy that appears to have been re-appeared in the QED formulation in a FV with PBCs? The answer lies in the "shift symmetry of the action, the fact that:

$$A_\mu(x) \to A^b_\mu(x) \equiv A_\mu(x) + \frac{b_\mu}{TL^3} \equiv A_\mu(x) + \partial_\mu \Lambda(x)$$

leaves the action invariant. Note that in Fourier space:

$$\tilde{A}_\mu(k) \to \tilde{A}_\mu(k) + ik_\mu \underset{\substack{\downarrow \\ \text{periodic part of gauge}}}{\tilde{\Lambda}_p(k)} + \frac{2\pi}{e\hat{Q}} \begin{cases} \frac{m_\mu}{L}, & \mu = 1,2,3 \\ \frac{m_\mu}{T}, & \mu = 0 \end{cases} \times \delta_{k,0}$$

with integer m_μ. Note that this will ensure that the transfered matter fields satisfy PBCs:

$$\psi(x) \to e^{ie\hat{Q}\Lambda(x)}\psi(x)$$

Since: $\Lambda(x) = \Lambda_p(x) + \frac{2\pi}{e\hat{Q}} \sum_{m_0, m_i} \left(\frac{m_0}{T} t + \frac{m_i}{L} x_i\right), m_0, m_i \in \mathbb{Z}$

Two comments are in order: First shift transformation is not a symmetry of the infinite-volume theory as A_μ fields must vanish at infinite boundary, and second, because of the shift symmetry of the FV theory with PBCs, there are infinite number of identical field configurations that are different by a constant shift, making the laplacian of the theory non-invertible.

So what we saw from these two diagnostics, the origin of the pathalogies with the FV QED with PBCs is the photon zero mode. Therefore, it is not hard to guess that any remedy must be modifying the zero mode and its contributions. Here, we briefly mention four such remedies.

☐ solutions to zero mode problem:

○ QED_{TL} : $\tilde{A}_\mu(q=0)=0$

Well, the first solution is to remove the zero mode all together from the dynamics. This solution is a direct outcome of performing a Fadeev-popov gauge fixing.

Exercise1: By inserting the condition: $\int db\, \delta[\int_{\mathbb{T}^4} d^4x\, \overset{b}{A}(x)] = 1$ into the path integral of QED in a FV with PBCs, show that the photon propagator becomes well defined, and is given by: $D^{(TL)}_{\mu\nu}(x-y) = \frac{1}{TL^3}\sum'_{k\in\mathbb{T}^4} \frac{\delta_{\mu\nu}}{k^2} e^{ik\cdot(x-y)}$, where $'$ means the $k=0$ term of the sum is removed.

Now consider the gauge fields coupled to fermions through

$$S_{int} = \int d^4x\, j_\mu(x) A^\mu(x)$$

obviously, this term is not invariant under $A_\mu \to A_\mu^b$, and the treatment above breaks down unless we make a modification to the current as well such that the new interacting action is:

$$S_{int}' = \int d^4x \, A_\mu(x) \left[J^\mu(x) - \frac{1}{TL^4} \int d^4y \, J^\mu(y) \right]$$

what does this mean? Well, it just means that the removal of the photon zero mode is accomplished by introducing a uniform charge density over the spacetime volume. This also makes it clear why such a process restore Gauss' Law. One introduces a charge that cancels out the embedded charge in the volume, making everything consistent with PBCs imposed!

what are the issues with this? Obviously non-locality! If $j_\mu = \bar{\psi}\gamma_\mu\psi$ for example, equation above means that A_μ at x couples to fermions at all point in the spacetime volume. While this non-locality goes away as $T \to \infty$, $L \to \infty$, the finite volume theory lacks a well defined "reflection-positive transfer matrix" which introduce subtleties, an example of which we will mention when we consider FV corrections to the mass of charged particles in this theory.

○ QED_{TL} : $\tilde{A}_\mu(q=0)=0$

Alternatively, we can avoid non-locality in time and only remove the spatial zero mode of the photon. This means that we are only fixing the shift symmetry associated with :

$$A_\mu(x) \to A_\mu^{(b)}(x) = A_\mu(x) + \frac{b_\mu(t)}{L^3}$$

This give rise to the same photon propagator as in QED_{TL} except now only $\vec{k}\neq 0$ Fourier component is fixed. Hence, the interacting action is :

$$S_{int} = \int d^4x\, A_\mu(x)\left[J^\mu(x) - \frac{1}{L^3}\int d^3y\, J^\mu(y)\right].$$

should we still worry about non-locality in space? Both yes and no! No because such non-locality goes away anyway as $L\to\infty$, and yes because quantum corrections can get affected by the IR physics (the constant charge density) and it will be difficult to decouple UV and IR physics, see for example the discussions regarding the careful construction of an effective field theory for such a non-local theory in Ref. arXiv:1810.05923.

○ QED_{C^*} : PBCs $\rightarrow$ C^*BCs

Since the origin of zero mode problem is PBCs, one can come up with alternative BCs that naturally don't give rise to a zero mode for the photon. Charge Conjugate BCs are one example. All the fields here undergo a charge conjugation at the boundary and the photon field therefore obeys anti-periodic BCs:

$$A_\mu(x+L) = A_\mu^C(x) = -A_\mu(x)$$

Exercise 2: Show that with the C^*BCs, the photons will not have any zero mode. Write down the Fourier decomposition of the photon propagator.

This, on surface may appear a minor modification to the theory. However, such a boundary condition has profound consequences on charge and flavor conservations, and in fact partially breaks them! The origin of this is not hard to understand since the fields change charge and flavor number as they go around the boundary. Such violation of conservation laws are however exponential in the volume and can be ignored in numerical simulations. In short, while QED_{C^*} provides a local formulation of QED in a FV, it is a much more complex construct than QED_{TL} or QED_{L}.

○ QED_m : $m_\gamma \neq 0$

Obviously if the photon had mass, there would be no zero modes and QED interactions would be effectively cutoff at distances of the order of Compton wavelength of the photon. A non-zero mass for the photon breaks gauge invariance, and imply no Guass' law. It is also a local formulation for QED in a FV with any BCs. One can compute observables in such a theory and once the infinite volume is taken, perform an extrapolation to $m_\gamma \to 0$. Note that for this method to be useful, $m_\gamma \ll m$, where m is the mass of the lightest hadron in the theory so that there is a clear separation between UV and IR in the theory.

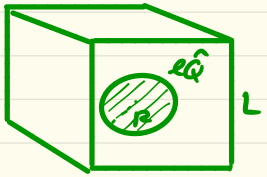
☐ Computing observables with QED_L

For simplicity, and given the popularity of QED_L, for the remainder of discussions, we consider only this formulation. The generalization of the analysis below to other formulation below is straightforward upon replacing the photon propagator with the corresponding form in each formulation.

○ A charged sphere

How does the self energy of a classical charged sphere gets modified if enclosed in a cubic volume with PBC? This can serve as a warm-up example. It also teaches us about the nature of QED FV corrections and shares similar features with corrections to masses of fields in quantum field theory.

Exercise 3: Consider a charge sphere with radius R and charge $e\hat{Q}$ spread uniformly over its volume. By performing a $1/L$ expansion, show that at leading orders, the self energy of the sphere is given by:



$$U(R,L) = \frac{3}{5}\frac{e^2\hat{Q}^2}{4\pi R} + \frac{e^2\hat{Q}^2}{8\pi R}\left(\frac{R}{L}\right)c_1 + \frac{e^2\hat{Q}^2}{10R}\left(\frac{R}{L}\right)^3 + \dots$$

where: $c_1 = \left(\sum_{\vec{n}\neq 0} - \int d^3n\right)\frac{1}{|\vec{n}|} = -2.83729$, for $n \in \mathbb{Z}^3$.*

Note that in QED_L the Coulomb potential can be written as: $V(\vec{r}-\vec{r}\,') = \frac{e\hat{Q}}{L^3}\sum_{\vec{k}\neq 0}\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}}{\vec{k}^2}$, $k = \frac{2\pi\vec{n}}{L}$.

The result of this calculation implies that FV corrections due to QED_L are polynomial in $1/L$, which is a stronger volume dependence than exponential and can not be ignored. Further, as we will see, the $O(1/L)$

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* For a derivation of FV sums, see: Hasenfratz, Leutwyler (1989).

volume correction is the same as that to the mass of any particle in QFT. The underlying reason for this being that FV effects are IR physics that don't probe the short-distance detail of system at leading order.

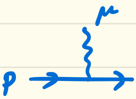
○ Mass of hadrons

From a quantum theory perspective, the reason the mass of a composite or elementary field is sensitive to the FV and BCs is that it can, for example, emit a photon, the photon can then go around the "world" and come back and be reabsorbed by the field. As the propagating photon sees the boundary, and as such a radiative correction is the leading-order correction to the self energy of the particle in field theory, the mass of the particle receives FV corrections.

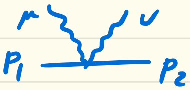
As an example, let's consider the case of a scalar fundamental particle that interacts with photons through: $\mathcal{L}_{scalar} = (D_\mu \phi)^\dagger (D_\mu \phi) - m^2 \phi^\dagger \phi$

where : $D_\mu \phi = \partial_\mu \phi + ie\hat{Q}A_\mu \phi$. Then the Feynman rules for this theory are simply:

$= \frac{i}{p^2-m^2+i\epsilon}$



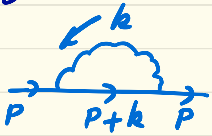
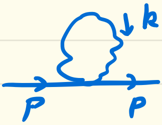
$= -ie\hat{Q}(p+p')_\mu$



$= 2ie^2\hat{Q}^2 g_{\mu\nu}$

$= \frac{-ig_{\mu\nu}}{k^2+i\epsilon}$ [Feynman gauge]

The self energy of field ϕ at $O(\alpha)$ can be obtained from:

$-i\Sigma^{(\phi)}(p) =$  + 

$$= \frac{1}{L^3}\sum_{\vec{k}\neq 0}\int\frac{dk^0}{(2\pi)}\left[\frac{i}{(p+k)^2-m^2+i\epsilon}(-ie\hat{Q})^2(2p+k)^2\frac{-i}{k^2+i\epsilon}\right.$$
$$\left.(ie^2\hat{Q}^2)\frac{-i}{k^2+i\epsilon}g_\mu^{\ \mu}\right]$$

Exercise4: By performing an expansion in small $\frac{1}{mL}$, show that: $-i\Sigma^{(\phi)}(\vec{p}=0) = -\frac{ie^2\hat{Q}^2}{L^3}\sum_{\vec{k}\neq 0}\left[\frac{m}{|\vec{k}|^2}+\frac{1}{|\vec{k}|}+\cdots\right]$.

Note that: $\vec{k}=\frac{2\pi}{L}\vec{n}, n\in\mathbb{Z}$.

Now since the self energy modifies the bare mass of the field, i.e., $m^2 \to m^2+\Sigma(p^2=m^2)$, at $O(\alpha)$, we get:

$$\delta m^{(\phi)} = \frac{e^2\hat{Q}^2}{8\pi L}c_1\left[1+\frac{2}{mL}\right]+\cdots$$

Note that the first term is the same as the leading-order correction to the self energy of a charged sphere! Take the charged sphere as $m \to \infty$ limit of a particle and you can already see why the $o(e^2/L)$ corrections are equal! Further, there is a rigorous proof for the universality of the $o(e^2/L, e^2/L^2)$ terms: They are independent of the spin and structure of the particles considered!

Exercise 5: Evaluate the self energy of the a point-like charged particle in QED (spin-$1/2$ electron for example), and show that the QED FV corrections to the mass at $o(e^2/L, e^2/L^2)$ are the same as for spin-0 particles we just considered.

You may now ask what would have happened if we removed all $k=0$ modes of the photon instead of $\vec{k}=0$ only? One can show that in QED_{TL}, the corrections to the self energy of a scalar point-like particle is:

$$\delta m^{(\phi)} = \frac{e^2 \hat{Q}^2}{2L} c_1 \left[1 + \frac{2}{mL} \left(1 + \frac{\pi}{2c_1} \frac{T}{L} \right) \right] + \cdots$$

This expression is clearly problematic if one attempt to take the $T \to \infty$ limit first. This is a clear symptom of non-locality of the theory in time. Of course if T/L is not large in a LQCD calculation but $mL \gg 1$, such a problematic term can be numerically small, justifying LQCD+QED calculations that have implemented this scheme in the past, but for high-precision calculations, QED_L is a better formulation, see e.g., the precise calculation of proton-neutron mass difference in arXiv:1406.4088.

○ Muon magnetic moment

Different formulations of QED in a FV can be used to assess the size of volume corrections to a range of quantities. An interesting example is the muon magnetic moment.

Exercise 6: Review the derivation of the anomalous magnetic moment of muon in QED at $O(\alpha = e^2/4\pi)$. Then perform the same calculation this time in QED_L to show that:

$$\frac{g_\mu - 2}{2} = \frac{\alpha}{2\pi}\left[1 + \frac{\pi c_1}{m_\mu L} + O\left(\frac{1}{m_\mu^2 L^2}\right)\right]$$

what volume is needed to reach 1ppm precision in this quantity?

BONUS

Note that current precision calculations with LQCD are based on indirect methods that isolates the hadronic contributions only and hence don't suffer from such a large FV effect.

☐ prospect of LQCD+QED calculations

Finally, to conclude this lecture, we note that all the formulations of QED in a FV mentioned here are already implemented in LQCD+QED computation of various observables such as hadron masses and hadronic vacuum polarization, meson leptonic decays, etc. There is also extensive research on how to extract observables such as charged-particle scattering, decay/transition amplitudes with initial/final charged states, etc. If you are interested in such formal developments, this is a great time to get involved and contribute!

Lecture II: QCD in a finite volume

To be covered in today's lecture:

- ☐ General features of QCD in a finite volume with PBCs
  arXiv: 1409.1966
- ☐ Finite-volume corrections to single-hadron observables:
  An original paper: Luescher 1986
  - ○ Example 1: Nucleon mass
    arXiv: 0403015
  - ○ Example 2: Nucleon axial charge
    arXiv: 0403015

☐ General features of QCD in a finite volume with PBCs

Quantum chromodynamics (QCD) is an interesting theory. Despite QED where we had the issue with the propagation of massless photons, in QCD the states that go on shell and propagate are not the massless gluons, but instead confined massive objects: mesons, baryons, or even glueballs! This is the statement that QCD has a mass gap. This means that we don't really have to reformulate the theory in a FV to make it well-defined, since there is no Gauss' law to satisfy: there is no charged (under SU(3) charged) quarks or gluons at confinement scale or lower, which we are interested in. Since the lightest hadronic states in the theory are pions, they are the ones setting the size of finite volume corrections to a range of quantities.

Further, since the FV correction concern effect at the boundaries, these are considered IR effects and hence to determine them, we don't need to know all details of short-distance physics. This is great, since the reason we perform LQCD calculations is that we don't have the analytic dependence of quantities such as masses on the parameters of the short-distance theory, in this case QCD. The fact that FV effects are IR physics, means that we can use effective descriptions of the theory at low energy's, with which we can analytically calculate observables (not everything!) and estimate leading FV effects. Here, we work out an example of this method to calculate volume corrections to the mass of the nucleon, and in an exercise you'd be applying the same techniques to the nucleon's axial charge.

☐ Finite-volume corrections to single-hadron observables:

Here we focus of nucleon's properties, but with the right EFTs, one can look at other single-hadron observables too.

○ Example 1: Nucleon mass

In order to estimate the FV corrections to the mass of the nucleon, a nice framework is chiral perturbation theory (χPT). You will learn all about in subsequent lectures from Prof. Epelbaum, so here I simply state the form of Lagrangean at leading order in the expansion parameter of the theory p/Λ_χ, m_π/Λ_χ, where p is a typical momenta, m_π is the mass of the pion, and Λ_χ is the scale of chiral symmetry breaking. Since nucleons are heavy, a more convenient formulation of the Lagrangian is what is called "heavy baryon χPT". In this formulation, the mass of the nucleon is subtrated from the dynamics, leaving a NR two-component nucleon field. Expressing nucleon momentum as: $P_\mu = M_N^{(0)} v_\mu + l_\mu$

where v_μ is a velocity four-vector, which is $v_\mu = (1,0,0,0)$ in the rest frame of the nucleon. l_μ is a residual momentum that carries the rest of momentum not associated with the mass. The kinetic energy Lagrangian is:

$$\mathcal{L}_N = \bar{N}[i\partial\cdot v]N + M_N^{(0)}\bar{N}N + \cdots$$

Here, N is a two-component vector in both spin and isospin spaces: $N = \begin{pmatrix} N_\downarrow \\ N_\uparrow \end{pmatrix}$, $N = \begin{pmatrix} n \\ p \end{pmatrix}$.

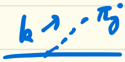
The relevant interations of the nucleons for our purpose are those with the pions, and can be described at LO by:

$$\mathcal{L}_{\pi N} = -\frac{g_A}{f_\pi}\bar{N}(\vec{\sigma}\cdot\vec{\partial})(\vec{\tau}\cdot\vec{\pi})N$$

Here $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are pauli matrices in spin space and $\vec{\tau} = (\tau_1, \tau_2, \tau_3)$ are pauli matrices in isospin space. $g_A = 1.27$ is the nucleon axial charge and $f_\pi \simeq 130$ MeV is the pion decay constant. The feynman rules relevant for us are:

$$= \frac{i}{p\cdot v - M_N^{(0)} + i\epsilon}$$

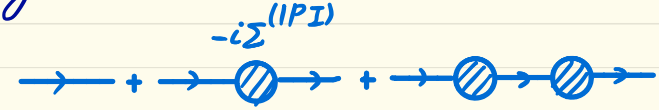
$$= -4 c_1 m_\pi^2 \quad \text{with} \quad c_1 = -0.93 \pm 0.10 \ \text{GeV}^{-1}$$



$$= \frac{g_A}{f_\pi} k_i \sigma_i \tau_j$$ From insertions of quark mass matrix

Now we have all the ingredients to carry out the calculation of FV effects to the nucleon mass. Note first that the "radiative" corrections to the mass of the nucleon arise from interactions with pions. The nucleon mass can then by obtained from fully dressed nucleon propagator:

$D_N =$



$$= \frac{i}{p\cdot v - M_N^{(0)} + i\epsilon}\left[1 - i\Sigma^{(1PI)}\frac{i}{p\cdot v - M_N^{(0)} + i\epsilon} + \left(-i\Sigma^{(1PI)}\frac{i}{p\cdot v - M_N^{(0)} + i\epsilon}\right)^2 + \dots\right]$$

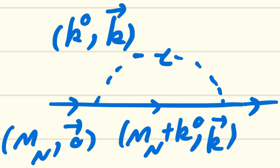
$$= \frac{i}{p\cdot v - M_N^{(0)} - \Sigma^{(1PI)} + i\epsilon} = \frac{iZ_N}{p\cdot v - M_N + i\epsilon}$$

Here, $M_N^{(0)}$ is the bare nucleon mass and $\Sigma^{(1PI)}$ is the one-particle irreducible self-energy function. The pole of the fully dressed prapagator gives the mass of the nucleon:

$$p\cdot v = M_N \Rightarrow \left[p\cdot v - M_N^{(0)} - \Sigma^{(1PI)}\right]_{p\cdot v = M_N} = 0 \Rightarrow M_N = M_N^{(0)} + \Sigma^{(1PI)}\Big|_{p\cdot v = M_N}$$

Now we have to identify in the theory the leading diagrams contributing to $\Sigma^{(1PI)}$. They are:

$$= -4c_1 m_\pi^2 \equiv -i\Sigma_{LO}$$



$$= \left(\frac{-g_A}{f_\pi}\right)\left(\frac{-g_A}{f_\pi}\right) \times \frac{3}{2} \int \frac{d^4k}{(2\pi)^4} \vec{k}^2 \frac{i}{k^0 - i\epsilon} \frac{i}{k^{0\,2} - \vec{k}^2 - m_\pi^2 + i\epsilon}$$

$$\equiv -i\Sigma_{NLO}$$

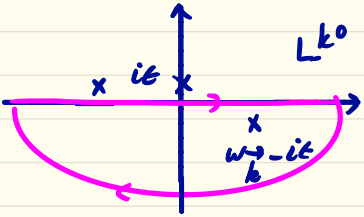
where we have chosen to work at rest frame of the nucleon since we are interested in the corrections to the mass.

Exercise 7: Derive/justify the factor of $3/2\,\vec{k}^2$ in the loop expression above. Note that: $\vec{\tau}\cdot\vec{\pi} = \begin{bmatrix} \pi^0/\sqrt{2} & \pi^+ \\ \pi^- & -\pi^0/\sqrt{2} \end{bmatrix}$.

To get one step closer to evaluating this integral, we can perform integration over k^0: $\left[\omega_{\vec{k}} \equiv \sqrt{\vec{k}^2 + m_\pi^2}\right]$

$$-i\Sigma_{NLO} = -\frac{3 g_A^2}{2 f_\pi^2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\pi} \frac{(-2\pi i)}{\omega_{\vec{k}}(2\omega_{\vec{k}})} \vec{k}^2$$

$$= \frac{3 i g_A^2}{4 f_\pi^2} \int \frac{d^3k}{(2\pi)^3} \frac{\vec{k}^2}{\vec{k}^2 + m_\pi^2}$$



First, you may note that this integral is UV divergent, introducing a dependence on the scale that must be renormalized.

However, we are not interested in deriving this known result here. What we are interested in is to obtain the finite and infinite volume difference in this quantity. Such a UV divergence is present in a finite volume and cancels out in the difference. Note that for this discussions, we have assumed that the time extent of the spacetime volume is infinity, so that the only finite-size corrections are in the spatial directions, again in a finite cubic volume with periodic boundary conditions, such that: $\begin{cases} k^0 \text{ continuous} \\ \vec{k} = \frac{2\pi}{L}\vec{n},\ n \in \mathbb{Z}^3 \end{cases}$

Therefore: $\delta\Sigma \equiv \Sigma(L) - \Sigma(\infty)$

$$= \underbrace{\left(\Sigma_{LO}(L) - \Sigma_{LO}(\infty)\right)}_{0} + \left(\Sigma_{NLO}(L) - \Sigma_{NLO}(\infty)\right) + \cdots$$

$$= -\frac{3g_A^2}{4f_\pi^2}\left[\frac{1}{L^3}\sum_{\vec{k}=\frac{2\pi\vec{n}}{L}} - \int\frac{d^3k}{(2\pi)^3}\right]\frac{\vec{k}^2}{\vec{k}^2+m_\pi^2} + \underset{\substack{\downarrow \\ \text{higher orders}}}{\cdots}$$

A powerful relation is the Poisson resummation formula:

$$\frac{1}{L^3}\sum_{\underset{\substack{\downarrow \\ k = 2\pi\vec{n}/L,\ n\in\mathbb{Z}^3}}{\vec{k}}} f(\vec{k}) = \sum_{\underset{\substack{\downarrow \\ m\in\mathbb{Z}^3}}{\vec{m}}} \int\frac{d^3k}{(2\pi)^3} f(k)\, e^{i\vec{k}\cdot\vec{m}L}$$

Using this, we already see that the first term in the sum is the infinite-volume value, leaving a purely finite volume contributions in the difference:

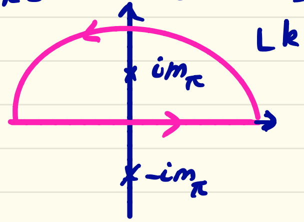
$$\delta\Sigma = -\frac{3g_A^2}{4f_\pi^2}\sum_{\vec{m}\neq 0}\int\frac{d^3k}{(2\pi)^3}\frac{\vec{k}^2}{\vec{k}^2+m_\pi^2}e^{i\vec{m}\cdot\vec{k}L}$$

$$= -\frac{3g_A^2}{4f_\pi^2}\sum_{\vec{m}\neq 0}\frac{(2\pi)}{(2\pi)^3}\int_0^\infty dk\,\vec{k}^2\frac{\vec{k}^2}{\vec{k}^2+m_\pi^2}\int_{-1}^{1}d(\cos\theta)\,e^{i|\vec{m}||\vec{k}|L\cos\theta}$$

$$= -\frac{3g_A^2}{16\pi^2 f_\pi^2}\sum_{\vec{m}\neq 0}\int_0^\infty dk\,\frac{k^4}{k^2+m_\pi^2}\frac{1}{i|\vec{m}|kL}\left(e^{i|\vec{m}|kL}-e^{-i|m|kL}\right)$$

$$= i\frac{3g_A^2}{16\pi^2 f_\pi^2}\sum_{\vec{m}\neq 0}\frac{1}{|\vec{m}|L}\int_{-\infty}^{\infty}dk\,\frac{k^3}{k^2+m_\pi^2}e^{i|\vec{m}|kL}$$

$[k \equiv |\vec{k}|]$



$$= \frac{3g_A^2}{16\pi f_\pi^2}\sum_{\vec{m}\neq 0}\frac{e^{-|\vec{m}|m_\pi L}}{|\vec{m}|L}$$

$$= \frac{3g_A^2}{16\pi f_\pi^2}m_\pi^2\left[\frac{e^{-m_\pi L}}{L}\times 6+\cdots\right] = \delta M_N \equiv M_N(L)-M_N(\infty)$$

Exercise 8: Write down explicitly the contributions from terms up to and including $O(e^{-2m_\pi L})$ in δM_N. plot as a function of $m_\pi L$ contributions from each of these terms, and compare with the exact evaluation. Use $a \lesssim m_\pi L \lesssim 6$ for the range of plot.

This example clearly demonstrates that FV corrections to the mass of stable hadrons, such as nucleons, are exponentially suppressed in volume. It also serves as an example on how the knowledge of a low-energy effective field theory allows to determine leading volume effects. It turned out that volume corrections to other properties of single hadrons are also exponentially suppressed in volume.

Exercise 9: Consider the following chiral perturbation theory lagrangean:

$$\mathcal{L}_{N\gamma} = \frac{e}{4M_N} F^{\mu\nu}\left[\mu_0 \bar{N}\sigma_{\mu\nu}N + \mu_1 \bar{N}\sigma_{\mu\nu}\tau_3^{(\xi^\dagger)}N\right]$$

that describes the magnetic moment of the nucleon through coupling to the electromagnetic field strength tensor at lowest orders.

$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. Here, $\sigma_{\mu\nu} = \frac{1}{4}[\gamma_\mu, \gamma_\nu]$ and nucleons are in relativistic four-component spinor representation. μ_0 and μ_1 are two low-energy const. and $\tau_3^{(\xi^+)} = \frac{1}{2}(\xi^+\tau^3\xi + \xi^+\tau^3\xi)$ with: $\xi = e^{\frac{i\vec{\pi}\cdot\vec{\tau}}{f_\pi}}$.

Show that at $O(g_A^2/f_\pi^2)$, the FV corrections to the magnetic moment of nucleon is:

$$\delta\mu \equiv \mu(L) - \mu(\infty) = -\frac{g_A^2}{12\pi f_\pi^2} M_N m_\pi \sum_{\vec{m}\neq 0}\left(1 - \frac{2}{m_\pi |\vec{m}| L}\right) e^{-m_\pi |\vec{m}| L}$$

BONUS

An interesting point regarding the expressions we just derived is that these can be used to simultaneously extrapolate both in volume and in the pion mass. If a lattice QCD calculation is performed at a larger quark mass, then as long as the associated pion mass is not too high such that χPT can be still applicable, one can use the expressions obtained to extrapolate to $m_\pi^{\text{phys.}}$.

This is another example of the benefits of an EFT study of observables.

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

- ○ Introduction and qualitative picture
- ○ A derivation based on field theory
  arXiv:0507006 arXiv:1409.1966
- ○ Extension to multi-channel 2→2 scattering
  arXiv:1204.1110
  arXiv:1409.1966
- ○ Bound states in a finite volume
  arXiv:1108.5371 arXiv:1107.1272
  arXiv:1309.3556
- ○ 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

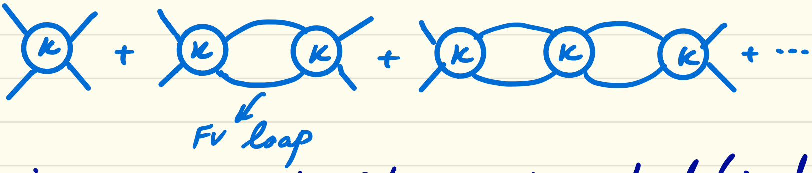
○ Introduction and qualitative picture

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 gaurranteed 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 sector, 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 signiture. There is in fact a no-go theorem, stated and proved by Maini-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→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.

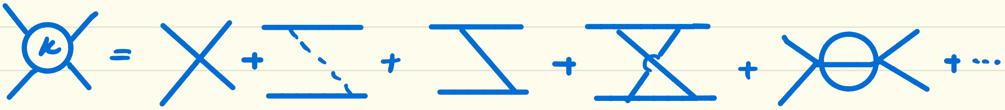
○ A derivation based on field theory

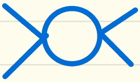
Once again, we consider a generic low-energy effective theory in which hadrons are the degrees of freedom, but beside this, we make no other assumptions or truncation in the EFT expansion. Our goal is to identify the FV corrections to the energy of two hadrons that go as powers of $1/L$. The two-hadron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

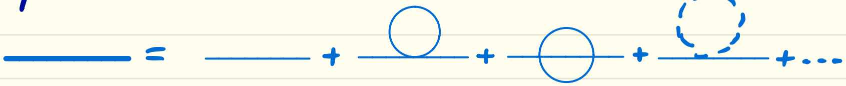
Let us now define a FV "amplitude" in this hadronic theory with one caveat. The notion of amplitude in a FV theory doesn't make sense since there is no asymptotic states, however what we are interested here are the FV energies which are the poles of FV correlation function, and these poles are the same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

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

where K is a 2→2 Bethe-Salpeter kernel defined as:



Baiscally, this include every 2→2 irriducaible diagram allowed in the theory except for those that include "s-channel" loaps, 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:

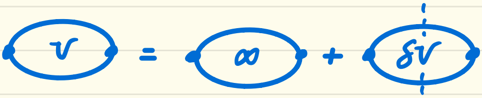
i) Below three-particle inelastic thresholds, the 2→2 kernel κ is close to its infinite-volume counterpart up to exponential corrections in mL where m is the mass of the lightest hadron relevant to the given process. This is because off-shell states can not reach the boundaries of volume and give rize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

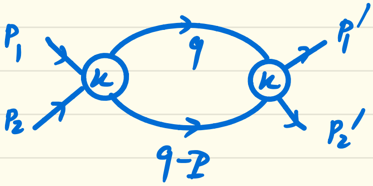


where δV denated purely FV function contributing to the loop. It arises from the condition that both the particles running in the loop go on-shell, and hence the function itself is evaluated on-shell. These functions will be the subject of the rest of the discussions.

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

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

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



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:

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

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:

$$[\delta G^V]_{lm,l'm'} = [G^V - G^\infty]_{lm,l'm'} = -i\kappa_{lm,l_1m_1}\,\delta\mathcal{G}^V_{l_1m_1,l_2m_2}\,\kappa_{l_2m_2,l'm'}$$

where:
$$\delta\mathcal{G}^V_{l_1m_1,l_2m_2} = i\frac{p^*\xi}{8\pi E^*}\Big[\delta_{l_1,l_2}\delta_{m_1,m_2} + i\frac{4\pi}{p^*}\sum_{l,m}\frac{\sqrt{4\pi}}{p^{*l}} \times$$
$$c^{\vec{P}}_{lm}(p^{*2})\int d\Omega\, Y^*_{l_1m_1}Y^*_{lm}Y_{l_2m_2}\Big]$$

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

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 $\delta\mathcal{G}^V_{l_1m_1,l_2m_2}$ 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→2 elastic scattering amplitude. We start with $-iM^V$ expansion in terms of G^V and K:

$$iM^V = (-iK) + (-iK)\, iG^V (-iK) + \cdots$$

$$= (-iK) + (-iK)\, (iG^\infty + i\delta G^V)(-iK) + \cdots$$

$$= \underbrace{(-iK) + (-iK)\, iG^\infty (-iK) + \cdots}_{iM^\infty} +$$

$$\underbrace{(-iK + (-iK)\, iG^\infty (-iK) + \cdots)}_{iM^\infty}\, i\delta G^V \underbrace{(-iK + (-iK)\, iG^\infty (-iK) + \cdots)}_{iM^\infty} +$$

$$(iM^\infty)\, i\delta G^V (iM^\infty)\, i\delta G^V (iM^\infty) + \cdots$$

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

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, M^V diverges at a set of discrete FV energies, E_n^*. Therefore:

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

This is the relation between the infinite-volume scattering amplitude M^∞ 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. We discuss further generalizations of this formula, as well as its applications in actual lattice QCD calculations of two-hadron systems in the next lecture.

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→2 elastic scattering amplitude can be decomposed as:

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