# 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:
  - o $QED_{TL}$ : $\tilde{A}_\mu(q=0) = 0$
    arXiv:1810.05923 arXiv:0804.2044
  - o $QED_L$ ; $\tilde{A}_\mu(t, \vec{q}=0) = 0$
    arXiv:1810.05923 arXiv:1406.4088
  - o $QED_{C^*}$ : PBCs $\rightarrow$ $C^*$BCs
    arXiv:1509.01636
  - o $QED_m$ : $m_\gamma \neq 0$
    arXiv:1507.08916
- ☐ Computing observables with $QED_L$
  - o A charged sphere
    arXiv:1402.6741
  - o Mass of hadrons
    arXiv:1810.05923
  - o 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 connecting 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

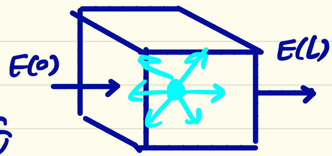
In all subsequent lectures, I will be assuming a continuum QFT. The strategies on how to mitigate discretization effects and how to take the continuum limit of a lattice QCD calculation are/will be covered in other lectures.

## ☐ 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:

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

This incompatibility arises from the photon zero mode.

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

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 Fourier decomposition of $A_\mu$ 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: $D_{\mu\nu}(x-y) = \frac{1}{TL^4}\sum_{k\in\Pi^4} \frac{\delta_{\mu\nu}}{k^2} e^{ik\cdot(x-y)}$ .

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 Fadaeev-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:

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

leaves the action invariant. Note that in Fourier space:

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

with integer $m_\mu$. 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 $A_\mu$ 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.

> Exercise 1: By inserting the condition: $\int db\, \delta\left[\int_{\mathbb{T}^4} d^4x\, A^b(x)\right]=1$ 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 every thing 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 $A_\mu$ 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.

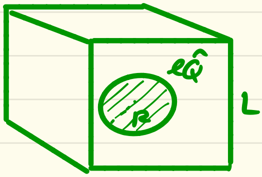
☐ Computing observables with $QED_L$

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.

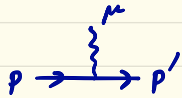
○ Mass of hadrons

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.

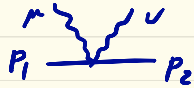
As an example, let's consider the case of a scalar fundamental particle that interacts with photons through:
$$\mathcal{L}_{scalar} = (D_\mu \phi)^\dagger (D_\mu \phi) - m^2 \phi^\dagger \phi$$

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

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



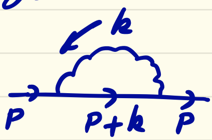
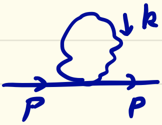

$= -ie\hat{Q}(p+p')_\mu$




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


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

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

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


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

**Exercise 4:** By performing an expansion in small $\frac{1}{mL}$, show that : $-i\Sigma^{(\phi)}(\vec{p}=0) = -\dfrac{ie^2\hat{Q}^2}{L^3} \displaystyle\sum_{\vec{k} \neq 0} \left[ \frac{m}{|\vec{k}|^2} + \frac{1}{|\vec{k}|} + \cdots \right]$.

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.

o 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?

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!