Finite-size effects in lattice QCD+QED_L

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In transition: Bern $\longrightarrow$ Lund $\longrightarrow$ Edinburgh

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Overview

- Motivation: Precision tests of the Standard Model
- Isospin-breaking needed $\implies$ Simulate Lattice QCD+QED
- Several talks about QED in finite volume: $\mathrm{QED_L}$
- My goal today:
  1. What is $\mathrm{QED_L}$?
  2. What about finite-size effects in the simulations?
  3. What lies ahead?
- Reaching the infinite-volume limit:
  1. Simulations at different volumes: Fits
  2. Analytical correction for finite-size effects: Loop calculations

QED in a finite volume

- Gauss' law: Difficult to define charged states in finite volume with periodic boundary conditions
(photon zero-momentum modes and absence of mass gap)
- Several prescriptions (see the other talks here!)

1. $\mathrm{QED_C}$: Charge-conjugated boundary conditions
[Kronfeld, Wiese 1991–1993; RC* 2019]
2. $\mathrm{QED_M}$: Photon mass m_γ
[Endres, Shindler, Tiburzi, Walker-Loud 2016; Bussone, Della Morte, Janowski 2018]
3. $\mathrm{QED_\infty}$: Do the QED part in infinite volume
[Feng, Jin 2018]
4. $\mathrm{QED_L}$: Exclude photon zero-mode on each time-slice
[Hayakawa, Uno 2008]

$$\mathrm{QED_L}: \quad \sum_{\mathbf{k}} \longrightarrow \sum_{\mathbf{k}}{}' = \sum_{\mathbf{k}\neq 0}$$

- Each has advantages/drawbacks : $\mathrm{QED_L}$ simple but non-local

Finite-size effects

- Massless photon + no zero-mode ($\mathrm{QED_L}$ and $\mathrm{QED_C}$)

  $V = \mathbb{R} \times L^3$: $\implies$ Finite-size effects (FSEs) in observable $\mathcal{O}(L)$:

$$\Delta\mathcal{O}(L) = \mathcal{O}(L) - \mathcal{O}_{\mathrm{IV}} = C_0 + C_{\log} \log m_P L + C_1 \frac{1}{m_P L} + C_2 \frac{1}{(m_P L)^2} + \ldots$$

- Scaling in L is observable-dependent:
  e.g. self-energy $C_0 = C_{\log} = 0$
- Coefficients depend on physical particle properties: masses, charges, structure (form-factors):
  Point-like + structure-dependent
- NB: Coefficients are prescription-dependent!

- $\mathrm{QED_M}$ and QED_∞: no power-law effects

Finite-size effects in $\mathrm{QED_L}$

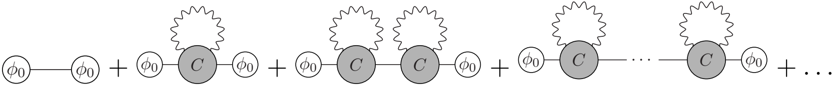
$$\Delta\mathcal{O}(L) = \mathcal{O}(L) - \mathcal{O}_{\mathrm{IV}} = C_0 + C_{\log} \log m_P L + C_1 \frac{1}{m_P L} + C_2 \frac{1}{(m_P L)^2} + \dots$$

- In the following:
  1. How does one get the analytical scaling?
  2. What is the current status and the future of this?

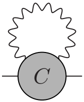
- Based on/biased towards [Davoudi, Savage 2014; BMW 2015; RM-123/Soton 2017; Davoudi, Harrison, Jüttner, Portelli, Savage 2019; Bijnens, Harrison, H-T, Janowski, Jüttner, Portelli 2019; Di Carlo, Hansen, H-T, Portelli 2021]

Finite-size effects in $\mathrm{QED_L}$

- Observable $\mathcal{O}$ with a virtual order α-correction from a photon loop
- Example: Pseudoscalar self-energy, i.e. mass m_P
- Given by pole of Euclidean QCD+QED 2-point correlator

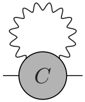


- Relevant object: Compton scattering amplitude



Finite-size effects in $\mathrm{QED_L}$

- Relevant object: Compton scattering amplitude



- Let $k = (k_0, \mathbf{k})$ be the photon momentum
- Finite-size effects in $\mathcal{O}(L)$ given by:

$$\Delta\mathcal{O}(L) = \mathcal{O}(L) - \mathcal{O}_{\mathrm{IV}} = \left(\frac{1}{L^3} \sum_{\mathbf{k}}{}' - \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \right) \int \frac{dk_0}{2\pi} f_{\mathcal{O}}(k_0, \mathbf{k}, \ldots)$$

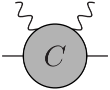
- The integrand $f_{\mathcal{O}}(k_0, \mathbf{k}, \ldots)$ depends on the observable and all scales
- Soft photons travel far: Expand in small $|\mathbf{k}| = \frac{2\pi|\mathbf{n}|}{L} \implies$ expansion in L

$$\Delta\mathcal{O}(L) = C_0 + C_{\log} \log m_P L + C_1 \frac{1}{m_P L} + C_2 \frac{1}{(m_P L)^2} + \ldots$$

The Compton scattering amplitude

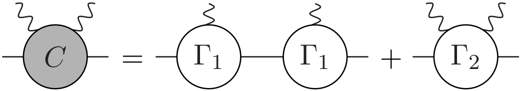
- Need to define kernels: Compton scattering amplitude

$$C_{\mu\nu}(p,k,q) =$$



$$\lim_{p^2 \to -m_{P,0}^2} C_{\mu\nu}(p,k,-k) = e^2 \int \mathrm{d}^4x\, e^{-ik\cdot x}\, \langle P, \mathbf{p}|\, T\left\{J_\mu(x) J_\nu(0)\right\} |P, \mathbf{p}\rangle$$

- Step 1: Decompose into irreducible vertex functions $\Gamma_1 = \Gamma_\mu$, $\Gamma_2 = \Gamma_{\mu\nu}$



- Amplitude $C_{\mu\nu}(p,k,q)$ satisfies Ward identities:
  - Γ_μ and $\Gamma_{\mu\nu}$ must satisfy them as well, but arbitrary separation!

Decomposing vertex functions

- Step 2: Form-factor decomposition (structure-dependence!)

$$\Gamma_\mu(p,k) = (2p+k)_\mu\, F(k^2,(p+k)^2,p^2) + k_\mu\, G(k^2,(p+k)^2,p^2)$$

- Contains both on-shell and off-shell dependence

$$F^{(1,0,0)}(0,-m_P^2,-m_P^2) \equiv F'(0) = -\langle r_P^2\rangle/6$$

- $F^{(0,0,n)}(0,-m_P^2,-m_P^2)$: Unphysical derivative! $\longrightarrow$ Must always cancel in the end!
- How must they cancel, and what about $G(k^2,(p+k)^2,p^2)$?

Decomposing vertex functions

- Step 3: Use Ward identities, e.g.

$$k_\mu \Gamma^\mu(p,k) = D(p+k)^{-1} - D(p)^{-1}$$

- Define full propagator ($Z(p^2)$: z_n [BMW 2015; RM-123/Soton 2017])

$$D(p) = \frac{Z(p^2)}{p^2 + m_P^2}$$

- Ward identity yields G as a function of F and

$$F(0, p^2, -m_P^2) = F(0, -m_P^2, p^2) = Z(p^2)^{-1}$$

- Example relation: $z_1 = F^{(0,0,1)}(0, -m_P^2, -m_P^2)$
- Unphysical derivative! $\longrightarrow$ Must always cancel in the end!
- Equivalently: We could put all non-physical quantities to zero directly

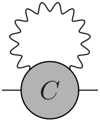
$$F(k^2, (p+k)^2, p^2) \to F(k^2) = 1 + k^2 F'(0) + \dots$$
$$Z(p^2) \to 1$$

The k_0-integral

- Where are we?

$$\Delta\mathcal{O}(L) = \mathcal{O}(L) - \mathcal{O}_{\mathrm{IV}} = \left(\frac{1}{L^3} \sum_{\mathbf{k}}{}' - \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \right) \int \frac{dk_0}{2\pi} f_{\mathcal{O}}\left(k_0, \mathbf{k}, \ldots\right)$$

- Step 4: Do k_0-integral and expand integrand in $1/L$ via $\mathbf{k} = \frac{2\pi\mathbf{n}}{L}$

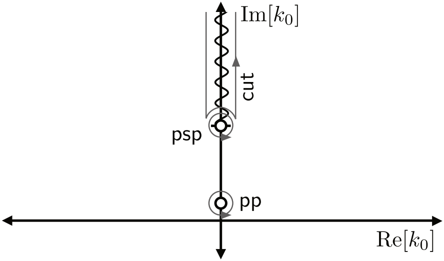


$$= \left(\frac{1}{L^3} \sum_{\mathbf{k}}{}' - \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \right) \int \frac{dk_0}{2\pi}$$

$$\times \left\{ \frac{\Gamma_\mu(p,k)\, Z\left((p-k)^2\right) \Gamma_\mu(p-k,-k)}{k^2\left[(p-k)^2 + m_P^2\right]} + \frac{1}{2} \frac{\Gamma_{\mu\mu}(p,k,-k)}{k^2} \right\}$$

- Poles: Photon, Pseudocalar

The k_0-integral



- The poles are not enough! Branch-cut on the imaginary axis

$$\int \frac{dk_0}{2\pi} = \sum_{\text{poles}} + \int_{\text{cut}} \frac{dk_0}{2\pi}$$

- Smooth function on cut: add/subtract zero-mode $\mathbf{k} = 0$ in sum

$$\left(\frac{1}{L^3} \sum_{\mathbf{k}}{}' - \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \right) \int_{\text{cut}} \frac{dk_0}{2\pi} \overset{\text{Poisson}}{=} -\frac{1}{L^3} \int_{\text{cut}} \frac{dk_0}{2\pi} \bigg|_{\mathbf{k}=0} + \mathcal{O}(e^{-m_P L})$$

- Branch-cut: Specific $1/L^3$ term from $\mathrm{QED_L}$ prescription

Finite-size effects in the mass

- Can use our knowledge of the Compton scattering amplitude decomposition to give $\Delta m_P^2(L)$ (c_j finite-size coefficients)

$$\Delta m_P^2(L) = e^2 m_{P,0}^2 \Bigg\{ \frac{c_2}{4\pi^2 m_{P,0} L} + \frac{c_1}{2\pi (m_{P,0} L)^2} + \frac{\langle r_P^2 \rangle c_0}{3 m_{P,0} L^3} + \frac{\mathcal{C}}{(m_{P,0} L)^3} + \mathcal{O}\left[\frac{1}{(m_{P,0} L)^4}, e^{-m_{P,0} L} \right] \Bigg\}$$

- Leading two terms: point-like ([Davoudi, Savage 2014; BMW 2015; RM-123/Soton 2017])
- Structure-dependence the same as in NRsQED! [Davoudi, Savage 2014]
- Branch-cut: Specific to $\mathrm{QED_L}$ (not in $\mathrm{QED_C}$ [Lucini, Patella, Ramos, Tantalo 2016])
- Need $\mathcal{C}$ to make a prediction:
  1. Defined in terms of Compton tensor integrated to infinity
  2. Can cancel other contributions at order $1/L^3$
  3. For the mass: $\mathcal{C} > 0$

Our method

- Model-independent and relativistic set-up, including structure-dependence
- Given form factor decomposition, we can stop at any order
- Everything depends on finite-volume coefficients c_j
- Branch-cut specific at order $1/L^3$ in $\mathrm{QED_L}$
- NB: Approach relies on power-law/logarithmic FSEs
  $\implies$ would not work for $\mathrm{QED_M}$

$\longrightarrow$ How can we now use what we have learned?

Leptonic decays

- Infrared-divergent process:

$$\Gamma\left(P^- \to \ell^- \nu_\ell[\gamma]\right) = \Gamma_0 + \Gamma_1(\Delta E_\gamma)$$

- RM-123/Soton strategy 2015: Add and subtract universal (point-like) Γ_0^{uni}

$$\Gamma_0 + \Gamma_1(\Delta E_\gamma) = \lim_{L\to\infty}[\Gamma_0(L) - \Gamma_0^{\mathrm{uni}}(L)] + \lim_{m_\gamma\to 0}[\Gamma_0^{\mathrm{uni}}(m_\gamma) + \Gamma_1(m_\gamma, \Delta E_\gamma)]$$

- RM-123/Soton 2017: $\Gamma_0^{\mathrm{uni}}(L)$ calculated to give

$$\Gamma_0(L) - \Gamma_0^{\mathrm{uni}}(L) \sim \mathcal{O}\left(\frac{1}{L^2}\right)$$

- Our proposal: Replace $\Gamma_0^{\mathrm{uni}}(L)$ by

$$\Gamma_0^{(n)}(L) = \Gamma_0^{\mathrm{uni}}(L) + \sum_{j=2}^{n} \Delta\Gamma_0^{(j)}(L)$$

- $\Delta\Gamma_0^{(j)}(L)$ are here the FSEs of order $1/L^j$, containing both point-like and structure terms

Leptonic decays

- The residual volume-scaling is thus

$$\Gamma_0(L) - \Gamma_0^{(n)}(L) \sim \mathcal{O}\left(\frac{1}{L^{n+1}}\right)$$

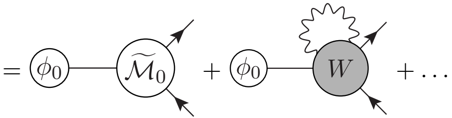
- Define the dimensionless FV function $Y^{(n)}(L)$ as

$$\Gamma_0^{(n)}(L) = \Gamma_0^{\mathrm{tree}}\left[1 + 2\frac{\alpha}{4\pi}\, Y^{(n)}(L)\right] + \mathcal{O}\left(\frac{1}{L^{n+1}}\right)$$

- NB: $Y^{(1)}(L) = Y(L)$ of [RM-123/Soton, 2017] in different approach

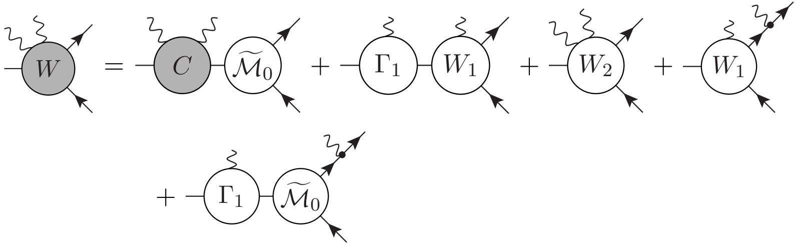
- Euclidean correlator for the decay $P^- \to \ell^- \nu_\ell$

$$C_W^{rs}(p, p_\ell) = \int \mathrm{d}^4 z\, e^{ipz}\, \langle \ell^-, \mathbf{p}_\ell, r; \nu_\ell, \mathbf{p}_{\nu_\ell}, s|\, \mathrm{T}[\mathcal{O}_W(z)\phi^\dagger(0)]\, |0\rangle$$



- Need to define kernels: Play the same game

Leptonic decays



- W_1 and W_2 depend on unphysical off-shell derivatives of the decay constant: f_n [RM-123/Soton 2017]
- W_1: $A_1(k^2,(p+k)^2)$, $V_1(k^2,(p+k)^2)$, $H_{1,2}(k^2,(p+k)^2)$: appear in $P^- \to \ell^- \nu_\ell \gamma^{(*)}$
  - On-shell: $F_A^P = A_1(0,-m_P^2)$ and $F_V^P = V_1(0,-m_P^2)$
  - Known from chiral perturbation theory [Bijnens, Ecker, Gasser 1992], lattice [RM-123/Soton 2020], experiment [...] (Discrepancies [RM-123/Soton 2020])
- W_2: Structure-dependence starting at $1/L^4$ from $P^- \to \ell^- \nu_\ell \gamma^{(*)} \gamma^{(*)}$

Finite-size effects

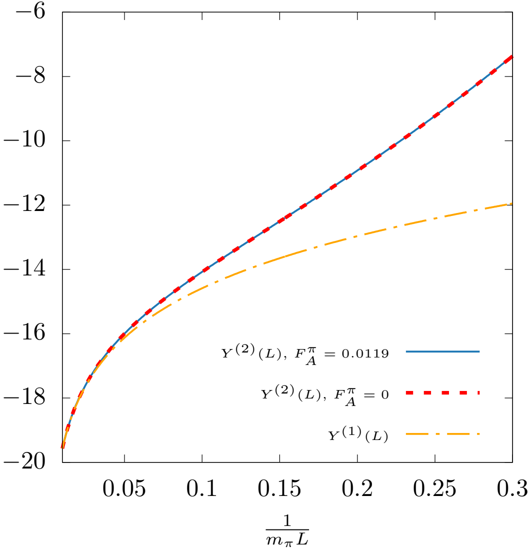
- Diagrams give $Y^{(n)}(L)$ for $n = 2$ as

$$Y^{(2)}(L) = \frac{3}{4} + 4\,\log\left(\frac{m_\ell}{m_W}\right) + \frac{c_3 - 2\,c_3(\mathbf{v}_\ell)}{2\pi} - 2\,A_1(\mathbf{v}_\ell) + 2\,\log\left(\frac{m_W L}{4\pi}\right)$$
$$- 2\,A_1(\mathbf{v}_\ell)\left[\log\left(\frac{m_P L}{4\pi}\right) + \log\left(\frac{m_\ell L}{4\pi}\right)\right] - \frac{1}{m_P L}\left[\frac{(1+r_\ell^2)^2\,c_2 - 4\,r_\ell^2\,c_2(\mathbf{v}_\ell)}{1-r_\ell^4}\right]$$
$$+ \frac{1}{(m_P L)^2}\left[-\frac{F_A^P}{f_P}\,\frac{4\pi\,m_P\,[(1+r_\ell^2)^2\,c_1 - 4\,r_\ell^2\,c_1(\mathbf{v}_\ell)]}{1-r_\ell^4} + \frac{8\pi\,[(1+r_\ell^2)\,c_1 - 2\,c_1(\mathbf{v}_\ell)]}{(1-r_\ell^4)}\right]$$

- All unphysical quantities vanish, i.e. we could put $f_n = z_n = 0$ from the start (as they must at all orders in $1/L$)
- Only F_A^P appears
- Charge radii $\langle r_P^2 \rangle$ cancel between diagrams due to charge conservation
- Point-like agreement with RM-123/Soton: Different representations

$$c_3 = -\pi\,(4 + K_P - 4\,\log 4\pi)$$

Numerical results: Physical Pion



- The $1/L^2$-correction is sizeable
- NB: Point-like $1/L^2$ completely dominates

Convergence of the finite-volume expansion

- The $1/L^3$ correction can be evaluated in a point-like approximation (neglecting the $1/L^3$ structure-dependence and branch-cut):

$$Y^{(3),\mathrm{pt}}(L) = Y^{(2)}(L) + \frac{32\pi^2 c_0 \,(2 + r_\ell^2)}{(m_P L)^3 (1 + r_\ell^2)^3}$$

- For pions one finds at $L/a = 48$

$$Y_\pi^{(1)}(48) \approx -12.33$$

$$Y_\pi^{(2)}(48) \approx -8.93 \longleftarrow \frac{51}{(m_\pi L)^2}$$

$$Y_\pi^{(3),\,\mathrm{pt}}(48) \approx -12.53 \longleftarrow \frac{-209}{(m_\pi L)^3}$$

- Extreme shift in going to $1/L^3$ [see talk by Di Carlo]

  $\longrightarrow$ Large structure-dependence/branch-cut?

- We defined all necessary kernels to evaluate $1/L^3$

- Branch-cut situation different from the self-energy case

Convergence of the finite-volume expansion

- What about the higher-order point-like terms?

$$Y^{(4),\mathrm{pt}}(L) - Y^{(3),\mathrm{pt}}(L) = 0$$

$$Y^{(5),\mathrm{pt}}(L) - Y^{(4),\mathrm{pt}}(L) = -\frac{4\pi^4\, c_{-2}\left(r_\ell^{14} + 9r_\ell^{12} + 37r_\ell^{10} + 93r_\ell^{8} + 163r_\ell^{6} + 1051r_\ell^{4} + 2871r_\ell^{2} - 385\right)}{3\left(r_\ell^2+1\right)^7 (m_P L)^5}$$

$$Y^{(6),\mathrm{pt}}(L) - Y^{(5),\mathrm{pt}}(L) = 0$$

$$Y^{(7),\mathrm{pt}}(L) - Y^{(6),\mathrm{pt}}(L) = \frac{8\pi^6\, c_{-4}}{9\left(r_\ell^2+1\right)^{11}(m_P L)^7}\left\{r_\ell^2\left[7\left(r_\ell^{12} + 13r_\ell^{10} + 79r_\ell^{8} + 299r_\ell^{6} + 794r_\ell^{4} + 1586r_\ell^{2} + 1998\right)r_\ell^8 + 9802r_\ell^6 + 99027r_\ell^4 + 323799r_\ell^2 - 63835\right] - 15111\right\}$$

- However, $c_{-2j} = 0$ for all j

$\Longrightarrow$ No point-like contributions through order $1/L^7$

- Structure-dependence can still appear, but cf. exponential FSEs...
- Same story for mass:

$$\Delta m_P^2(L) = \ldots + e^2 m_P^2\left\{\frac{\pi^2\, c_{-2}}{2\,(m_P L)^5} - \frac{2\pi^4 c_{-4}}{(m_P L)^7} + \frac{15\pi^6\, c_{-6}}{2\,(m_P L)^9}\right\}$$

Conclusions

- With model-independent principles it is indeed possible to predict FSEs beyond the point-like approximation (only physical form-factors and derivatives appear $\leftarrow$ needed from lattice, experiments, ChPT, ...)
- Our approach: General and easy to go to higher orders (software)

$$\Delta\mathcal{O}(L) = C_0 + C_{\log} \log m_P L + C_1 \frac{1}{m_P L} + C_2 \frac{1}{(m_P L)^2} + \left(C_3^{\mathrm{pole}} + C_3^{\mathrm{cut}}\right) \frac{1}{(m_P L)^3} + C_4 \frac{1}{(m_P L)^4} + \dots$$

- Peculiarity in $\mathrm{QED_L}$: Branch-cut terms appear at order $1/L^3$
- Crucial to understand branch-cuts and/or estimate them for $1/L^3$ and beyond
  1. Self-energy
  2. Leptonic decays
  3. Hadronic vacuum polarisation
- Things for the future: Semi-leptonic decays, $K \to \pi\pi$, ...