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Charged hadrons in a finite box

Agostino Patella CERN & Plymouth University

based on:

B. Lucini, AP, A. Ramos, N. Tantalo, Charged hadrons in local finite-volume QED+QCD with C^{*} boundary conditions, arXiv:1509.01636.

Lattice QCD



- A regularization of QCD (it is QCD, not a model of QCD). The lattice spacing a is the UV cutoff.
- The only known consistent way to define QCD at all energy scales: from the high-energy perturbative regime all the way down to pion physics.
- When restricted to a finite box, suitable for numerical calculation of the path integral.
- Limits to be taken in numerical calculations

 $a
ightarrow 0 \; , \qquad L
ightarrow \infty$

Isospin-breaking effects

- Most numerical simulations neglect isospin-breaking effects (i.e. they treat the u and d quarks as undistinguishable).
- The isosymmetric limit is a very good approximation of the real world. Yet, isospin breaking effects are necessary to explain the stability of matter as we know it.
- Two equally-important sources of isospin breaking effects:

$$rac{m_u - m_d}{M_p} \simeq 0.3\% \qquad lpha_{em} = 0.7\% \qquad rac{M_n - M_p}{M_n} \simeq 0.1\%$$

- Lattice QCD+QED provides a way to calculate isospin breaking effects from first principles.
- Is this relevant? FLAG world average, isosymmetric limit:

 $F_K/F_\pi = 1.194(5) \sim 0.4\%$ $F_+^{K\pi} = 0.9661(32) \sim 0.3\%$

Isospin breaking corrections, as estimated in χ PT:

$$F_{K}/F_{\pi} \sim 1\%$$
 $F_{+}^{K\pi} \sim [0.5, 3]\%$

Antonelli *et al.*, An Evaluation of $|V_{us}|$ and precise tests..., Eur.Phys.J. C69 (2010) 399-424. Cirigliano *et al.*, Kaon Decays in the Standard Model, Rev.Mod.Phys. 84 (2012) 399.

Two ways for QCD+QED on the lattice

Expand observables with respect to α_{em} and simulate QCD only. de Divitiis et al. (RM123), Leading isospin breaking effects on the lattice, Phys.Rev. D87 (2013) 11, 114505. Carrasco et al., QED Corrections to Hadronic Processes in Lattice QCD, Phys.Rev. D91 (2015) 7, 074506.

E.g. Cottingham formula for the mass correction:

$$\Delta m = -\frac{e^2}{4m} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2} \int d^4x \ e^{-ikx} \langle h | \mathsf{T}\{j_\mu(x)j_\mu(0)\} | h \rangle_{c,QCD} + O(e^4)$$

Pros: Only $O(\alpha_{em}^0)$ observables.

Cons:

Complex observables (e.g. a 4-point functions for mass correction). Fermionic disconnected diagrams.

Two ways for QCD+QED on the lattice

Simulate QCD+QED on the lattice.

Borsanyi *et al.* (BMW), Ab initio calculation of the neutron-proton mass difference, Science 347 (2015) 1452-1455.



Pros: Simpler observables (e.g. 2-point functions for mass correction).

Cons:

Signal is typically $O(\alpha_{em})$.

QCD+QED in finite volume

If we want to measure the mass of the proton on the lattice, we need to be able to put a nonzero charge in a finite box.

> On a torus with periodic boundary conditions, the Gauss law forbids a nonzero charge.

$$\partial_k E_k(x) = \rho(x) \quad \Rightarrow \quad Q = \int d^3 x \ \rho(t, \mathbf{x}) = \int d^3 x \ \partial_k E_k(t, \mathbf{x}) = 0$$

I want to explore an old idea...

Wiese, C periodic and G periodic QCD at finite temperature, Nucl. Phys. B375, 45 (1992). Kronfeld, Wiese, SU(N) gauge theories with C periodic boundary conditions. 1. Topological structure, Nucl. Phys. B357 (1991) 521.

Kronfeld, Wiese, SU(N) gauge theories with C periodic boundary conditions. 2. Small volume dynamics, Nucl. Phys. B401 (1993) 190.

Polley, Boundaries for $SU(3)(C) \times U(1)$ -el lattice gauge theory with a chemical potential, Z. Phys. C59, 1993.

 C* boundary conditions provide a framework to describe a certain class of electrically-charged states in a rigorous way. This class is wide enough to include most of the spectroscopic applications.

C* boundary conditions

$$A_{\mu}(x + L\mathbf{k}) = -A_{\mu}(x) \qquad \psi(x + L\mathbf{k}) = C^{-1}\bar{\psi}^{T}(x) \qquad \bar{\psi}(x + L\mathbf{k}) = -\psi^{T}(x)C$$



Electric flux can escape the torus and flow into the mirror charge

$$Q(t) = \int d^3 x \ \rho(t, \mathbf{x}) = \int d^3 x \ \partial_k E_k(t, \mathbf{x}) \neq 0$$

Overview

- Other ways to deal with Gauss law in a finite box
- Symmetries of QED with C* boundary conditions (QED_C)
- ► Some finite-volume effects in QED_C

Charge particles and zero modes

$$A_{\mu}(x) \rightarrow A_{\mu}(x) + rac{2\pi n_{\mu}}{L} , \quad \psi(x) \rightarrow e^{rac{2\pi i n_{\mu} \times \mu}{L}} \psi(x)$$

$$\langle \psi(x)\bar{\psi}(y) \rangle \to e^{\frac{2\pi i n \mu(x-y)\mu}{L}} \langle \psi(x)\bar{\psi}(y) \rangle \quad \Rightarrow \quad \langle \psi(x)\bar{\psi}(y) \rangle = 0$$

Charge particles and zero modes

 $QED + Feynman gauge \Rightarrow$ electron two-point function $\langle \psi(x)\bar{\psi}(y) \rangle$ However in finite volume, large gauge transformations *survive* a local gauge fixing

$$A_{\mu}(x)
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Large gauge transformations shift the zero-modes of the photon field.

Various constraints on some momentum components of the photon field. e.g. Hayakawa, Uno, QED in finite volume and finite size scaling effect on electromagnetic properties of hadrons, Prog. Theor. Phys. 120 (2008) 413-441.

$$\int d^4x \; A_\mu(x) = 0 \;,\; \text{or} \quad -\frac{\pi}{L} < \int d^4x \; A_\mu(x) < \frac{\pi}{L} \;,\; \text{or} \quad \int d^3x \; A_\mu(t,x) = 0$$

Widely used, but the constraint is non-local.

- Give a small mass to the photon. Endres, Shindler, Tiburzi, Walker-Loud, Massive photons: an infrared regularization scheme for lattice QCD+QED, arXiv:1507.08916 [hep-lat]. Interesting recent proposal, local QFT.
- C* boundary conditions: the gauge field is antiperiodic (no zero-mode). Local QFT.

Locality

Microcausality

$$[A(t, \mathbf{x}), B(t, \mathbf{y})] = 0$$
 for $\mathbf{x} \neq \mathbf{y}$

- Equations of motion are local differential equations: time evolution of fields in x is determined only by the value of fields in an arbitrarily small neighbourhood of x.
- Local action

$$Z = \int_{\substack{\text{b.c.'s}\\\text{local constraints}}} e^{-S} , \qquad S = \int d^4x \ \mathcal{L}(x)$$

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Locality is a core property of QFT. It guarantees, e.g.

- Renormalizability by power counting
- Volume-independence of renormalization constants
- Operator product expansion
- Effective-theory description of long-distance physics
- Symanzik improvement program

▶ ...

Symmetries of QED_C

$$\begin{aligned} \mathcal{L} &= \frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \sum_{f} \bar{\psi}_{f} (\mathcal{D}_{f} + m_{f}) \psi_{f} \\ A_{\mu} (x + L\mathbf{k}) &= -A_{\mu} (x) \qquad \psi(x + L\mathbf{k}) = C^{-1} \bar{\psi}^{T} (x) \qquad \bar{\psi}(x + L\mathbf{k}) = -\psi^{T} (x) C \end{aligned}$$

Translations: momentum P is conserved.

Charge conjugation: C is conserved. A translation by Lk concides with charge conjugation

$$e^{iLP_k} = C$$

Because of the b.c.s, and eigenstate of the P_k is automatically and eigenstate of C. Periodic states have C = +1 and antiperiodic states have C = -1.

- Parity: P is conserved.
- Flavour symmetry is partially broken:

$$\psi_f \to e^{i\alpha}\psi_f \qquad \bar{\psi}_f \to e^{-i\alpha}\bar{\psi}_f$$

leaves the b.c.s invariant iff $e^{i\alpha}=\pm 1.~(-1)^{F_f}$ is conserved.

Electric charge is a linear combination of flavour charges

$$Q = \sum_{f} n_{f} q_{el} F_{f}$$

Electric charge Q is not conserved but $(-1)^{Q/q_{el}}$ is.

Quantum numbers in QED_C

For simplicity, we consider only electrons and muons $(q_{el} = 1)$.

$$[P_k, C] = [P_k, (-1)^{F_f}] = [C, (-1)^{F_f}] = [P_k, (-1)^Q] = [C, (-1)^Q] = 0$$

Consider a Hamiltonian eigenstate with

$$\mathbf{P} = \mathbf{0}$$
 $C = +1$ $(-1)^{F_e} = -1$ $(-1)^{F_{\mu}} = 1$ $(-1)^{Q} = -1$

This state is a mixture of states with

 $F_e = \pm 1, \pm 3, \pm 5, \ldots$ $F_\mu = 0, \pm 2, \pm 4, \ldots$ $Q = \pm 1, \pm 3, \pm 5, \ldots$

The ground state in this channel in the infinite-volume limit becomes the *C*-even combination of a single electron and a single positron.

Finite-volume charged states = States with $(-1)^Q = -1$

Messages:

- Ther residual symmetry is enough to construct single-electron and single-muon states, but not e.g. two-electron states.
- The spurious mixing decays exponentially in the $L \rightarrow \infty$ limit.

Charge violation in QED_C

In infinite volume

Charge violation in QED_C

In finite volume with C* boundary conditions



Charge violation in QED_C



With C* b.c.s the following transitions are allowed

 $\Delta F_f = 0 \mod 2$, $\Delta Q = 0 \mod 2$

A single-electron state can mix with a three-electron state but *not* with a single-photon state or a single-muon state

 Flavour-violation processes involve flavourful particles (which are massive) traveling around the torus and they are therefore exponentially suppressed in the volume

Conservation of each flavour number is violated in units of 2

$$Q = \sum_{f}^{N_f} q_f F_f \qquad F = \sum_{f}^{N_f} F_f \qquad B = \frac{F}{3} \qquad \Delta F_f = 0 \mod 2$$

If L is large enough, only colourless particles can travel around the torus

 $\Delta Q = 0 \mod 2$, $\Delta B = 0 \mod 2$, $\Delta F = 0 \mod 6$

- Pseudoscalar mesons (the pions, the kaons, D and B) cannot mix with lighter states and are therefore stable
- The proton cannot mix with states having B = 0 and it remains the lightest state with $(-1)^B = -1$
- ▶ The neutron cannot mix with states having B = 0 or $Q = \pm 1$ and it remains the lightest state with $(-1)^B = -1$ and $(-1)^Q = 1$
- Flavour-violation processes involve flavourful particles (which are massive) traveling around the torus and they are therefore exponentially suppressed in the volume



$$C(t; L) = \sum_{\mathbf{x}} \langle \Xi_{+}(t, \mathbf{x})^{\dagger} \Xi_{+}(0) \rangle = C_{
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The mixing with lighter states is generated by a loop of strange hadrons wrapping around the torus, that cannot go on-shell \Rightarrow exponential suppression

$$\begin{aligned} |C_{< M_{\Xi^{\pm}}}(t;L)| &\leq \exp\left\{-2\mu L + \mathcal{O}(\ln L)\right\} e^{-tM_{p}} \\ \mu &= \left[M_{K^{\pm}}^{2} - \left(\frac{M_{\Xi^{-}}^{2} - M_{\Lambda^{0}}^{2} + M_{K^{\pm}}^{2}}{2M_{\Xi^{-}}}\right)^{2}\right]^{1/2} \end{aligned}$$



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$$\begin{aligned} |C_{$$

$$\frac{\Delta m(L)}{m} = \frac{e^2}{4\pi} \left\{ \frac{q^2 \xi(1)}{2mL} + \frac{q^2 \xi(2)}{\pi (mL)^2} - \frac{1}{4\pi m L^4} \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell} (2\ell)!}{\ell! L^{2(\ell-1)}} \mathcal{T}_{\ell} \xi(2+2\ell) \right\} + \dots$$

▶ Very similar to BMW formula for QED_L, but some important differences

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• The boundary conditions are encoded in the generalized zeta function $\xi(s)$

$$\xi(s) = \sum_{\mathbf{n}\neq \mathbf{0}} \frac{(-1)^{\sum_{j \in C} n_j}}{|\mathbf{n}|^s}$$

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- ▶ Non-universal (i.e. spin- and structure-dependent) corrections are order $1/L^4$. Notice that these are of order $1/L^3$ in QED_L. This extra suppression is a direct consequence of locality.

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- The coefficients of the 1/L and $1/L^2$ are completely fixed by charge and mass (universal)
- Non-universal (i.e. spin- and structure-dependent) corrections are order 1/L⁴. Notice that these are of order 1/L³ in QED_L. This extra suppression is a direct consequence of locality.
- The non-universal corrections are related to the forward Compton amplitude for the scattering of a soft photon on the hadron at rest

$$\mathcal{T}_\ell = \left. rac{d^\ell}{d(\mathbf{k}^2)^\ell} \, T^\mu_\mu(|\mathbf{k}|,\mathbf{k})
ight|_{\mathbf{k}=0}$$

Summary

- QCD+QED with C* boundary conditions is a local QFT in finite volume, and provides a framework to describe a certain class of electrically-charged states in a rigorous and gauge-invariant way.
- ▶ C* boundary conditions partially break flavour (and charge) conservation. F_f is not conserved but $(-1)^{F_f}$ is.
- ► Several interesting states are not affected by the finite-volume mixing (p, n, π^{\pm} , K^{\pm} , K_0 , Λ^0 , D^{\pm} , D^0 , D_s^{\pm} , B^{\pm} , B^0 , Σ^{\pm} , Σ^0)
- Some states are affected by the finite-volume mixing, e.g. Ξ⁻ or Ω⁻, but the mixing with lighter states is exponentially suppressed with the volume (with a generally large exponent).
- ▶ Non-unversal finite-volume corrections to the masses of stable charged hadrons are $1/L^4$ rather than $1/L^3$ (thanks to locality).
- Operator mixing is not affected by breaking of flavour symmetry (thanks to locality).
- QCD+QED with C* boundary conditions can be formulated on the lattice with a compact U(1). Charged states can be described in a gauge-invariant way.
- QCD+QED with C* boundary conditions has a mild sign problem with Wilson fermions (but not with chiral fermions), analogous to the one of a single flavour with periodic boundary conditions.

What's next

- \blacktriangleright We are working on the numerical implementation of QCD+QED with C* boundary conditions.
- We will start from pilot studies (QED in isolation, electroquenched aproximation, study of finite volume effects...).
- If we convince ourselves that this is the best approach, we will consider simulations closer to physics.
- We would like to derive a finite-volume formula for the matrix elements, in analogy to the one for the mass.

Backup slides

Dirac interpolating operator:

$$\Psi(t,\mathbf{x}) = e^{-i \int d^3 y \, \Phi(\mathbf{y}-\mathbf{x}) \partial_k A_k(t,\mathbf{y})} \psi(t,\mathbf{x})$$

where $\Phi(x)$ is the electric potential of a unit charge in a box with C^{*} b.c.'s

$$\partial_k \partial_k \Phi(\mathbf{x}) = \delta^3(\mathbf{x})$$

 $\Phi(\mathbf{x} + L\mathbf{k}) = -\Phi(\mathbf{x})$

Nontrivial fact: such an electric potential exists!

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• $\Psi(t, \mathbf{x})$ is odd under the global gauge transformation

$$egin{aligned} & A_k(t, \mathbf{x})
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Nontrivial fact: such an electric potential exists!

$$\int d^3x \ \Psi(t,{\bf x})|0\rangle$$

This state has the following properties

invariant under infinitesimal gauge transformations

- ▶ *C* = +1
- ▶ $(-1)^Q = -1$

The charged-particle mass is defined in a gauge-invariant fashion:

$$\langle \Psi(t, \mathbf{x}) \overline{\Psi}(0)
angle \simeq A(\mathbf{x}) e^{-tm}$$