Humboldt/DESY lattice seminar

Electrically-charged hadrons in a finite box

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*Charged hadrons in local finite-volume QED+QCD with $C^*$ boundary conditions*  
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**openQxC code**  
Isabel Campos, Martin Hansen, Marina Marinkovic, Patrick Fritzsch, AP, Alberto Ramos, Nazario Tantalo
Motivations

- In the real world up and down quarks have different masses and electric charges.

- Isospin-breaking effects are typically a few percent effects:

\[
\frac{m_u - m_d}{M_p} \simeq 0.3\% \quad \alpha_{\text{EM}} \approx 0.7\% \quad \frac{M_n - M_p}{M_n} \simeq 0.1\%
\]

- From FLAG16 [Aoki et al., arXiv:1607.00299] and [PDG review, Rosner et al., 2016], [Cirigliano et al., Rev. Mod. Phys. 84, 399 (2012)]

\[
\begin{align*}
 f_{\pi^\pm} &= 130.2(1.4) \text{ MeV} \quad \text{err} = 1\% \\
f_{K^\pm} &= 155.6(0.4) \text{ MeV} \quad \text{err} = 0.3\% \\
f_+(0) &= 0.9704(24)(22) \quad \text{err} = 0.5\%
\end{align*}
\]

\[
\begin{align*}
\delta_{\text{QED}}^{\chi_{\text{PT}}}(\pi^- \to \ell^- \bar{\nu}) &= 1.8\% \\
\delta_{\text{QED}}^{\chi_{\text{PT}}}(K^- \to \ell^- \bar{\nu}) &= 1.1\% \\
\delta_{\text{QED}}^{\chi_{\text{PT}}}(K \to \pi \ell \bar{\nu}) &= [0.5, 3]\%
\end{align*}
\]
Part I

Theoretical aspects of QED in finite volume
No charged states in a periodic box

In a finite box with periodic boundary conditions, Gauss law forbids states with nonzero charge

\[ eQ = e \int d^3x \ j_0(t, x) = \int d^3x \ \partial_k E_k(t, x) = 0. \]

If we want to calculate the mass of the proton, we would like to be able to have a single proton in our lattice (rather than a proton-antiproton system).

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- Break translational invariance in space in various ways, e.g. introduce a static charge in a point. The effect of the static charge does not vanish in the infinite volume.
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- Introduce a classical uniform charge density. It seems that it is impossible to contract a gauge-invariant momentum operator. Theoretically poorly understood (nothing is published on this topic). Also the zero-mode dynamics generates an irregular perturbation theory in finite volume (e.g. powers of \( e \) in masses).
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- **Add a mass to the photon (and break gauge invariance).** In Minkowski spacetime, the theory is not manifestly unitary (negative-norm states). In Euclidean space, the Hamiltonian is not hermitean. One needs to project over the correct physical Hilbert space. Also \( m \to 0 \) and \( L \to \infty \) limits do not commute.
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- Break locality in various ways by chopping and restricting some Fourier modes of the photon field. Absence of transfer matrix, break down of renormalization by local counterterms.
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- Break locality in various ways by chopping and restricting some Fourier modes of the photon field. Absence of transfer matrix, break down of renormalization by local counterterms.
- Use C-parity (aka $C^*$) boundary conditions in the spatial direction.
C* boundary conditions

\[ A_\mu(x + Lk) = -A_\mu(x) \quad \psi(x + Lk) = C^{-1}\bar{\psi}^T(x) \quad \bar{\psi}(x + Lk) = -\psi^T(x)C \]

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

\[ Q(t) = \int d^3x \, \rho(t, x) = \int d^3x \, \partial_k E_k(t, x) \neq 0 \]
\[ \mathcal{L} = \frac{1}{4} F_{\mu \nu} F_{\mu \nu} + \sum_f \bar{\psi}_f (\not{D}_f + m_f) \psi_f \]

\[ A_\mu(x + Lk) = -A_\mu(x) \quad \psi(x + Lk) = C^{-1} \bar{\psi}^T(x) \quad \bar{\psi}(x + Lk) = -\psi^T(x)C \]

- **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:
  \[ \psi_f \to e^{i\alpha} \psi_f \quad \bar{\psi}_f \to e^{-i\alpha} \bar{\psi}_f \]
  
  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.
Flavour violation in Q[C+E]D

\[ \sum_x \langle [\Xi^- (t, x)]^\dagger \Xi^- (0) \rangle = C_{< M_{\Xi^-} (t; L)} + C_{\geq M_{\Xi^-} (t; L)} \]

\[ C_{< M_{\Xi^-} (t; L)} \simeq A(L) e^{-tM_{\Xi^-}(L)} + \ldots \quad C_{\geq M_{\Xi^-} (t; L)} \simeq B(L) e^{-tM_{\Xi^-}(L)} + \ldots \]
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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 ⇒ exponential suppression

\[ |C_{< M_{\Xi^-}} (t; L)| \leq \exp \{ -2 \mu L + O(\ln L) \} e^{-t M_p} \]

\[ \mu = \left[ M_{K^\pm}^2 - \left( \frac{M_{\Xi^-}^2 - M_{\Lambda^0}^2 + M_{K^\pm}^2}{2M_{\Xi^-}} \right)^2 \right]^{1/2} \]
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

\[
|C_{<M_{\Xi^-}}(t; L)| \leq \exp\left\{-2\mu L + O(\ln L)\right\} e^{-tM_p(L)} \approx 10^{-10} \times e^{-tM_p} \quad \text{for } M_\pi L = 4
\]

\[
\mu = \left[M_{K^\pm}^2 - \left(\frac{M_{\Xi^-}^2 - M_{\Lambda^0}^2 + M_{K^\pm}^2}{2M_{\Xi^-}}\right)^2\right]^{1/2}
\]
Flavour violation in $\mathbb{Q[C+E]}D_\mathbb{C}$

- Renormalization of composite operators is not affected by the flavour violation due to the boundary conditions.

- In a local theory, the divergent part of the renormalization constants does not depend on the volume (this is why renormalization constants can be calculated at finite volume and used in infinite volume).

- The divergent part of the renormalization constants in $\mathbb{Q[C+E]}D_\mathbb{C}$ is the same as in infinite volume and is therefore insensitive of the flavour breaking.
In infinite volume it is possible to define gauge-invariant interpolating operators for charged states. These operators must be non-local, however they can be chosen to be local in time.
Interpolating operators for electrically-charged states

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- In covariant gauge, the Hilbert space includes non physical states (positive-norm longitudinal states and negative-norm states). One needs to project by hand on the physical Hilbert space. E.g. in the Gupta-Bleuler formalism (in Heisenberg picture)

\[ \partial_\mu A^\dagger_\mu(x)|\psi\rangle = 0 \]
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- In gauge-invariant quantization, the Hilbert space contains only positive-norm state. Physical states are selected by requiring gauge invariance, i.e. they are automatically generated by gauge-invariant operators.
Interpreting operators for electrically-charged states

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- In gauge-invariant quantization, the Hilbert space contains only positive-norm state. Physical states are selected by requiring gauge invariance, i.e. they are automatically generated by gauge-invariant operators.

- With minimal effort, we can construct gauge-invariant interpolating operators for charged states. So why should we bother to fix the gauge?
Interpolating operators for electrically-charged states

- The mass of a charged particle is gauge invariant. Obvious yet non trivial in covariant gauge...
Interpolating operators for electrically-charged states

▶ The mass of a charged particle is gauge invariant. Obvious yet non trivial in covariant gauge...

▶ Dirac interpolating operator in infinite volume:

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

where \( \Phi(x) \) is the electric potential of a unit charge

\[ \partial_k \partial_k \Phi(x) = \delta^3(x) \]
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Dirac interpolating operator in infinite volume:

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\[ \partial_k \partial_k \Phi(x) = \delta^3(x) \]

\( \Psi(t, x) \) is invariant under infinitesimal gauge transformations with a compact support

\[ A_k(t, x) \rightarrow A_k(t, x) + \partial_k \lambda(t, x) \quad \psi(t, x) \rightarrow e^{i \lambda(t,x)} \psi(t, x) \]

\[ e^{-i \int d^3 y \, \Phi(y-x) \partial_k A_k(t,y)} \rightarrow e^{-i \int d^3 y \, \Phi(y-x) \partial_k A_k(t,y)} e^{-i \int d^3 y \, \Phi(y-x) \partial_k \partial_k \lambda(t,y)} = \]

\[ = e^{-i \int d^3 y \, \Phi(y-x) \partial_k A_k(t,y)} e^{-i \lambda(t,x)} \]

\[ \Psi(t, x) \] is charged under global gauge transformations

\[ A_k(t, x) \rightarrow A_k(t, x) \quad \psi(t, x) \rightarrow e^{i \alpha} \psi(t, x) \]

The electron mass is manifestly gauge invariant

\[ M = -\lim_{t \rightarrow \infty} \frac{d}{dt} \ln \int d^3 x \, \langle \Phi(t, x) \bar{\Phi}(0) \rangle \]
Interpolating operators for electrically-charged states

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Interpolating operators for electrically-charged states

- The mass of a charged particle is gauge invariant. Obvious yet non trivial in covariant gauge...

- Dirac interpolating operator in infinite volume:
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  \Psi(t, x) = e^{-\imath \int d^3y \Phi(y-x) \partial_k A_k(t, y)} \psi(t, x)
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  \]
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  A_k(t, x) \rightarrow A_k(t, x) \quad \psi(t, x) \rightarrow e^{i\alpha} \psi(t, x)
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- The electron mass is manifestly gauge invariant
  \[
  M = - \lim_{t \rightarrow \infty} \frac{d}{dt} \ln \int d^3x \langle \Phi(t, x) \tilde{\Phi}(0) \rangle
  \]
Interpolating operators for electrically-charged states

The Dirac interpolating operator can be constructed also in finite volume

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

provided that the Poisson equation has solutions

$$\partial_k \partial_k \Phi(x) = \delta^3(x)$$

The Poisson equation has no solutions on a torus with periodic boundary conditions, while it admits a unique solution with C-parity boundary conditions

$$\Phi(x + Lk) = -\Phi(x)$$
Part II

A simulation code for QCD+QED with C* boundary conditions
Add the U(1) gauge field \( u_\mu(x) \)...

...and its dynamics, i.e. the U(1) gauge action, but also the U(1) component of the fermionic forces (the construction of the MD integrator has to be tweaked as well).

\[
F_\mu(x) = -\partial^U S_f(\phi, U, u) \\
f_\mu(x) = -\partial^u S_f(\phi, U, u)
\]

Couple matter to the U(1) field via the Dirac operator.

Implement \( C^* \) boundary conditions.

A single flavour with \( C^* \) boundary conditions requires the Pfaffian of the Dirac operator, i.e. the fourth-root of \( D^\dagger D \). Implement general rational approximation.

Extend the flag and parameter database, if you know what it is. If you don’t, you are lucky, stay away from it!
$C^*bc$ are trivial enough for the gauge field, but not so for the fermion fields

$$U_\mu(x + L_\rho \hat{\rho}) = U_\mu(x)^*$$

$$\int [d\bar{\psi}] [d\psi] \exp(\bar{\psi}, D[U]\psi) \neq \det D(U)$$

because $\psi$ and $\bar{\psi}$ are not independent fields

$$\psi(x + L\hat{k}) = C^{-1}\bar{\psi}^T(x)$$
**C* boundary conditions**

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\[ \psi(x + L \hat{k}) = C^{-1} \bar{\psi}^T(x) \]

Put \( \psi \) and \( C^{-1} \bar{\psi}^T \) in the same field...

\[ \chi(x) = \begin{pmatrix} \psi(x) \\ C^{-1} \bar{\psi}^T(x) \end{pmatrix} \quad \chi(x + L \hat{k}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \chi \equiv K \chi \]

From the point of view of gauge-transformations, \( \chi \) lives the the \( \Box \oplus \tilde{\Box} \) representation of the gauge group. A little bit of algebra shows that

\[ (\bar{\psi}, D[U] \psi) = - (\chi, KCD[U \oplus U^*] \chi) \]

\[ U \oplus U^* = \begin{pmatrix} U & 0 \\ 0 & U^* \end{pmatrix} \]

\[ \int [d\bar{\psi}] [d\psi] \exp(\bar{\psi}, D[U] \psi) = \text{Pf} KCD[U \oplus U^*] = \left( \det D^\dagger D[U \oplus U^*] \right)^{1/4} \]
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The Dirac operator acts not on a single pseudofermion, but a pair of pseudofermions which are swapped by the boundary conditions. For one of the two, the \( U_\mu(x) \) matrix in the hopping term of the Dirac operator has to be replaced with \( U_\mu^*(x) \). No way!
\[
\left( \det D^\dagger D[U \oplus U^*] \right)^{1/4} \propto \int [d\Phi] [d\Phi^\dagger] \exp \left\{ -\Phi^\dagger (D^\dagger D[U \oplus U^*])^{-1/4} \Phi \right\}
\]

\[
\Phi(x + L\hat{k}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi \equiv K\Phi
\]
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Orbifold construction

\[
\left( \det D^\dagger D[U \oplus U^*] \right)^{1/4} \propto \int \left[ d\tilde{\phi} \right] \left[ d\tilde{\phi}^\dagger \right] \exp \left\{ -\tilde{\phi}^\dagger (D^\dagger D[\tilde{U}])^{-1/4} \tilde{\phi} \right\}
\]

\[
\tilde{U}_\mu(x) = \begin{cases} U_\mu(x) & x \in \text{fundamental lattice} \\ U_\mu^*(x - \hat{L}) & x \in \text{mirror lattice} \end{cases}
\]

\[
\tilde{\phi}(x) = \begin{cases} \Phi_1(x) & x \in \text{fundamental lattice} \\ \Phi_2(x - \hat{L}) & x \in \text{mirror lattice} \end{cases}
\]

1 C* boundary conditions \Rightarrow Periodic boundary conditions
Orbifold construction

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\]

2,3 C* boundary conditions \(\Rightarrow\) Periodic b.c. in 1 + Shifted b.c. in 2,3
Orbifold construction

- Double the lattice in direction 1, and use shifted boundary conditions in directions 2 and 3 if necessary.

- Initialize the gauge field such that $U_\mu(x + L_1 \hat{1}) = U_\mu(x)^*$.

- Draw the momenta such that $\pi_\mu(x + L_1 \hat{1}) = \pi_\mu(x)^*$.

- Replace the MD evolution equation for the momenta with
  \[
  \pi'_\mu(x) = \pi_\mu(x) + \epsilon [F_\mu(x) + F_\mu(x + L_1 \hat{1})^*]
  \]
Orbifold construction

- Double the lattice in direction 1, and use shifted boundary conditions in directions 2 and 3 if necessary.

- Initialize the gauge field such that $U_\mu(x + L_1 \hat{1}) = U_\mu(x)^*$. 

- Draw the momenta such that $\pi_\mu(x + L_1 \hat{1}) = \pi_\mu(x)^*$. 

- Replace the MD evolution equation for the momenta with
  
  $$\pi'_\mu(x) = \pi_\mu(x) + \epsilon [F_\mu(x) + F_\mu(x + L_1 \hat{1})^*]$$

How much do we lose in performance by doubling the lattice?

- The gauge field and momenta get updated twice (in the fundamental and mirror lattice). We lose a factor 2x here.

- In the momentum update, the whole mirror lattice has to be copied into the fundamental lattice. The impact of this operation is unclear at the moment.

- The Dirac operator acts on a single flavour defined on the double lattice, instead than on two flavours defined on the fundamental lattice. The performance is unaffected.

In simulations that are heavily dominated by the inversion of the Dirac operator, the effect of the orbifold construction should be moderate.
Fundamental degree of freedom: $A_\mu(x)$

**Compact action**

\[ u_\mu(x) = e^{iA_\mu(x)} \]

\[ S = \beta_{U(1)} \sum_{x\mu\nu} [1 - \text{tr} u_{\mu\nu}(x)] \]

**Non-compact action**

\[ S = \frac{1}{4e_0^2} \sum_{x\mu\nu} \left[ \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) \right]^2 + \frac{\lambda}{2} \sum_x \left( \sum_\mu \partial_\mu^* A_\mu \right)^2 \]
The Dirac operator is given by

\[ D\psi(x) = (m_0 + 4)\psi(x) + \]

\[ + \frac{1}{2} \sum_\mu \left\{ H_\mu(x)(1 - \gamma_\mu)\psi(x + \hat{\mu}) + H_\mu(x - \hat{\mu})\dagger(1 + \gamma_\mu)\psi(x - \hat{\mu}) \right\} + \]

\[ + \sum_{\mu\nu} \frac{i}{4} \sigma_{\mu\nu} \left[ c_{sw,3} \hat{F}_{\mu\nu}(x) + c_{sw,1} \hat{f}_{\mu\nu}(x) \right] \psi(x) \]

The hopping term contains the U(3) field

\[ H_\mu(x) = U_\mu(x)[u_\mu(x)]^q \]

which depends on the electric charge \( q \) of the field \( \psi \). From the programming point of view, one has to calculate \( H_\mu(x) \) and replace a pointer in the Dirac operator.
We have a beta version of the openQxD code (temporary name!). The testing is at a very advanced stage. What is missing

- Noncompact U(1) action
- Fourier acceleration for the U(1) field
- Combine twisted mass reweighting with the RHMC
- Documentation
- Study the effect of the electric charge on the deflation subspace
Conclusions

▶ When aiming at the percent precision, isospin breaking corrections must be included. Activity in this direction has been growing significantly in the past few years.

▶ QED and QCD are very different theories. Inclusion of QED effects implies a shift in the standard paradigm of lattice simulations.

▶ Description of charged states in a finite box is somewhat challenging. Effects of nonlocality are not systematically understood. I advocate the use of setups that are theoretically under control.

▶ Numerical calculations of masses are already at an advanced stage from the technical point of view. The challenge ahead is the full calculation of radiative corrections to decay rates.

▶ A simulation code for QCD+QED, based on openQCD, is at a very advanced stage of development. A beta version will be available by the Lattice conference.

Thank you!