Inclusion of isospin breaking effects in lattice simulations

Antonin J. Portelli
(University of Southampton)
What’s new?
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  - update of quark masses and Dashen’s theorem corrections using electro-quenched simulations
  - new insights on finite-volume effects
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  - new full $N_f = 1+1+1$ QCD+QED simulations
  - preliminary results for the baryon octet splittings
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  - new set of $N_f = 1+1+1+1$ full QCD+QED simulations
  - extensive analytical/numerical study of finite-volume effects
  - high precision computation of the hadron spectrum splittings (continuum, infinite volume and physical point extrapolation)
• Motivations
• Update on electro-quenched results
• Lattice QED
• Full QCD+QED simulations
• Isospin splittings in the hadron spectrum
• Summary & outlook
Motivations
Isospin symmetry breaking

- Isospin symmetric world: up and down quarks are particles with identical physical properties.
Isospin symmetry breaking

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<table>
<thead>
<tr>
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<tr>
<td><strong>up</strong></td>
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source: [PDG, 2013]
Isospin symmetry breaking

- Isospin symmetric world: up and down quarks are particles with identical physical properties.

- Isospin symmetry is explicitly broken by:
  - the up and down quark mass difference
    \[ |m_u - m_d|/\Lambda_{QCD} \simeq 0.01 \]
  - the up and down electric charge difference
    \[ \alpha \simeq 0.0073 \]

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source: [PDG, 2013]
Well known experimentally:

\[ M_n - M_p = 1.2933322(4) \text{ MeV} \]

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Nucleon mass splitting

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  source: [PDG, 2013]
- needed for proton stability
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needed for proton stability
determines through \( \beta^- \)-decay the stable nuclide chart

**Source:** [PDG, 2013]
Well known experimentally:

\[ M_n - M_p = 1.2933322(4) \text{ MeV} \]

source: [PDG, 2013]

- needed for **proton stability**
- determines through \( \beta \)-decay the **stable nuclide chart**
- initial condition for **Big-Bang nucleosynthesis**
Dashen’s theorem

- In the SU(3) chiral limit [Dashen, 1969]:

\[ \Delta_{\text{QED}} M_K^2 = \Delta_{\text{QED}} M_\pi^2 + O(\alpha m_s) \]
Dashen’s theorem

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- How large are the corrections? FLAG parametrisation:
  \[ \varepsilon = \frac{\Delta_{\text{QED}} M_K^2 - \Delta_{\text{QED}} M_\pi^2}{\Delta M_\pi^2} \]
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- \( \varepsilon \) is important to determine light quark mass ratios
Update on electro-quenched results
EQ results for the baryon spectrum

EQ results for $\varepsilon$

- [Maltman and Kotchan, 1990]
- [Donoghue et al., 1993]
- [Bijnens, 1993]
- [Baur and Urech, 1996]
- [Bijnens and Prades, 1997]
- [Donoghue and Perez, 1997]
- [Gao et al., 1997]
- [Moussallam, 1997]
- [Duncan et al., 1996] (quenched QCD)
- [RBC-UKQCD, 2007]
- [RBC-UKQCD, 2010]
- [RM123, 2013]
- [BMWc, Q, 2014] (preliminary)
- [MILC, 2014] (preliminary)
EQ results for light quark masses

F. Sanfilippo plenary talk on quark masses: right after this talk
Lattice QED
Non-compact lattice QED

- Naively discretised Maxwell action:

\[ S[A_\mu] = \frac{1}{4} \sum_{\mu,\nu} (\partial_\mu A_\nu - \partial_\nu A_\mu)^2 \]
Non-compact lattice QED

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- Pure gauge theory is free, it can be solved exactly
Non-compact lattice QED

- Naively discretised Maxwell action:

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S[A_\mu] = \frac{1}{4} \sum_{\mu,\nu} (\partial_\mu A_\nu - \partial_\nu A_\mu)^2
\]

- Pure gauge theory is **free**, it can be solved **exactly**

- Gauge invariance is preserved
Zero-mode subtraction

Finite volume: **momentum quantisation**

\[
\alpha \int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2} \cdots \quad \leftrightarrow \quad \alpha \frac{1}{V} \sum_k \frac{1}{k^2} \cdots
\]
Finite volume: \textit{momentum quantisation}

\[ \alpha \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2} \cdots \Rightarrow \frac{\alpha}{V} \sum_k \frac{1}{k^2} \cdots \]

Possibly IR divergent, but not for physical quantities
Zero-mode subtraction

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Possibly IR divergent, but not for physical quantities

Contains a straight 1/0!
Zero-mode subtraction

- This problem can be solved by removing zero modes
Zero-mode subtraction

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- **Many possible schemes:**
  modification of $A_\mu(k)$ on a set of measure 0
Zero-mode subtraction

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- Many possible schemes: modification of $A_\mu(k)$ on a set of measure 0
- Different schemes: different finite volume behaviours
Zero-mode subtraction

- This problem can be solved by removing zero modes
- Many possible schemes:
  modification of $A_\mu(k)$ on a set of measure 0
- Different schemes: different finite volume behaviours
- Some more interesting than others
QED$_{\text{TL}}$ zero-mode subtraction

- QED$_{\text{TL}}$: $A_\mu(0) = 0$
  Mostly used in all simulations so far
QED$_{TL}$ zero-mode subtraction

- **QED$_{TL}$**: $A_\mu(0) = 0$
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- With QED$_{TL}$, the $T \to \infty$, $L = \text{cst.}$ limit can diverge:

\[
\frac{\alpha}{V} \sum_{k \neq 0} \frac{1}{k^2} \ldots \quad \longrightarrow \quad \frac{\alpha}{L^3} \int \frac{dk_0}{2\pi} \sum_k \frac{1}{k^2} \ldots
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- **QED\textsubscript{TL} does not have reflection positivity**
Example — 1-loop $\text{QED}_{TL}$ [BMWc, 2014]:

\[
m(T, L) \underset{T,L \to +\infty}{\sim} m \left\{ 1 - q^2 \alpha \left[ \frac{\kappa}{2mL} \left( 1 + \frac{2}{mL} \left[ 1 - \frac{\pi}{2\kappa} \frac{T}{L} \right] \right) \right] \right. \\
\left. - \frac{3\pi}{(mL)^3} \left[ 1 - \frac{\coth(mT)}{2} \right] - \frac{3\pi}{2(mL)^4} \frac{L}{T} \right\}
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up to exponential corrections, with $\kappa = 2.83729 \ldots$
QED\textsubscript{TL} finite-volume effects

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Divergent finite volume effects with \( T \to \infty, L = \text{cst.} \)

Same behaviour independently discovered by MILC
QED$_L$ zero-mode subtraction

- QED$_L$: $A_\mu(k_0, 0) = 0$
  inspired from [Hayakawa & Uno, 2008]
QED\textsubscript{L} zero-mode subtraction

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- QED$_L$ finite volume effects:

$$m(T, L) \xrightarrow{T,L\to+\infty} m \left\{ 1 - q^2 \alpha \left[ \frac{\kappa}{2mL} \left( 1 + \frac{2}{mL} \right) - \frac{3\pi}{(mL)^3} \right] \right\}$$

inverse powers of $L$, independent of $T$
Finite-volume effects

Pure QED simulations (quenched) from [BMWc, 2014]
Finite-volume effects

- What about composite particles (QCD + QED)?
Finite-volume effects

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- [Hayakawa & Uno, 2008]: SU(3) PQChPT
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- [Davoudi & Savage, 2014]: NREFTs mesons, baryons, nuclei and HVP

\[ m(L) \sim m \left\{ 1 - q^2 \alpha \left[ \frac{\kappa}{2mL} \left( 1 + \frac{2}{mL} \right) + O \left( \frac{1}{L^3} \right) \right] \right\} \]
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- [BMWc, 2014]: Ward identities: NLO is universal
- parallel talk by C. Lehner: tomorrow 15:35
Full QCD+QED simulations
# Full QCD + QED projects

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<th>PACS-CS</th>
<th>QCDSF-UKQCD</th>
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<td>1205.2961</td>
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<td>clover</td>
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<td>$N_f$</td>
<td>2+1</td>
<td>1+1+1</td>
<td>1+1+1</td>
<td>1+1+1+1</td>
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<td>method</td>
<td>reweighting</td>
<td>reweighting</td>
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<td>250</td>
<td>195</td>
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<td>0.09</td>
<td>0.08</td>
<td>0.06 — 0.10</td>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>$L$ (fm)</td>
<td>1.8</td>
<td>2.9</td>
<td>1.9 — 2.6</td>
<td>2.1 — 8.3</td>
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<tr>
<td>$#L$</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>11</td>
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Starting simulation program by MILC: **R. Zhou talk Monday 14:15**
[BMWc, 2014]: QED simulations

- No mass gap: large autocorrelations!
[BMWc, 2014]: QED simulations

- No mass gap: large autocorrelations!
- One can determine exactly an MD Hamiltonian that removes all memory in the QED Markov chain:

\[
H = \frac{1}{2TL^3} \sum_{\mu,k} \left\{ |\hat{k}|^2 |A_{\mu,k}|^2 + \frac{\pi}{4|\hat{k}|^2} |\Pi_{\mu,k}|^2 \right\}
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- Clover term greatly reduces discretisation errors
[BMWc, 2014]: QED simulations

![Graph showing the 1x1 compact plaquette of the photon as a function of HMC trajectories for naive HMC and improved HMC.](image)

- **Naive HMC**
- **Improved HMC**
Isospin splittings in the hadron spectrum
[QCDSF, 2014]: progress summary
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- $N_f = 1+1+1$
- full QCD+QED simulations in progress
[QCDSF, 2014]: progress summary

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- start from the SU(3) symmetric point and move keeping $m_u + m_d + m_s$ constant
[QCDSF, 2014]: progress summary

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G. Schierholz parallel talk: tomorrow 14:15
[BMWc, 2014]: mass splitting calculation
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- many smeared sources per configurations (O(100))
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- Systematic error based on BMW's histogram method. Weights are based on the goodness of the fits, flat and Akaike’s information criterion (overfitting is penalised)
[BMWc, 2014]: mass splitting calculation

- many smeared sources per configurations (O(100))
- electric charge renormalisation using **Wilson flow**
- small extrapolation to the physical point (similar to [BMWc, 2013])
- Systematic error based on BMW's histogram method. Weights are based on the goodness of the fits, flat and Akaike’s information criterion (**overfitting is penalised**)
- O(500) analyses per mass splitting
[BMWc, 2014]: finite-volume study

(A) \( \chi^2 / \text{dof} = 0.86 \)

(B) \( \chi^2 / \text{dof} = 0.90 \)
[BMWc, 2014]: result summary

\[ \Delta_{CG} = \Delta M_N - \Delta M_\Sigma + \Delta M_\Xi \] (Coleman-Glashow relation)
What is the mass difference between $\Xi_{cc}^+$ and $\Xi_{cc}^{++}$ (including sign)?
- I do not care how you calculate it (HQET, Lattice, ...), JUST DO IT

J. Engelfried, LHC Workshop 2013, Trento

\[ \Delta M = \Delta M_N - \Delta M_\Sigma + \Delta M_\Xi \] (Coleman-Glashow relation)
Results for the nucleon mass splitting

\[
(M_n - M_p)_{QED} \quad (MeV)
\]

\[
(M_n - M_p)_{QCD} \quad (MeV)
\]

[Gasser & Leutwyler, 1982]

- no beta-decay

- experiment
Results for the nucleon mass splitting

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[Walker-Loud et al., 2012]
[NPLQCD, 2007]
no beta-decay

experiment
Results for the nucleon mass splitting

\( (M_n - M_p)_{QED} \) (MeV)

\( (M_n - M_p)_{QCD} \) (MeV)

-2.5
-2
-1.5
-1
-0.5
0

1 1.5 2 2.5 3 3.5 4 4.5

[Gasser & Leutwyler, 1982]
[Walker-Loud et al., 2012]
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Results for the nucleon mass splitting

\[(M_n - M_p)_{\text{QED}} \text{(MeV)}\]

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Results for the nucleon mass splitting

\[ (M_n - M_p)_{\text{QED}} (\text{MeV}) \]

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[Gasser & Leutwyler, 1982]
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[NPLQCD, 2007]
[QCDSF, 2012]
[RM123, 2013]
[Shanahan et al., 2012]

no beta-decay
experiment
Results for the nucleon mass splitting

\[(M_n - M_p)_{\text{QED}} (\text{MeV})\] vs. \[(M_n - M_p)_{\text{QCD}} (\text{MeV})\]

- [Gasser & Leutwyler, 1982]
- [Walker-Loud et al., 2012]
- [NPLQCD, 2007]
- [QCDSF, 2012]
- [RM123, 2013]
- [Shanahan et al., 2012]
- no \textit{beta}-decay
- experiment
- [RBC-UKQCD, 2010]
Results for the nucleon mass splitting

\[ (M_n - M_p)_{\text{QED}} \] (MeV)

\[ (M_n - M_p)_{\text{QCD}} \] (MeV)

[Gasser & Leutwyler, 1982]
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no beta-decay

experiment

[RBC-UKQCD, 2010]
[BMWc, 2013] (EQ)
Results for the nucleon mass splitting

\[ (M_n - M_p)_{\text{QED}} \] (MeV)

\[ (M_n - M_p)_{\text{QCD}} \] (MeV)

-2.5 -2 -1.5 -1 -0.5 0 1 1.5 2 2.5 3 3.5 4 4.5

- [Gasser & Leutwyler, 1982]
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- [QCDSF, 2014]
Summary & outlook
Summary

- We now have a good understanding of QCD+QED on a finite lattice
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Finite-size effects on masses are now well controlled
Summary

- We now have a good understanding of QCD+QED on a finite lattice
- Finite-size effects on masses are now well controlled
- [BMWc, 2014]: full simulations of the low-energy SM with a potential precision of $O[(N_c m_b^2)^{-1}, \alpha^2] \sim 10^{-4}$
Summary

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- Unquenched computations of the light quark masses and Dashen’s theorem corrections
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- Compute corrections to matrix elements
  \( (K_{\ell 3}, K \rightarrow \pi\pi, \ldots) \)
- QCD+QED to compute hadronic corrections to anomalous magnetic moments.
Thank you!
Backup
QED simulations

\[ L(m_{2L},m_L) \]

\[ L_{m_{L}=2} \]

unsmeared, Wilson

smeared, clover
[BMWc, 2014]: charge renormalisation

\[ \Delta M_{\pi}^2 \text{[MeV}^2\text{]} \]

\[ \frac{e^2}{(4\pi)} \]

bare
renormalized

\[ \Delta \]
[BMWc, 2014]: charm discretisation effects

\[ \Delta D, \chi^2/\text{dof}=0.94 \]

\[ \Delta \Xi_{cc}, \chi^2/\text{dof}=1.30 \]