CALCULATION OF MASSES OF CHARGED HADRONS IN QCD+QED$_C$

SPEAKER: Madeleine Dale AUTHORS: RC* collaboration

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Motivation for QED inclusion

- Statistical error reduced to subpercent levels for certain quantities
- Statistical error $\sim$ systematic error due to neglecting QED effects
- Increasing precision further requires QED inclusion for accuracy

Collaboration

- This work forms part of the RC* collaboration which comprises of:
  - Lucius Bushnaq, Isabel Campos-Plasencia, Marco Catillo, Alessandro Cotellucci, Madeleine Dale, Patrick Fritzsch, Roman Grueber, Jens Luecke, Marina Marinkovic, Agostino Patella and Nazario Tantalo
- We have used computing time at the following centers:
  - Cineca
  - CSCS Swiss National Supercomputing Centre
  - North German Supercomputing Alliance (HLRN)
  - Poznan Supercomputing and Networking Center
- This talk is accompanied by talks given by Lucius Bushnaq, Roman Grueber and Jens Luecke

Objective

- Baryon masses (preliminary results):
  - Relevant by themselves and for calibration of QCD+QED

Formulations of QCD+QED

- Gauss's Law: only electrically net-neutral states belong to the physical Hilbert space on a torus (p.b.c.)
- Local gauge fixing?
  - Global zero modes not constrained by local gauge-fixing procedures
- QED_L formulation[1]:
  - Idea: Decouple zero-modes from gauge field dynamics through quenching some gauge field Fourier modes
  - Enforce constraint $\tilde{A}_\mu(t, \mathbf{0}) = \int_{L^3} d^3x A_\mu(t, \mathbf{x}) = 0$
  - Constraint is non-local $\rightarrow$ many properties of local QFTs are not automatic

[1] M. Hayakawa et al., QED in finite volume and finite size scaling effect on electromagnetic properties of hadrons (2008)

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QED_{C^*} formulation

- Advantage: Totally local formulation so renormalisability guaranteed[1]
- Method: Extend physical lattice with mirror lattice of opposite electric charges
- $U(1)$ gauge field anti-periodic in space $\rightarrow$ spatial zero-modes sum to zero
- Spectra of electrically-charged states can be calculated without PT or gauge-fixing

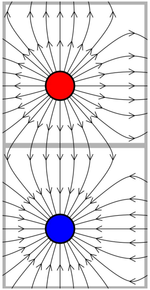


Figure: C* boundary conditions

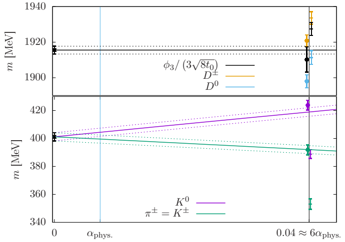
[1] B. Lucini et al., Charged hadrons in local finite-volume QED+QCD with C^* boundary conditions (2015)

RC* collaboration effort

- Explored in detail in talk by Jens Lücke

ensemble	n. cnfgs	a	α_R	L	$m_{\pi^\pm} L$
QCD-32-1	2000	0.0539(3) fm	0	1.736(8) fm	3.52(4)
QCD-48-1	1082	0.0539(3) fm	0	1.736(8) fm	3.52(4)
Q*D-32-1	1993	0.0526(2) fm	0.04077(6)	1.682(5) fm	4.18(2)
Q*D-32-2	2001	0.0505(3) fm	0.04063(6)	1.62(1) fm	2.89(3)
Q*D-32-2+RW	2001	0.0510(2) fm	0.0407(1)	1.631(6) fm	3.24(3)

ensemble	volume	β	α	κ_u	$\kappa_d = \kappa_s$	κ_c	$c_{sw,SU(3)}$	$c_{sw,U(1)}$
QCD-32-1	64×32^3	3.24	0	0.13440733	0.13440733	0.12784	2.18859	0
QCD-48-1	80×48^3	3.24	0	0.13440733	0.13440733	0.12784	2.18859	0
Q*D-32-1	64×32^3	3.24	0.05	0.135479	0.134524	0.12965	2.18859	1
Q*D-32-2	64×32^3	3.24	0.05	0.135560	0.134617	0.129583	2.18859	1
Q*D-32-2+RW	64×32^3	3.24	0.05	0.1355368	0.134596	0.12959326	2.18859	1



Interpolate/extrapolate from lines of constant physics

Baryon masses for calibration

BMW Summary plot

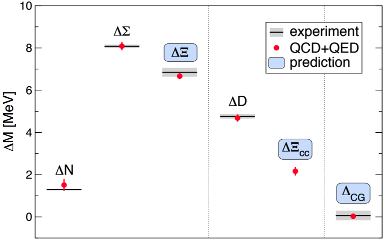


Figure: Mass differences[1]

- BMW calculation in $QCD + QED_L$ formulation remains reference calculation
- $QCD + QED_C$: totally local formulation to act as a check on $QCD + QED_L$ results without reliance on gauge-fixing

[1] BMW Collaboration, Ab initio calculation of the neutron-proton mass difference, Fig. 2 (2015)

Baryon correlators

- Baryon correlators are notoriously noisy
- We use both Gaussian fermion smearing and Wilson gauge smearing[1] to lengthen the plateau and reduce noise

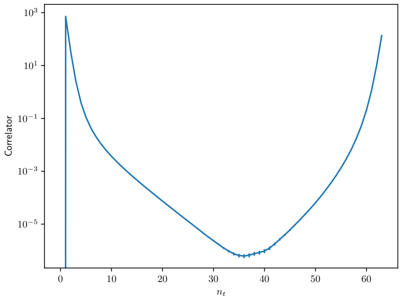


Figure: Neutron correlator with no smearing

[1] In spatial dimensions only; not applied in propagator inversion but instead on fermion smearing

Smeared correlators

- In order to optimise our results, calculate for several smearing levels
- These can also be used to construct Generalised Eigenvalue Problem

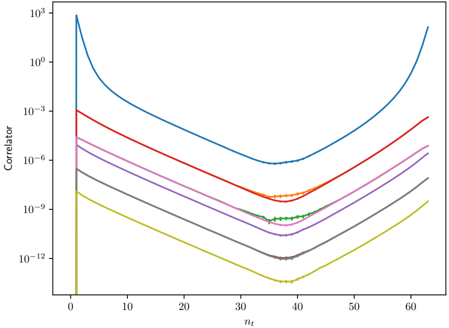
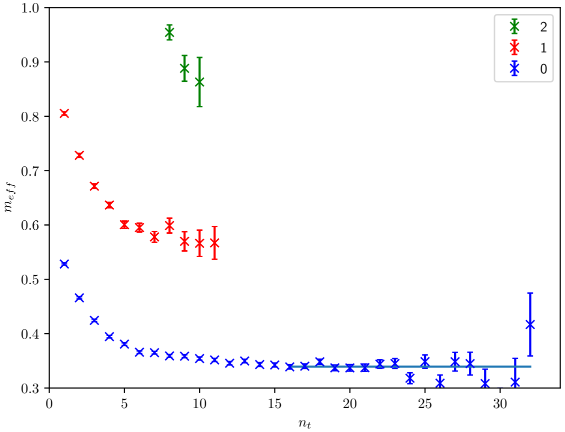


Figure: Neutron correlator with different levels of fermion smearing

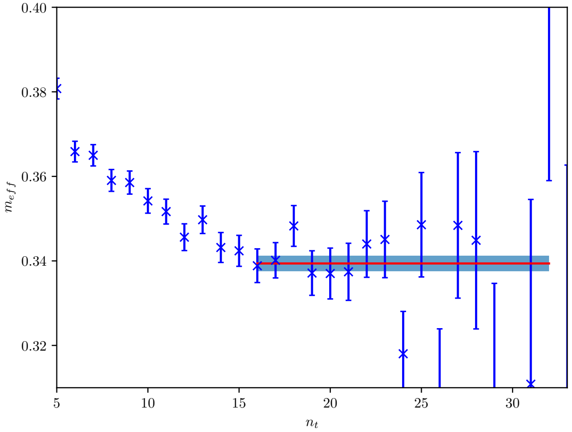
Proton

- Interpolating operator:
  $\mathcal{O} = \Psi \Psi^T C \gamma_5 \Psi$
- Parity projected and folded:
  $C(t) = C^+(t) - C^-(T - t)$



Proton

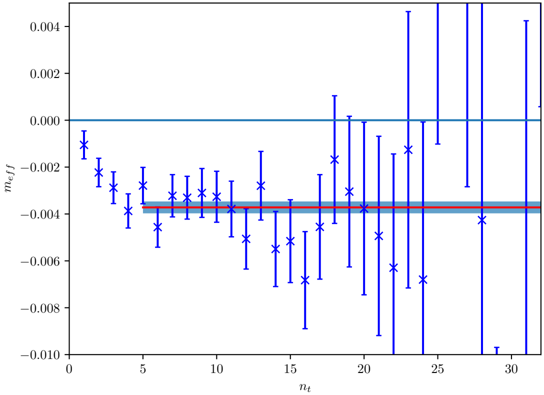
- Proton:
  $m_p = 1272(9)$ MeV
- FV-corrected [1] proton:
  $m_{p,\mathrm{FV}} = 1277(9)$ MeV
- Neutron:
  $m_n = 1291(6)$ MeV
- For reference:
  $m_\pi = 496(2)$ MeV
  $\alpha_R \sim 0.04$



[1] Universal FV-correction using formula from B. Lucini et al., Charged hadrons in local finite-volume QED+QCD with C^* boundary conditions (2015)

P-N mass difference

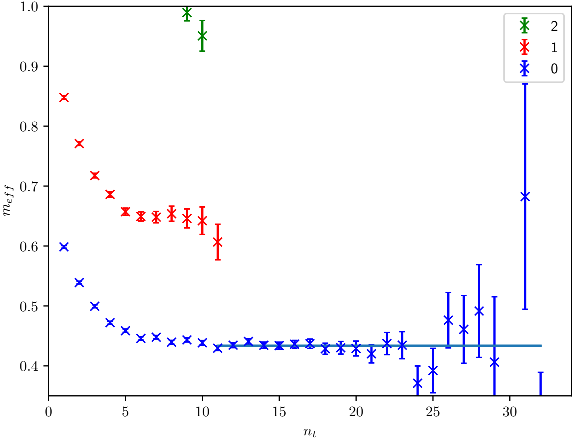
- P-N mass difference:
  $m_p - m_n = -14(1)$ MeV
- FV-corrected[1] P-N mass difference:
  $m_{p,\mathrm{FV}} - m_n = -9(1)$ MeV
- For reference:
  $m_\pi = 496(2)$ MeV
  $\alpha_R \sim 0.04$



[1] Universal FV-correction using formula from B. Lucini et al., Charged hadrons in local finite-volume QED+QCD with C^* boundary conditions (2015)

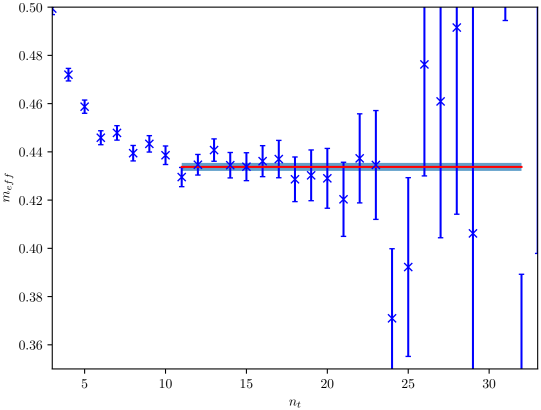
Omega baryon

- Interpolating operator $\mathcal{O} = \Psi\Psi^T C\gamma_i \Psi$ for i=1,2,3
- Spin-projected to spin-3/2 state: $P_{ij}^{\frac{3}{2}} = \delta_{ij} - \gamma_i\gamma_j$
- Parity projected and folded: $C(t) = C^+(t) - C^-(T-t)$



Omega baryon

- Ω baryon:
  $m_\Omega = 1629(10)$ MeV
- FV-corrected[1] Ω baryon:
  $m_{\Omega,\mathrm{FV}} = 1633(10)$ MeV
- For reference:
  $m_\pi = 496(2)$ MeV
  $\alpha_R \sim 0.04$



[1] Universal FV-correction using formula from B. Lucini et al., Charged hadrons in local finite-volume QED+QCD with C^* boundary conditions (2015)

Summary and outlook

- RC* collaboration: baryon masses in full QCD+QED simulations
- QCD+QED_C: totally local formulation; our results don't require perturbation theory or gauge-fixing
- Extended basis of interpolating operators
  - Good signals for spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ baryons at $m_\pi = 496(2)$ MeV and $\alpha_{\text{em}} \sim 6\alpha_{\text{phys}}$
- Future:
  - Extrapolate to physical point?
  - Investigate numerically the flavour violating contributions to Ω baryons
    - Expect these to be highly suppressed from theory

Thanks for listening

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- The work was supported by CINECA that granted computing resources on the Marconi supercomputer to the LQCD123 INFN theoretical initiative under the CINECA-INFN agreement.
- We acknowledge access to Piz Daint at the Swiss National Supercomputing Centre, Switzerland under the ETHZ's share with the project IDs go22 and go24.
- The work was supported by the North-German Supercomputing Alliance (HLRN) with the project bep00085.

Details

- 3 C^* dimensions
- Periodic bcs in time
- $N_T = 64, \; N_L = 32$
- $1 + 2 + 1$ simulation
- $\alpha_R \sim 0.04$
- $\beta = 3.24$
- 1912 configurations
- 4 hits per configuration at random timeslices
- Smeared point-source
- Gaussian smearing: nsteps $= (0, 200, 400)$; eps $= 0.5$
- Wilson smearing: nsteps $= 180$; eps $= 0.02$

Flavour mixing caveat

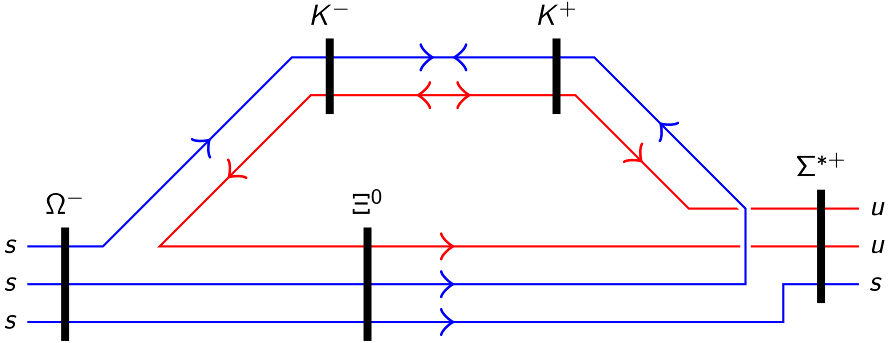
- C^* boundary conditions allow some flavour violation as particles travel around the torus
- Colourless particles only (given large enough box) may violate flavour under the conditions:

$$\Delta Q = 0 \text{ mod } 2; \Delta B = 0 \text{ mod } 2; \Delta F = 0 \text{ mod } 6$$

- Induced by disconnected contractions $\langle \Psi(\mathbf{0})\Psi^T(\mathbf{x})\rangle$
- Proton/neutron is the lightest charged/neutral state with $B = 1$
- Omega baryon mixing can satisfy these mixing conditions
- Any flavour violation is exponentially suppressed with volume[1]
- Future work: calculation of disconnected contractions

[1] B. Lucini et al., Charged hadrons in local finite-volume QED+QCD with C^* boundary conditions (2015)

Example of flavour mixing for Ω



Gauge dressing factor

- Define electrically charged state using a dressing factor (e.g. Dirac factor):

$$\Psi(t,\vec{x}) = \underbrace{e^{-i\int_{L^3} d^3y\,\Phi(\vec{y}-\vec{x})\partial_k A_k(t,\vec{y})}}_{\Theta(t,\vec{x})}\,\psi(t,\vec{x})\;,\quad \partial_k\partial_k\Phi(\vec{x}) = \delta^3(\vec{x})\;,\quad \Phi(\vec{x}+L\vec{k}) = -\Phi(\vec{x})$$

- Ψ is then invariant under local gauge transformations...

$$\psi(x) \mapsto e^{i\alpha(x)}\,\psi(x)\;,\qquad A_\mu(x) \mapsto A_\mu(x) + \partial_\mu\alpha(x)$$

$$\Theta(t,\vec{x}) \mapsto \; e^{-i\int_{L^3} d^3y\,\Phi(\vec{y}-\vec{x})\partial_k\partial_k\alpha(t,\vec{y})}\,\Theta(t,\vec{x}) = \; e^{-i\alpha(t,\vec{x})}\,\Theta(t,\vec{x})$$

- ... so a gauge invariant correlator $\int_{L^3}\langle\Psi(t,\mathbf{x})\bar{\Psi}(\mathbf{0})\rangle$ can be constructed
- Non-trivial aside: $\phi(x)$, electric potential of a charge in a box with C^* boundary conditions, exists!

Gauge dressing factor

- Define electrically charged state using a dressing factor:
  $\Psi(t,\vec{x}) = \Theta(t,\vec{x})\psi(t,\vec{x})$
- $\Psi(t,\vec{x})$ is not invariant under global gauge transformations; it is electrically charged!
- Dirac's factor is not unique

$$\Theta_J(x) = e^{i\int_{L^3} d^4y\, J_\mu(y-x)A_\mu(y)}\,, \quad \partial_\mu J_\mu(x) = \delta^4(x)\,, \quad J_\mu(x+L\vec{k}) = -J_\mu(x)$$

- We choose the 'string' gauge factor:

$$\Theta_{\mathbf{s}}(x) = e^{-\frac{i}{2}\int_{-x_k}^{0} ds\, A_k(x+s\vec{k})}\, e^{\frac{i}{2}\int_0^{L-x_k} ds\, A_k(x+s\vec{k})}\,;$$

$$J_\mu(x) = \frac{1}{2}\delta_{\mu k}\,\mathrm{sign}(x_k)\prod_{\nu\neq k}\delta(x_\nu)$$

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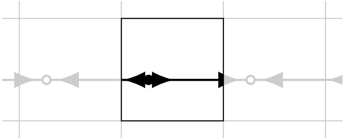
QED$_C$ on the lattice



$$S = \frac{2}{e^2} \sum_{x,\mu\nu} [1 - P_{\mu\nu}(x)] + \sum_x \bar{\psi}(x) D[U^2] \psi(x)$$

$$U_\mu(x) = 1 + \frac{i}{2} A_\mu(x) + \cdots$$

- Lattice implementation requires an unconventional coupling of the matter fields to the gauge fields

$$D[U^2] = m + \frac{1}{2} \sum_\mu \left\{ \gamma_\mu \left(\nabla^*_\mu[U^2] + \nabla_\mu[U^2] \right) - \nabla^*_\mu[U^2] \nabla_\mu[U^2] \right\}$$

$$\nabla_\mu[U^2]\psi(x) = U^2_\mu(x)\psi(x+\mu) - \psi(x)$$

$$U_\mu(x) \mapsto \Omega(x) U_\mu(x) \Omega^{-1}(x+\mu) \,, \qquad \psi(x) \mapsto \Omega^2(x)\psi(x)$$

- The gauge invariant interpolating operator can then be simply implemented as (no square roots!)

$$\Psi(x) = \prod_{s=-x_k}^{-1} U_k^{-1}(x + s\vec{k}) \, \psi(x) \prod_{s=0}^{L-x_k-1} U_k(x + s\vec{k})$$

Finite volume corrections

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

Dependence on boundary conditions is contained *only* in the generalized zeta functions

	$1C^\star$	$2C^\star$	$3C^\star$
$\xi(1)$	-0.77438614142	-1.4803898065	-1.7475645946
$\xi(2)$	-0.30138022444	-1.8300453641	-2.5193561521
$\xi(4)$	0.68922257439	-2.1568872986	-3.8631638072

$$\xi(s) = \sum_{\vec{n}\neq\vec{0}} \frac{(-1)^{\langle\vec{n}\rangle}}{|\vec{n}|^s}\,, \qquad \langle\vec{n}\rangle = \sum_{i\in\{C^\star\text{ b.c.}\}} n_i$$

Smeared correlators

- Act on interpolating operator $\mathcal{O}$ with:

$$S = (1 + \kappa_g H)^N S_0, \quad H(\mathbf{n},\mathbf{m}) = \sum_{j=1}^{n_{\text{dims}}} \Big(U_j(\mathbf{n})\delta(\mathbf{n}+\hat{j},\mathbf{m}) + U_j(\mathbf{n}-\hat{j})^\dagger \delta(\mathbf{n}-\hat{j},\mathbf{m}) \Big);$$

$$\dot{V}_t(x,k) = -g_0^2 \delta_{x,k} S_w(V_t) V_t(x,k),$$

$$\text{where } \delta_{x,k} f(U) = T^a \delta^a_{x,k} f(U), \quad \delta^a_{x,k} f(U) = \frac{d}{ds} f(e^{sX} U)|_{s=0},$$

$$X(y,i) = \begin{cases} T^a & \text{if}(y,i) = (x,k), \\ 0 & \text{otherwise.} \end{cases}$$

$$\text{with initial condition } V_t(x,k)|_{t=0} = U(x,k)$$

Generalised Eigenvalue Problem

- Spectral decomposition of two-point function:

$$
\begin{aligned}
C_{ij}(t) &= \langle \mathcal{O}_i(t) \tilde{\mathcal{O}}^\dagger{}_j(t) \rangle, \\
&= \langle \mathcal{O}_i(t) e^{-\hat{H}t} \tilde{\mathcal{O}}^\dagger{}_j(0) \rangle, \\
&= \sum_{n=1}^{\infty} Z_i^n \tilde{Z}_j^{n*} e^{-E_n t},
\end{aligned}
$$

where

$$
\begin{aligned}
\hat{H}|n\rangle &= E_n |n\rangle, \\
Z_i^n &= \langle 0|\mathcal{O}_i|n\rangle, \\
\tilde{Z}_j^{n*} &= \langle n|\tilde{\mathcal{O}}^\dagger{}_j|n\rangle
\end{aligned}
$$

Generalised Eigenvalue Problem

- Express in matrix form
$$C(t) = Z\Lambda\tilde{Z}^{\dagger},$$
where
$$\Lambda = \text{diag}(\lambda_1(t), \lambda_2(t), \ldots), \qquad E_1 < E_2 < E_3 \ldots$$
- Using
$$Q^{\dagger} = (Z)^{-1}, \qquad \tilde{Q} = (\tilde{Z}^{\dagger})^{-1},$$
rewrite as
$$Q^{\dagger}C(t)\tilde{Q} = \Lambda(t).$$
- Factorise $\Lambda = \Lambda(t - t_0)\Lambda(t_0)$, finally get GEVP:
$$C(t)\tilde{Q} = C(t_0)\tilde{Q}\Lambda(t - t_0),$$
- Enforcing Hermiticity of correlator ensures real eigenvalues