Including isospin breaking in lattice QCD calculations:
QED (+ QCD) in a finite volume

Laurent Lellouch

CPT Marseille
CNRS & Aix-Marseille U.

Borsanyi, Dürr, Fodor, Hoelbling, Katz, Krieg, Lellouch, Lippert, Portelli, Szabo, Toth
Budapest-Marseille-Wuppertal collaboration (BMWc)

(based mainly on Science 347 '15, arXiv:1502.06921)

Motivations for isospin breaking in lattice calculations

- Plays critical role in fundamental quantities, e.g.
  - *n-p* mass difference required for BBN and existence and stability of matter as we know it (BMWc '14, see Hoelbling's talk)
  - knowledge of individual *u* and *d* masses, limited by determination of EM corrections (FLAG '13)
- Improving indirect search for new physics
  - → important flavor observables are precisely computed in LQCD today: e.g. $\mathrm{err}(m_{ud}), \mathrm{err}(m_s) \sim 2\%$, $\mathrm{err}(m_s/m_{ud}) \lesssim 1\%$, $\mathrm{err}(F_K) \sim 1\%$, $\mathrm{err}(F_K/F_\pi) \sim 0.5\%$, $\mathrm{err}(F_+^{K\pi}(0)) \sim 0.8\%$
  - → to go beyond, need to account for isospin breaking
- Expected $\sim$ 0.15 ppm precision in new Fermilab & JPARC $(g-2)_\mu$ experiments will require inclusion of isospin breaking effects in HVP contribution
- Hadronic contributions to $(g-2)_\mu$ (e.g. HLbyL à la Blum et al '14) may be best obtained by including QED in LQCD calculations
- Required for understanding heavier nuclei and eventually precision nuclear physics

Isospin symmetry and its breaking

Nature has a near $SU(2)$-isospin symmetry

$$\left(\begin{array}{c} u \\ d \end{array} \right) \longrightarrow \exp[i\vec{\theta}\cdot\frac{\vec{\tau}}{2}] \left(\begin{array}{c} u \\ d \end{array} \right)$$

Only broken by small, often competing effects

	u	d
m_q [FLAG 13]	$2.16(11)\,\mathrm{MeV}$	$4.68(16)\,\mathrm{MeV}$
e_q	$\frac{2}{3}e$	$-\frac{1}{3}e$

$$3\,\frac{m_d - m_u}{M_N} \sim 1\% \qquad \text{and} \qquad (Q_u^2 - Q_d^2)\,\alpha \sim 1\%$$

Small $\Rightarrow$ can compute perturbatively in α & $(m_d - m_u)$ ...
...but mixing w/ nonperturbative QCD

$\Rightarrow$ **nonperturbative QCD tool**
$\Rightarrow$ **include QED and** $m_u \neq m_d$

Including isospin breaking in LQCD calculations

$$S_{\mathrm{QCD+QED}} = S^{\mathrm{iso}}_{\mathrm{QCD+QED}} + \frac{1}{2}(m_u - m_d)\int(\bar{u}u - \bar{d}d) + ie\int A_\mu j_\mu\,, \qquad j_\mu = \bar{q}Q\gamma_\mu q$$

(1) operator insertion method (Blum et al '06-, RM123 '12-)

$$\langle\mathcal{O}\rangle_{\mathrm{QCD+QED}} = \langle\mathcal{O}\rangle^{\mathrm{iso}}_{\mathrm{QCD}} - \underbrace{\frac{1}{2}(m_u - m_d)\langle\mathcal{O}\int(\bar{u}u - \bar{d}d)\rangle^{\mathrm{iso}}_{\mathrm{QCD}}}_{(a)}$$
$$+ \underbrace{\frac{1}{2}e^2\langle\mathcal{O}\int_{xy} j_\mu(x)D_{\mu\nu}(x-y)j_\nu(y)\rangle^{\mathrm{iso}}_{\mathrm{QCD}}}_{(b)} + \text{hot}$$

- ✓ no new simulations
- ✓ directly get desired order in α
- ✓ no renormalization of α at LO

- x difficult observables
- x quark-disconnected diagrams not yet included

(2) direct method (Eichten et al '97, Blum et al '07, '10, BMWc '10-, MILC '10-, BNL '15, Endres et al '15)

Include $m_u \neq m_d$ and QED directly in simulation

- ✓ much simpler observables
- ✓ quark-disconnected diagrams for free
- ✓ full calculation done & it works (BMWc '14)

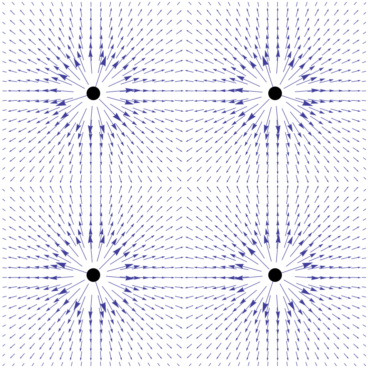
- x desired effect often subleading in α
- x new, difficult simulations, including QED

(3) any combination of (1) & (2)

All must deal with problem of QED in FV and potentially large FV effects

No net charge in a periodic box: classical EM

Electric field of a point charge cannot be made periodic and continuous



Gauss's law forbids a net charge in a periodic box

$$\vec{\nabla} \cdot \vec{E}(x) = \rho(x) \Rightarrow Q = \int d^3x\, \rho(t, \vec{x}) = \int_\partial d\vec{S} \cdot \vec{E}(t, \vec{x}) = 0$$

Localized charge in a periodic box: modified EM

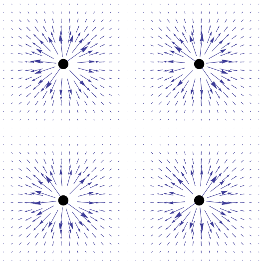
- Introduce uniform, time-independent background current c_μ as new variable $(\Omega = \Pi_{\mu=0}^{3} L_\mu)$

$$\partial_\nu F_{\mu\nu}(x) = j_\mu(x) - \frac{L_\mu}{\Omega} c_\mu$$

- Allow it to adjust such that

$$c_0 = \int d^3x\, j_0(x) \qquad \text{which implies} \qquad \int d^3x\, \partial_i F_{0i}(x) = 0$$

and Gauss' law satisfied even with net j_μ, and similarly in other directions



Presence of localized charge allowed at cost of EM modification that vanishes in IV limit

Elimination of zero modes: TL vs L prescriptions

TL prescription:

- Modified EM obtained from $(\partial_\nu c_\mu = 0)$

$$\mathcal{L}(x) = \frac{1}{4} F_{\mu\nu} F_{\mu\nu}(x) - \left(j_\mu(x) - \frac{L_\mu c_\mu}{\Omega} \right) A_\mu(x)$$

- EoM associated with c_μ

$$\int d^4x\, A_\mu(x) = 0 \quad \Rightarrow \quad \tilde{A}_\mu(k=0) = 0$$

L prescription:

- TL does not allow introducing and removing charges or currents (as in charged particle propagators)

  $\Rightarrow$ consider $c_\mu \to c_\mu(t)$

- EoM associated with $c_\mu(t)$

$$\int d^3x\, A_\mu(t, \vec{x}) = 0, \quad \forall t \quad \Rightarrow \quad \tilde{A}_\mu(k_0, \vec{k} = \vec{0}) = 0, \quad \forall k_0$$

Zero-mode problem in finite-volume QED

Path integral view

e.g. in $\partial_i A_i = 0$ Coulomb gauge

$$S = \frac{1}{2}\int d^4x \left[\sum_i (\partial_i A_0)^2 + \sum_i (\partial_0 A_i)^2 + \sum_{i\neq j}(\partial_j A_i)^2\right]$$

$$\Rightarrow \quad S = 0 \quad \text{for} \quad \begin{cases} \tilde{A}_0(k_0, \vec{k} = \vec{0}), & \forall k_0 \\ \tilde{A}_i(k = 0) \end{cases}$$

$\Rightarrow$ these zero modes can fluctuate wildly

$\Rightarrow$ problem for algorithms

Perturbative view

Usual perturbative calculations are not well defined

$$\alpha \int \frac{d^4k}{(2\pi)^4}\frac{1}{k^2}\cdots \quad \longrightarrow \quad \frac{\alpha}{TL^3}\sum_k \frac{1}{k^2}\cdots$$

$\uparrow$ possible IR divergences but not in physical qties

$\uparrow$ contains a straight 1/0!

Zero-mode problem in finite-volume QED

Problem can be solved by **removing zero mode(s)**

$\rightarrow$ modification of $\tilde{A}_\mu(k)$ on set of measure zero

$\rightarrow$ does not change infinite-volume physics

$\rightarrow$ physically equivalent to adding a canceling uniform charge distribution

- different schemes $\rightarrow$ different finite-volume behaviors
- some schemes more interesting than others

QED_{TL} zero-mode subtraction

- Set $\tilde{A}_\mu(k=0)=0$ on $T\times L^3$ four-torus (Duncan et al '96)
- Used in all previous studies
- Violates reflection positivity!

  $\rightarrow$ no hermitian Hamiltonian, states w/ non-positive norm

  $\rightarrow$ divergences when L fixed, $T\rightarrow\infty$

$$\frac{\alpha}{TL^3}\sum_{k\neq 0}\frac{1}{k^2}\cdots \quad \xrightarrow[T\to+\infty,L\ \text{fixed}]{} \quad \alpha\int\frac{dk_0}{2\pi}\frac{1}{L^3}\sum_{\vec{k}}\frac{1}{k^2}\cdots$$

Checked analytically in 1-loop spinor (also scalar) QED calculation

$$m(T,L) \underset{T,L\to+\infty}{\sim} m\left\{1-q^2\alpha\left[\frac{\kappa}{2mL}\left(1+\frac{2}{mL}\left[1-\frac{\pi}{2\kappa}\frac{T}{L}\right]\right) -\frac{3\pi}{(mL)^3}\left[1-\frac{\coth(mT)}{2}\right]-\frac{3\pi}{2(mL)^4}\frac{L}{T}\right]\right\}$$

with $\kappa=2.837\cdots$, up to exponentially-suppressed corrections

QED_L zero-mode subtraction

- Set $\tilde{A}_\mu(k_0, \vec{k}=0) = 0$ on $T \times L^3$ four-torus for all $k_0 = 2\pi n_0/T$, $n_0 \in \mathbb{Z}$
- Used here (orginally suggested in Hayakawa & Uno '08)
- Satisfies reflection positivity

  $\rightarrow$ fixing to Coulomb gauge, $\vec{\nabla}\cdot\vec{A}=0$, ensures existence of Hamiltonian

  $\rightarrow$ well defined asymptotic states

  $\rightarrow$ well defined $T, L \rightarrow \infty$ limit

Checked analytically in 1-loop spinor (and scalar) QED calculation

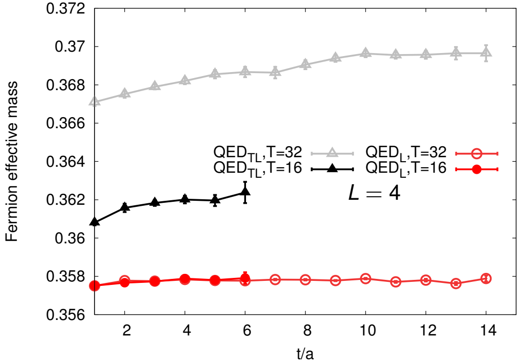
$$m(T,L) \underset{T,L\to+\infty}{\sim} m\left\{1 - q^2\alpha\left[\frac{\kappa}{2mL}\left(1+\frac{2}{mL}\right) - \frac{3\pi}{(mL)^3}\right]\right\}$$

with $\kappa = 2.837\cdots$, up to exponentially-suppressed corrections

$\Rightarrow$ only inverse powers of L and no powers in T

QED_{TL} vs QED_L: numerical tests

Numerical studies in pure spinor QED (w/out QCD, $e = \sqrt{4\pi/137}$, $am = 0.4$, $L/a = 4$)



QED_{TL}, as expected, has:

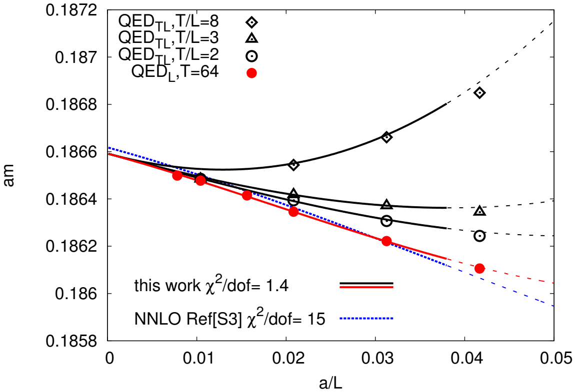
- no clear mass plateaux
- mass increases w/ T

As predicted, QED_L has none of these problems:

- ground state dominates at large t/a
- T-independent mass

QED_{TL} vs QED_L: numerical tests

Test pure QED simulations against our 1-loop finite-volume predictions (w/out QCD, $e = \sqrt{4\pi/137}$, $am = 0.2$, $L/a = 24, \cdots, 128$)



- Excellent agreement
- Both schemes give the same result in infinite volume
- QED_L cleaner and has more controlled infinite-volume limit

QED_L finite-volume effects for composite particles

In our point spinor and scalar QED_L calculations find

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

independent of particle spin (w/ $\kappa = 2.837\cdots$)

Same result found for:

- Mesons in $SU(3)$ PQ χPT (Hayakawa et al '08)
- Mesons/baryons in non-relativistic EFT (Davoudi et al '14)
- Classically: $1/L$ term is given by EM energy stored in system of a static charge in uniform canceling charge background in FV (BMWc '10, Davoudi et al '14)

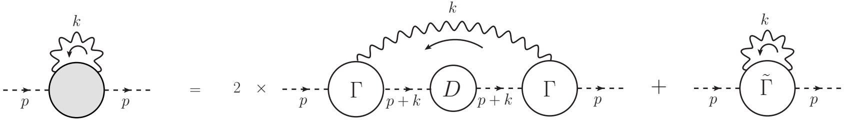
$\rightarrow$ leading $1/L$ and $1/L^2$ terms independent of particle spin and structure?

For a general field theory, this universality **follows from Ward identities** (BMWc '14), using Lüscher '86, under hypotheses satisfied here

$\rightarrow$ large leading FV effects can be removed analytically

QED$_L$ finite-volume effects for composite particles

- FV effects in particle masses come from difference in the on-shell self-energy (SE) in finite and infinite volumes
- For a composite charged particle, X, of mass m and charge q at $O(\alpha)$

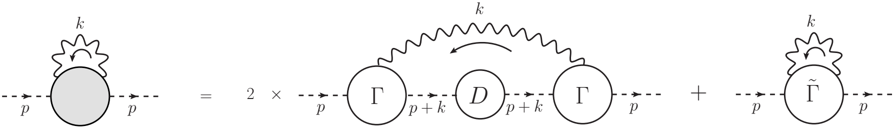


- D is full propagator & Γ_μ and $\tilde{\Gamma}_{\mu\nu}$ are full 1PI vertices
- D, Γ_μ and $\tilde{\Gamma}_{\mu\nu}$ are pure QCD functions (no QED)
- Obtained using re-written Poisson formula

$$\left(\frac{1}{L^3}\sum_{\vec{k}\in\frac{2\pi}{L}\mathbb{Z}^{3*}} - \int\frac{d^3k}{(2\pi)^3}\right) f(\vec{k}) = \left(\sum_{\vec{x}\in L\mathbb{Z}^{3*}} - \frac{1}{L^3}\int d^3x\right)\int\frac{d^3k}{(2\pi)^3} f(\vec{k})e^{i\vec{k}\cdot\vec{x}}$$

- Assumes that D, Γ_μ and $\tilde{\Gamma}_{\mu\nu}$ in FV can be replaced by IV counterparts (shown below)
- If $f(\vec{k})$ is analytic, FV corrections fall of faster than any power in $1/L$
- Corrections in powers of $1/L$ result from nonanalyticities in $f(\vec{k})$ associated w/ intermediate states going on shell in domain of integration

QED_L finite-volume effects for composite particles



- Make hypotheses well satisfied for cases of interest in our work
  - the photon is the only massless asymptotic state
  - the charged particle considered is stable (under strong interactions) and non-degenerate in mass

⇒ for on-shell SE diagram kinematics, energies flowing into D, Γ_μ and $\Gamma_{\mu\nu}$ are smaller than that of any other hadronic state

⇒ using analysis of Lüscher '86, $(p^2+m^2)D(p)$, Γ_μ and $\Gamma_{\mu\nu}$ are analytic for SE kinematics and equal to their IV counterparts up to exponentially suppressed volume corrections

⇒ only IR singularities that can arise in SE correspond to free γ propagator and to free charged particle X particle for $p^2=-m^2$ when $\vec{k}\to\vec{0}$

- Use analyticity of $(p^2+m^2)D(p)$, Γ_μ and $\Gamma_{\mu\nu}$ to expand integrand around on-shell point up to $O(k^0)$
- Use WTI's to cancel undesirable terms
- Find point-particle result up to and including $O(1/L^2)$, with structure-dependent $O(1/L^3)$ terms and a remainder that falls of at least like $1/L^3$ – QED

NREFT computation of QED FV corrections to masses

- Efficient method to compute FV effects: nonrelativistic EFT (NREFT) (Davoudi et al '14)
- In QED_L, FV corrections mainly given by γ exchange w/ $|\vec{k}| \sim 2\pi/L$
- NREFT gives what we want: expansions of particle properties in powers of its $|\vec{p}| \sim 2\pi/L$ and a complete description of the IR behavior of the theory, including singularities

PROBLEM (e.g. spin-$1/2$ case)

- Our relativistic QED_L computation gives (BMWc '14)

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

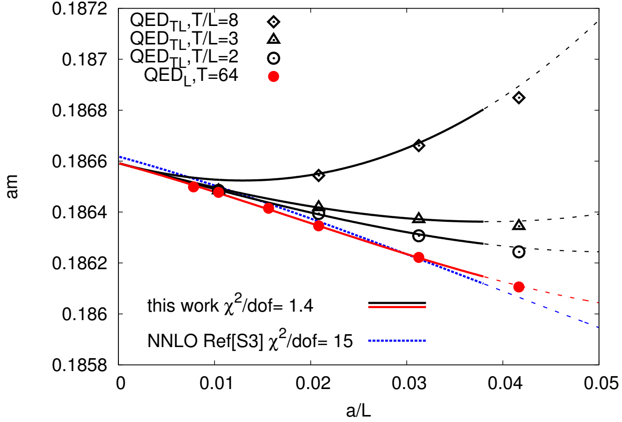
- Point-like reduction of Davoudi et al '14 NREFT calculation gives

$$\frac{3\pi}{(mL)^3} \longrightarrow \frac{3\pi}{2(mL)^3}$$

- Both cannot be simultaneously true!

QED_L: numerical test of coefficient of $1/L^3$ term

Test pure QED simulations against our 1-loop finite-volume predictions (w/out QCD, $e = \sqrt{4\pi/137}$, $am = 0.2$, $L/a = 24, \cdots, 128$)



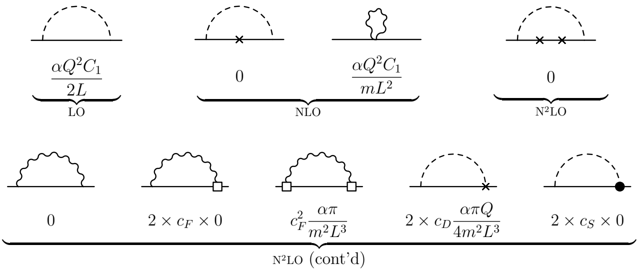
Relativistic value of coefficient (BMWc '14) is strongly favored over NREFT value of Davoudi et al '14

NREFT computation of QED FV corrections to masses

Repeat spinor NREFT calculation to N^{2}LO (Fodor et al '15), using (Caswell et al '86, Thacker et al '91, Labelle '92, Manohar '97, Luke et al '97, Chen et al '99, Hill et al '12, Lee et al '14)

$$\mathcal{L}_\psi = \psi^\dagger \left[iD_0 + \frac{|\vec{D}|^2}{2m} + c_F \frac{e}{2m}\vec{\sigma}.\vec{B} + c_D \frac{e}{8m^2}\vec{\nabla}\cdot\vec{E} + ic_S \frac{e}{8m^2}\vec{\sigma}\cdot(\vec{D}\times\vec{E} - \vec{E}\times\vec{D}) + O(\vec{p}^4) \right] \psi$$

FV contributions to spin-$1/2$ hadron/nucleus mass



Result fully agrees w/ Davoudi et al '14

$\Rightarrow$ go back to relativistic calculation to see what might be missing in NREFT computation

Revisiting relativistic QED FV calculation

In relativistic calculation expect:

1) IR singularities in on-shell self-energy integrand/summand are given by:
   - particle pole
   - positive and negative energy γ poles

2) antiparticle pole, which is $2m$ away, only contributes terms $\propto e^{-2mL}$

In fact, (2) is incorrect in QED_L:

$$\left(\frac{1}{L^3}\sum_{\vec{k}\in\frac{2\pi}{L}\mathbb{Z}^{3*}}-\int\frac{d^3k}{(2\pi)^3}\right)f(\vec{k})=\left(\frac{1}{L^3}\sum_{\vec{k}\in\frac{2\pi}{L}\mathbb{Z}^{3}}-\int\frac{d^3k}{(2\pi)^3}\right)f(\vec{k})-\frac{1}{L^3}f(\vec{0})$$

- $f(\vec{0})/L^3$ is $1/L^3$ FV effect not associated with any IR singularity and therefore missed by standard NREFT calculation

- Straightforward to show that antiparticle contribution to $f(\vec{0})/L^3$ gives missing $3\pi/2(mL)^3$ term!

NREFT with inclusion of antiparticle contributions

- In NREFT language, include antiparticles through (Labelle et al '97)

$$\mathcal{L}_{\mathrm{N^2LO}} = \mathcal{L}_\psi + \mathcal{L}_\chi + \mathcal{L}_{4f} + O(\vec{p}^4)$$

where $\mathcal{L}_\chi = \mathcal{L}_\psi$ w/ $\psi \to \chi$ and $q \to -q$, and

$$\mathcal{L}_{4f} = d_V \frac{\alpha}{m^2} (\psi^\dagger \vec{\sigma}\sigma_2 \chi^*) \cdot (\chi^T \sigma_2 \vec{\sigma} \psi) + O(\alpha^2, \vec{p}^4)$$

w/ $d_V = -\pi q^2 + O(\alpha)$ for point particles

$\Rightarrow$ new contribution to FV particle mass

$$\underbrace{-d_V \frac{3\alpha}{2m^2 L^3}}_{\mathrm{N^2LO}}$$

$\Rightarrow$ precisely the missing $3\pi/2(mL)^3$ term

- In fact, only $\vec{p} = \vec{0}$ modes of antiparticle are required

Lessons from RQED vs NRQED comparison in FV

- $|\vec{k}| = 0$ photons can couple antiparticles to particles

$\Rightarrow$ antiparticles must be dealt w/ carefully to allow subtraction of $|\vec{k}| = 0$ photon modes in FV

$\Rightarrow$ antiparticle dof's must be retained in NREFT

- When done, relativistic and NREFT calculations agree at they should

Conclusions and perspectives

- Isospin breaking corrections can be accounted for through

  (1) operator insertion method
  (2) direct method
  (3) a combination of (1) & (2)

- All methods, in lattice simulations, have to deal w/ non-trivial problem of putting QED in a finite box

- Proposed a solution based on Hayakawa et al '08: QED_L

- Modification of QED on a set of measure 0 which disappears in the IV limit
  $\Rightarrow$ FV momentum sums converge onto IV QED as $L \to 0$

- Performed many tests (1-loop analytical vs numerics, renormalizability up to 2-loops, EFT description, . . .)
  $\Rightarrow$ has passed them all w/ flying colors

- We were able to implement method (2) w/ QED_L in a full QCD + QED simulation and obtain significant results for isospin splitting in the stable hadron specturm over a year ago (BWMc '14, see Hoelbling's talk)

Conclusions and perspectives

- Alternatives are beginning to appear
  - QED_{TL}, used in all previous calculations and which we show is not reflection positive and has non-uniform $T, L \to \infty$ limit
  - $m_\gamma \neq 0$ (Enders et al '15): makes FV exponential in $m_\gamma L$ but need $1/L \ll m_\gamma \ll M_\pi$ which is a challenge for physical M_π on today's volumes
  - QED_∞ (Lehner et al '15): FV QCD + IV qQED and quarks in valence, in development
  - C^* boundary conditions (Polley '93, Lucini et al Lat '15):
    - Eliminate photon zero mode w/ $A_\mu(x+L\hat{e}_i) = -A_\mu(x_\nu)$ $\Rightarrow \psi(x+L\hat{e}_i) = C^{-1}\bar{\psi}^T(x)$ & $\bar{\psi}(x+L\hat{e}_i) = -\psi^T(x)C$
    - Using boundary conditions is a good way to get rid of unwanted modes
    - Charge and flavor violation, but generally exponentially suppressed in L
    - Gluons must also satisfy C^* boundary conditions $\Rightarrow$ re-use of $\alpha = 0$ configurations w/ periodic BCs (e.g. w/ "operator insertion method") not possible
    - Possible determinant positivity issues w/ non-chiral regularizations (e.g. Wilson fermions)
    - Computational cost and numerical tests?

Conclusions and perspectives

- Future applications:
  - QED corrections to HVP (Marinkovic et al Lat 15)
  - Hadronic LbyL (Blum et al '11-, see Izubuchi's talk)
  - QED corrections to hadronic amplitudes with real photons: develop methodology (Carrasco et al '15, see Martinelli's talk) and test numerically

$$\Gamma(\Delta E) = \lim_{V\to\infty}(\Gamma_0^{\rm lat} - \Gamma_0^{\rm pt})|_{O(\alpha)} + \lim_{V\to\infty}(\Gamma_0^{\rm pt}(\Delta E) + \Gamma_1^{\rm pt\ or\ lat}(\Delta E))|_{O(\alpha)}$$