Massive Photons: An Infrared Regularization Scheme for Lattice

The MIT Faculty has made this article openly available. Please share how this access benefits you. Your story matters.

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>As Published</td>
<td><a href="http://dx.doi.org/10.1103/PhysRevLett.117.072002">http://dx.doi.org/10.1103/PhysRevLett.117.072002</a></td>
</tr>
<tr>
<td>Publisher</td>
<td>American Physical Society</td>
</tr>
<tr>
<td>Version</td>
<td>Final published version</td>
</tr>
<tr>
<td>Accessed</td>
<td>Wed Dec 19 02:37:22 EST 2018</td>
</tr>
<tr>
<td>Citable Link</td>
<td><a href="http://hdl.handle.net/1721.1/110393">http://hdl.handle.net/1721.1/110393</a></td>
</tr>
<tr>
<td>Terms of Use</td>
<td>Article is made available in accordance with the publisher’s policy and may be subject to US copyright law. Please refer to the publisher’s site for terms of use.</td>
</tr>
<tr>
<td>Detailed Terms</td>
<td></td>
</tr>
</tbody>
</table>
Massive Photons: An Infrared Regularization Scheme for Lattice QCD + QED

Michael G. Endres,1,* Andrea Shindler,2,† Brian C. Tiburzi,3,4,5, and André Walker-Loud6,7,8,‡
1Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
2Department of Physics, City College of New York, New York, New York 10031, USA
3Graduate School and University Center, The City University of New York, New York, New York 10016, USA
4RIKEN BNL Research Center, Brookhaven National Laboratory, Upton, New York 11973, USA
5Department of Physics, College of William and Mary, Williamsburg, Virginia 23187-8795, USA
6Jefferson Laboratory, 12000 Jefferson Avenue, Newport News, Virginia 23606, USA
7Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
8School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA

(Received 10 August 2015; revised manuscript received 28 April 2016; published 10 August 2016)

Standard methods for including electromagnetic interactions in lattice quantum chromodynamics calculations result in power-law finite-volume corrections to physical quantities. Removing these by extrapolation requires costly computations at multiple volumes. We introduce a photon mass to alternatively regulate the infrared, and rely on effective field theory to remove its unphysical effects. Electromagnetic modifications to the hadron spectrum are reliably estimated with a precision and cost comparable to conventional approaches that utilize multiple larger volumes. A significant overall cost advantage emerges when accounting for ensemble generation. The proposed method may benefit lattice calculations involving multiple charged hadrons, as well as quantum many-body computations with long-range Coulomb interactions.

DOI: 10.1103/PhysRevLett.117.072002

Introduction.—Approximately 95% of the visible mass of the Universe arises from the binding of quarks into nucleons by the strong interactions of quantum chromodynamics (QCD). The relative mass difference between the proton and neutron is approximately 0.07%, and is attributed to two sources of isospin symmetry breaking in the standard model, namely, differences in the down and up quark masses and their electric charges. Although these breaking effects are minute, they play an essential role in our understanding of the Universe. For example, the primordial abundance of light nuclear elements in the early Universe is exquisitely sensitive to the excess mass of the neutron compared to the proton [1,2].

Lattice QCD (LQCD) provides a first-principles approach for determining isospin-breaking effects in hadronic and nuclear processes. There are a handful of LQCD calculations of the strong contribution to the nucleon mass splitting [2–8] and a comparable number that determine the electromagnetic corrections [4,6–16]. One impressive calculation includes both sources of isospin breaking simultaneously and yields, among other quantities, a postdiction for the nucleon isospin splitting with ~5σ statistical significance [8]. There exists an alternate means for determining the electromagnetic self-energy of the nucleon, from the Cottingham formula [17–20], which makes use of experimental cross sections as input to dispersion integrals. However, the uncertainty attained with this method [21–23] is not yet competitive with the LQCD calculations.

Although inclusion of electromagnetism in LQCD is theoretically straightforward [24,25], it presents practical challenges due to the long-range nature of the electromagnetic (QED) interactions. Specifically, such interactions give rise to power-law finite-volume (FV) corrections, and their removal via extrapolation requires computationally demanding simulations performed at multiple volumes. An analytic understanding of the power-law FV effects within such setups [8,26–28] has enabled reliable FV extrapolations of the single hadron spectrum.

Despite the successful application of present techniques, there are a number of reasons for considering new methods. Control over FV modifications to light nuclear binding energies seems to require particularly large volumes [26]. There are quantities in addition to the spectrum for which a precise knowledge of the QED modifications is needed, for example, corrections to hadronic matrix elements [29] and charged particle scattering [30], both of which suffer from infrared (IR) challenges. LQCD calculations are performed with multiple ultraviolet (UV) regulators, providing valuable cross-checks on the continuum extrapolation of many important quantities [31]. Multiple IR regulators can do the same for LQCD calculations that include QED, but to date, only a few other formulations have been considered [32–34]. Of those, only one is constructed with a local quantum field theory [33,34]. Finally, computationally efficient means of accounting for IR effects are always desirable, not just for lattice QCD + QED, but anywhere long-range Coulomb interactions are present (see, e.g., Ref. [35]).

Motivated by these considerations, we demonstrate the viability of an alternative IR regulator for lattice QCD + QED simulations: namely, the introduction of a photon...
mass $m_{f}$. Although a photon mass term manifestly violates gauge invariance, it maintains locality and its effects on hadronic quantities can be reliably quantified and accounted for within an effective field theory (EFT) framework. The introduction of a new scale $m_{f}$ implies an additional extrapolation within our approach. With the aid of analytic formulas, however, we demonstrate that for the spectrum, such extrapolations can be performed at a single volume and yield results that are consistent with conventional approaches. In the remaining sections, we present the salient features of our calculation.

Analytic considerations.—In continuum Euclidean spacetime, the $R_{ξ}$ gauge fixed action for the massive photon is given by

$$L_{γ} = \frac{1}{4} F_{μν}^{2} + \frac{1}{2ξ} (\partial_{μ}A_{ν})^{2} + \frac{1}{2} m_{γ}^{2} A_{μ}^{2},$$  

where $F_{μν} = \partial_{μ}A_{ν} - \partial_{ν}A_{μ}$; throughout this study, we work in Landau gauge, corresponding to the limit $ξ → 0$. An Abelian theory, such as QED, with a massive vector gauge field is still perturbatively renormalizable. This well-known result follows from the fact that it is possible to find a Becchi-Rouet-Stora-Tyutin (BRST) transformation that leaves the Lagrangian invariant up to a total divergence [36]. The BRST symmetry is preserved if one uses a gauge invariant UV cutoff [37], such as a spacetime lattice; thus, the renormalizability follows from the power-counting theorems for a lattice regularization [38].

We consider three forms of corrections to correlators and hadron mass differences at leading order in the fine-structure constant $α = e^{2}/(4π)$. These corrections arise from either the zero mode contribution to the partition function, the presence of a finite photon mass, or FV effects. The analytic forms of these corrections are determined from an EFT for hadrons of mass $M (M = m_{n}, m_{ρ}, m_{K^{0}})$ and charge $Q$; the naive expansion is in $m_{γ}/M$ (i.e., $Δ_{UV} = M$) [39]. The EFT is a generalization of non-relativistic QED [40] for hadrons that includes a photon mass shift $Δ_{γ}M(α,m_{γ}) = M(α,m_{γ}) - M(α,0)$, which is UV finite. These IR shifts are given by

$$Δ_{γ}M^{LO} = -\frac{α}{2} Q^{2} m_{γ},$$  

$$Δ_{γ}M^{NLO} = \left(Ce^{2} - \frac{α}{4π} Q^{2}\right) \frac{m_{γ}^{2}}{M}. \tag{3}$$

The leading-order (LO) expression is nonanalytic in the squared photon mass, whereas the next-to-leading-order (NLO) expression is analytic but arises from both loops and local contributions [42]; the next-to-next-leading-order (N$^{2}$LO) correction is of order $Δ_{γ}M^{(N^{2}LO)} = O(m_{γ}^{3}/M^{2})$. The latter two orders are accompanied by coefficients not fixed by the hadron charge.

(3) Finite volume: The effects of FV can similarly be calculated using a nonrelativistic QED approach. This is a finite photon mass generalization of that pursued by Refs. [26,27]. The FV corrections to the electromagnetic mass are written as $δ_{f}M(α,m_{γ},L) = M(α,m_{γ},L) - M(α,m_{γ},∞)$, and for charged hadrons are given up to NLO by

$$δ_{f}M^{LO} = 2παQ^{2} m_{γ} \left[I_{1}(m_{γ}L) - \frac{1}{(m_{γ}L)^{3}}\right],$$  

$$δ_{f}M^{NLO} = παQ^{2} \frac{m_{γ}^{2}}{M} \left[2I_{1/2}(m_{γ}L) + I_{3/2}(m_{γ}L)\right], \tag{4}$$

where

$$I_{n}(z) = \frac{1}{2 \pi^{2} n^{2} Γ(n)} \sum_{\nu ≠ 0} K_{\frac{n}{|\nu|}}(z|\nu|) \frac{|\nu|^{2-n}}{|\nu|^{2-n}} \tag{5}$$

and $ν ∈ \mathbb{Z}^{3}$. By contrast, the leading nonvanishing correction for neutral baryons [mesons] appears at N$^{2}$LO [next-to-next-to-next leading order (N$^{3}$LO)]. Because the zero mode of the temporal photon is treated exactly in Eq. (2), the FV corrections are calculated with this mode removed—a manifestation of which is the subtracted term appearing at LO.

Lattice parameters and ensembles.—Electroquenched numerical calculations of the hadron spectrum were performed using a modified version of the Chroma software suite [43]. Studies were performed using dynamical SU(3) flavor symmetric isotropic QCD gauge field configurations generated using a tadpole-improved Lüscher-Weisz gauge action and clover fermion action. The configurations correspond to a single lattice spacing $a = 0.1453(16)$ fm, three spatial extents $L ≈ 3.48$ fm, 4.64 fm, and 6.96 fm, and temporal extents $T > L$. The pion (kaon) and nucleon masses in physical units are $m_{π} = m_{K} = 807.9(9.1)$ MeV and $m_{n} = 1.634(18)$ GeV, respectively. This choice of masses ensures that the only appreciable FV corrections to hadron masses are those arising from QED effects. The QCD ensembles used in this work comprise 956
by postmultiplying each QCD configuration by a single function on QCD

isospin splittings have missing contributions that are

coupling does not renormalize and therefore we take

m by

The photon mass values considered in this work are given

discretized form of Eq.(1) (QED

removing\[11,24,25\] (QEDTL) \[45\], and a naive lattice

massless Coulomb gauge-fixed action with the zero mode

generated using two different lattice actions: a conventional

and therefore in the latter case, the path integration

over nonzero modes is well defined in the

limit.

The uncorrelated photon field configurations Aμ were

using different lattice actions: a conventional

massless Coulomb gauge-fixed action with the zero mode

removed \[11,24,25\] (QEDTL) \[45\], and a naive lattice
discretized form of Eq. (1) (QED\[\alpha\]), where the derivatives

are replaced by finite differences. Note that in Euclidean

space, Landau gauge is a complete gauge-fixing condition, and

therefore in the latter case, the path integration over nonzero

modes is well defined in the m \to 0 limit.

The photon mass values considered in this work are given

by mγ/\bar{m}_π \in [1/14, 1/7, 1/4, 1/3, 5/12, 1/2, 7/12, 1].

In both cases, results were obtained by computing correlation

functions on QCD + QED gauge configurations generated

by postmultiplying each QCD configuration by a single

\epsilon^\mu Q_\mu, where Q_u = 2/3, Q_d = Q_s = \tfrac{1}{3}.

In the electroquenched approximation with SU(3) flavor symmetry,
isospin splittings have missing contributions that are

O(\alpha^2), and are therefore negligible for this study.

In the electroquenched theory, the fine structure

coupling does not renormalize and therefore we take

it to be equal to its experimental value \alpha^{-1} = 137.036…,

measured in the Thomson limit. The presence of electromagnetic interactions demands renormalization

of the valence bare quark masses m_q, however. Since our lattice regulator breaks chiral symmetry, this leads to an

additive shift in the quark mass. We tune the valence quark masses so that, in the presence of electromagnetic

interactions, the neutral \bar{q}q meson mass m_{\bar{q}q} obtained

from the connected part of the \bar{q}q correlation function is

sufficiently close to the pion (kaon) mass \bar{m}_\pi. For our

electroquenched calculation, this choice of renormalization

is robust but the quark mass renormalization in the

full QCD + QED does not allow for a unique separation of the QED and QCD effects \[46\]. All measurements

were performed using valence quark masses \amu = -0.25501 and \amd = \ams = -0.24750

(the QCD bare quark mass is \amu = -0.2450); the resulting

misting for the charge neutral mesons was \Delta m_{\bar{q}q}/\bar{m}_\pi \leq 0.1% for all values of m_j/\bar{m}_\pi \leq 1,

where \Delta m_{\bar{q}q} \equiv m_{\bar{q}q} - \bar{m}_\pi.

The mistuning from strong isospin breaking can be

estimated using chiral symmetry. For the kaon, one finds

\[ \frac{\Delta m_{K^+,K^0}}{\bar{m}_K} \approx \frac{\Delta m_{\mu\mu} - \Delta m_{dd}}{2 \bar{m}_K} \lesssim 0.0004, \]

while the nucleon correction is given by

\[ \frac{\Delta m_{n,p}}{m_n} \approx \frac{\alpha_{n\mu}}{m_n} \left( \frac{\Delta m_{\mu\mu} - \Delta m_{uu}}{4\pi f_n m_n} \right) \frac{\bar{m}_n^2}{\bar{m}_\pi}. \]

We can estimate the parameter \alpha_{n\mu} from the LQCD
determination of the m_d - m_u contribution to the nucleon

mass splitting [2–8] and find \Delta m_{n,p}/\bar{m}_n \lesssim 0.0002. In both

cases, mistuning is a potentially sizable correction to our

results, which affects both the QEDTL and QED\[\mu\] determinations. Although a precise quark mass tuning

is required for practical applications, it is not needed in the

present proof-of-principle study \[47\].

Analysis and results.—Shell-shell and shell-point

correlation functions were estimated using a single

measurement per configuration, with a randomly chosen

spacetime source location. Following Ref. [9], we average

observables over +e and -e on each configuration in

order to exactly cancel off the \O(e) contributions to

FIG. 1. Zero-mode adjusted (filled) and unadjusted (open) effective mass difference for the kaon splitting (m_j/\bar{m}_\pi = 1/14 and L/a = 24). The diagonal grid lines have slope 2\epsilon; the red and blue points correspond to different sinks. The gray bands correspond to uncertainties on the extracted value for \Delta M_{\text{eff}}.

\begin{table}[h]
\begin{tabular}{|c|c|c|}
\hline
Splitting & K_L & \chi^2/DOF & \Delta M/M \times 10^3 \\
\hline
p-n & 1 & 0.07/2 & 0.73(05) \\
 & 2 & 0.03/1 & 0.70(13) \\
K^+ - K^0 & 1 & 0.29/2 & 3.71(06) \\
 & 2 & 0.17/1 & 3.68(20) \\
\hline
\end{tabular}
\caption{QEDTL induced mass splittings, extrapolated to $L \to \infty$ ($m_j = 0, K_L = 0$).}
\end{table}

FIG. 2. QEDTL induced mass differences, extrapolated to $L \to \infty$ (taking $K_L = 2$).
hadrons appearing in Eq. (2) nonperturbatively (for neutral
Both formulas treat the zero mode of the temporal photon
account for the backward propagating state by consider-
lattice of finite temporal extent

\[ \Delta \text{mass difference} \]

extract a clear signal for the mass difference. For the
exploiting the correlations between \( A \) and \( B \), we are able
extract a clear signal for the mass difference. For the
nucleons, we consider a generalized effective mass formula of the form

\[ M_{\text{eff, exp}}(\tau) = -\frac{1}{a} \log \frac{C(\tau + a)}{C(\tau)} + 2\tau + xa, \tag{8} \]

which neglects the backward propagation of states on a
lattice of finite temporal extent \( T \). For mesons, we account
for the backward propagating state by considering
a generalized effective mass formula of the form

\[ M_{\text{eff, cosh}}(\tau) = \frac{1}{a} \cosh^{-1} \left[ \frac{\cosh(\tau + a) + \cosh(\tau - a)}{2} \right] - xT, \tag{9} \]

where \( h(\tau, a) = xa(a - T + 2\tau) + \log[C(\tau + a)/C(\tau)] \).
Both formulas treat the zero mode of the temporal photon
field appearing in Eq. (2) nonperturbatively (for neutral
hadrons \( x = 0 \) and these expressions reduce to their
conventional forms). Although this contribution is neg-
ligible compared to the hadron masses, for the lattice
parameters considered it can be comparable in magnitude
to the mass differences we wish to extract. Figure 1
provides an explicit example of the behavior of \( \Delta M_{\text{eff}}(\tau) \)
for the kaon mass splitting, computed both with and
without the zero-mode contribution accounted for.

Mass differences were determined for all volumes and
photon masses via a correlated constant least-squares fit to
\( \Delta M_{\text{eff}} \) in the plateau region, as demonstrated in Fig. 1. An
analogous determination from exponential fits to a ratio of
correlation functions yielded consistent results. Systematic
uncertainties were estimated by varying the region over
which the fits were performed, and all uncertainties were
added in quadrature. The extracted mass shifts were
subsequently extrapolated to vanishing photon mass
and/or the infinite-volume limit using the fit formula

\[ \Delta M(\alpha, L, m_\gamma) = \Delta M(\alpha) + \sum_{k=0}^{K_L} \delta_{kL} M^{NLO}(\alpha, m_\gamma) + \sum_{k=0}^{K_L} \delta_{kL} M^{NLO}(\alpha, m_\gamma, L), \tag{10} \]

where \( \delta_{kL} \) and \( \delta_{kL} M^{NLO} \) indicate the order of each extrapolation.
In the case of mass splittings, an appropriate linear
combination of mass shift formulas was used. Note that
for the QED TL extrapolations, \( \delta_{kL} = 0 \); the appropriate FV
formulas for \( \delta_{kL} M^{NLO} \) retain \( T \) dependence, and may be
found in Ref. [8].

We carry out two independent analyses to test the viability
of our proposal: (1) an infinite-volume extrapolation of
QED TL induced mass differences, as is conventionally
performed, and (2) an \( m_\gamma \to 0 \) extrapolation of QED M
induced mass differences using data at a single FV, but
after having first removed the lowest order FV contributions
\( \delta_{kL} M \). Both types of extrapolation were performed using
Eq. (10), noting that many of the lowest-order contributions
are fixed by theory. Results for the first analysis, using all
three volumes, are provided in Table I and representative fits
are shown in Fig. 2. Results for the second analysis on the
smallest volume are provided in Table II for comparison, and
shown in Fig. 3. Analogous QED M extrapolations, per-
formed at each of the three volumes, are summarized in
Fig. 4 and are consistent not only with each other, but also
the QED$_{\text{TL}}$ extrapolations. In all cases, we find that the numerical and theoretical mass corrections are in excellent agreement down to at least $m_{\pi}L \sim 1$.

The most computationally demanding part of our calculation involves multiple inversions of the Dirac operator. Assuming, conservatively, a linear scaling with spacetime volume, the total inversion cost for $L/a = 32$ is $515/956 \times (32/24)^3 \sim 1.3$ times greater than that of $L/a = 24$. By comparison, the $L/a = 48$ inversion cost is $\sim 3.8$ times greater. The $L/a = 24$ extrapolations using $m_{\gamma}/\bar{m}_{\pi} \in [1/4, 1/2]$ data, provided in Table II, are consistent with those using all values of $m_{\gamma}$. The results are also consistent with the QED$_{\text{TL}}$ extrapolation using three volumes, provided in Table I, but required only 4/5 the computational cost. We therefore conclude that for the same precision and accuracy, the numerical cost of our QED$_{\gamma}$ calculation of the mass splittings is comparable to or less than that of QED$_{\text{TL}}$.

Conclusion.—This work demonstrates that it is possible to reliably estimate infinite-volume hadron mass differences induced by electromagnetism on a single lattice volume with QED$_{\gamma}$. Conservatively, the pionless EFT employed in this work is valid for $m_{\gamma} \ll 2m_{\pi}$ and $m_{\pi}L \gtrsim 4$. Provided these inequalities are satisfied, the analytic expressions obtained for the mass shift are valid up to $O(m_{\pi}^2/M^3, \alpha^2)$, and are independent of the pion mass; from our numerics, it appears that this order is sufficient to obtain reliable extrapolations of the mass shifts in the regime $m_{\gamma}/m_{\pi} \lesssim 1$ and $m_{\pi}L \gtrsim 1$.

On preexisting lattice configurations, and for equal computational cost, we obtain an equally precise uncertainty in extrapolated differences as compared to the traditional method. This cost comparison does not account for the significant overhead of generating the configurations in the first place. The results of our analysis pave the way for a more complete treatment of QED corrections using this approach. When considering more involved LQCD calculations, such as charged-particle scattering [30], our method provides a mass gap to produce a photon, thus increasing the range of energy for which the standard Lüscher method [48,49] for obtaining the scattering phase shift can be employed. It will be interesting to explore these types of calculations, and also to use our method with chiral fermions, which do not suffer from additive quark mass renormalization. Finally, it would be interesting to see if our method of screened interactions coupled with analytic extrapolation techniques is of benefit to quantum many-body calculations.

We would like to thank W. Detmold, R. Edwards, B. Joó, D. Richards, and K. Orginos for the use of the JLab–W&M QCD gauge field configurations and D. B. Kaplan, T. C. Luu, and M. J. Savage for useful conversations and correspondences. Additionally, we would like to thank A. Patella and N. Tantalo for stimulating discussions during the Lattice 2015 conference. We acknowledge the hospitality of the International Institute of Physics at the Federal University of Rio Grande de Norte and the Institute for Nuclear Theory at the University of Washington (Nuclear Reactions Workshop [50]), where portions of this work were completed. Computations for this study were carried out on facilities of the USQCD Collaboration, which are funded by the Office of Science of the U.S. Department of Energy. M. G. E was supported by U.S. Department of Energy Early Career Research Award No. DE-SC0010495, and moneys from the Dean of Science Office at MIT. B. C. T. was supported in part by a joint City College of New York-RIKEN/Brookhaven Research Center fellowship, a grant from the Professional Staff Congress of the CUNY, and by the U.S. National Science Foundation, under Grant No. PHY15-15738. A. W.-L. was supported in part by U.S. Department of Energy (DOE) Contract No. DE-AC05-06OR23177, under which Jefferson Science Associates, LLC, manages and operates the Jefferson Lab and by U.S. DOE Early Career Award Contract No. DE-SC0012180.

endres@mit.edu
a.shindler@fz-juelich.de
btiburzi@ccny.cuny.edu
awalker-loud@lbl.gov

[39] Dynamical pions must be accounted for when $m_\pi \gtrsim 2m_\rho$. This can be handled within chiral perturbation theory but is not considered in the present work.
[42] The local operator contributing at NLO is $\phi^3\phi^4\psi$, where the scalar $\phi$ picks up a vacuum expectation value, thereby Higgsing the photon. Whereas the operator $m_\gamma^2 A_\mu A_\mu \psi^4$ contributes to masses at $N^3\mathrm{LO}$, it is a prime example of a gauge noninvariant operator.
[45] Note that this formulation of QED violates reflection positivity, leading to the ill behavior of charged particle propagators for $T \to \infty$ at fixed $L$ [8]. Our QED$_T$ computation uses $T/L \sim 1$, for which the FV effect is mild.
[47] An additional mistuning effect arises because of the $T$ dependence of quark masses in QED$_T$ [8]. Addressing this is required for practical applications, or could be eliminated by using the QED$_L$ formulation.