

Massive photons: an infrared regularization scheme for lattice QCD+QED

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The commonly adopted approach for including electromagnetic interactions in lattice QCD simulations relies on using finite volume as the infrared regularization for QED. The long-range nature of the electromagnetic interaction, however, implies that physical quantities are susceptible to power-law finite volume corrections, which must be removed by performing costly simulations at multiple lattice volumes, followed by an extrapolation to the infinite volume limit. In this work, we introduce a photon mass as an alternative means for gaining control over infrared effects associated with electromagnetic interactions. We present findings for hadron mass shifts due to electromagnetic interactions (i.e., for the proton, neutron, charged and neutral kaon) and corresponding mass splittings, and compare the results with those obtained from conventional QCD+QED calculations. Results are reported for numerical studies of three flavor electroquenched QCD using ensembles corresponding to 800 MeV pions, ensuring that the only appreciable volume corrections arise from QED effects. The calculations are performed with three lattice volumes with spatial extents ranging from 3.4 - 6.7 fm. We find that for equal computing time (not including the generation of the lattice configurations), the electromagnetic mass shifts can be reliably extracted from computations on the smallest lattice volume with comparable or better precision than the conventional approach.

PACS numbers: 11.15.Ha, 12.38.-t, 12.38.Gc

INTRODUCTION

Approximately 95% of the visible mass of the universe arises from the confinement of quarks in 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 electromagnetic 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 prediction for the nucleon isospin splitting with $\sim 5\sigma$ 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 in-

put 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 straight-forward [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 corrections, and their removal via extrapolation requires computationally demanding simulations performed at multiple volumes. An analytic understanding of the power-law finite volume effects within such setups [26, 27] have enabled reliable finite volume 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 finite-volume modifications to light nuclear binding energies seem to require particularly large volumes [26]. There are quantities in addition to the spectrum for which precise knowledge of the QED modifications are needed, for example, corrections to hadronic matrix elements [28] and charged particle scattering [29], both of which suffer from infrared (IR) challenges. LQCD calculations are performed with a number of different ultraviolet (UV) regulators, providing valuable cross-checks on the continuum extrapolation of many important quantities [30]. Multiple IR regulators can do the same for calculations that include QED,

TABLE I. $\bar{q}q$ meson mass shifts.

m_γ/\bar{m}_π	am_γ	$\Delta m_{uu}/\bar{m}_\pi$	$\Delta m_{qq}/\bar{m}_\pi$ ($q = d, s$)
0	0	0.000560(40)(74)	0.00018210(33)(15)
1/14	0.0424471	0.001089(21)(14)	0.00029882(54)(36)
1/7	0.084894	0.001059(21)(15)	0.00029127(53)(36)
1/4	0.148565	0.000971(20)(17)	0.00026946(52)(43)
1/3	0.198087	0.000865(20)(19)	0.00024310(51)(46)
5/12	0.247608	0.000726(19)(20)	0.00020818(50)(48)
1/2	0.29713	0.000551(19)(21)	0.00016464(48)(51)
7/12	0.346652	0.000342(19)(21)	0.00011250(47)(53)
1	0.59426	-0.001184(16)(25)	-0.00026832(41)(60)

however, at present there are only a few other methods under development [31, 32]. Finally, computationally less demanding means of accounting for IR effects are always welcome.

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_γ . Although a photon mass term manifestly violates gauge-invariance, its effects on hadronic quantities can be reliably quantified and accounted for within an effective theory framework. The introduction of a new scale, m_γ , implies an additional extrapolation within our approach. With the aid of analytic formulas, however, we demonstrate that for the spectrum, a single extrapolation in m_γ at fixed volume is sufficient to achieve results 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

$$\mathcal{L}_\gamma = \frac{1}{4}F_{\mu\nu}^2 + \frac{1}{2\xi}(\partial_\mu A_\mu)^2 + \frac{1}{2}m_\gamma^2 A_\mu^2 \quad (1)$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$; throughout this study, we work in Landau gauge, corresponding to the limit $\xi \rightarrow 0$. 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 BRST transformation that leaves the Lagrangian invariant up to a total divergence [33]. Keeping in mind that the BRST symmetry is not a property of the continuum theory but rather of a gauge invariant ultraviolet cutoff [34], one can show that the renormalizability follows from the power-counting theorems for a lattice regularization [35].

We consider three forms of corrections to correlators and hadron mass differences at leading order in the fine-structure constant $\alpha = e^2/(4\pi)$. These corrections arise from either the zero mode contribution to the partition

function, the presence of a finite photon mass, or finite volume effects. The analytic forms of these corrections are determined from an effective theory for hadrons of mass M ($M = m_n, m_p, m_{K^+}$, and m_{K^0}) and charge Q , with a cutoff given by $\Lambda_{UV} \sim M$; the point-like treatment of hadrons is expected to break down at $\Lambda_{UV} \sim 2m_\pi$. The effective field theory is a generalization of nonrelativistic QED (NRQED) [36] for hadrons that includes a photon mass term, and additional operators unconstrained by gauge invariance.

(1) *Zero mode*: As demonstrated below, for sufficiently small m_γ , the zero mode of the temporal photon field appearing in Eq. 1 must be treated exactly. In that limit, the charged particle two-point function has the form

$$C(\tau) = Z e^{-M\tau - x\tau^2} \quad (2)$$

where Z is an overlap factor, and the zero-mode contribution appears in $x = (4\pi\alpha Q^2)/(2m_\gamma^2 L^3 T)$.

(2) *Photon mass*: The hadron's electromagnetic mass shift can be determined as a function of photon mass, order-by-order in an expansion in the hadron's Compton wavelength. With the electromagnetic mass written as $M(\alpha, m_\gamma)$, we define the mass shift $\Delta M(\alpha, m_\gamma) = M(\alpha, m_\gamma) - M(\alpha, 0)$, which is ultraviolet finite. These infrared shifts are given by

$$\begin{aligned} \Delta M^{LO} &= -\frac{\alpha}{2} Q^2 m_\gamma, \\ \Delta M^{NLO} &= \left(C e^2 - \frac{\alpha}{4\pi} Q^2 \right) \frac{m_\gamma^2}{M}. \end{aligned} \quad (3)$$

The leading-order (LO) expression is non-analytic in the squared photon mass, whereas the next-to-leading order (NLO) expression is analytic but arises from both loops and local contributions. The latter are accompanied by an unfixed parameter C . The NNLO correction is of order $\Delta M^{NNLO} = \mathcal{O}(m_\gamma^3/M^2)$.

(3) *Finite volume*: The effects of finite volume can similarly be calculated using an NRQED approach. This is a finite photon mass generalization of that pursued by [26, 27]. The finite volume corrections to the electromagnetic mass are written as $\delta_L M(\alpha, m_\gamma, L) = M(\alpha, m_\gamma, L) - M(\alpha, m_\gamma, \infty)$, and given up to NLO by

$$\begin{aligned} \delta_L M^{LO} &= 2\pi\alpha Q^2 m_\gamma \left[\mathcal{I}_1(m_\gamma L) - \frac{1}{(m_\gamma L)^3} \right], \\ \delta_L M^{NLO} &= \pi\alpha Q^2 \frac{m_\gamma^2}{M} \left[2\mathcal{I}_{1/2}(m_\gamma L) + \mathcal{I}_{3/2}(m_\gamma L) \right], \end{aligned} \quad (4)$$

where

$$\mathcal{I}_n(z) = \frac{1}{2^{n+\frac{1}{2}} \pi^{\frac{3}{2}} \Gamma(n)} \sum_{\nu \neq 0} \frac{K_{\frac{3}{2}-n}(z|\boldsymbol{\nu}|)}{(z|\boldsymbol{\nu}|)^{\frac{3}{2}-n}} \quad (5)$$

and $\boldsymbol{\nu} \in \mathbb{Z}^3$. The subtraction at LO is necessitated by the exact treatment of the zero mode of the temporal photon. In the limit $m_\gamma L \rightarrow 0$, and after all zero-mode contributions are subtracted, these expressions reduce to the known results: $\delta_L M^{LO} = \alpha Q^2 c_1/(2L)$ and

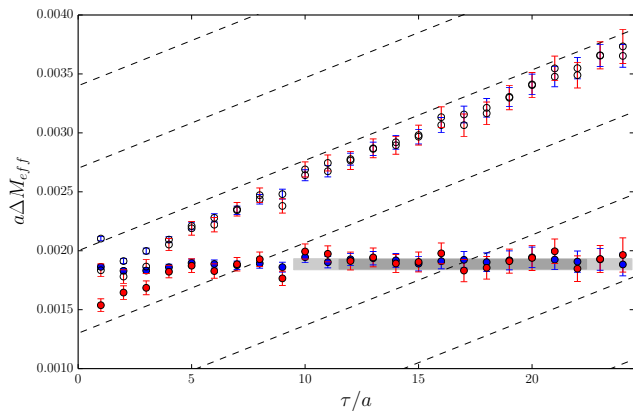


FIG. 1. Zero-mode adjusted (filled) and unadjusted (open) effective mass difference for the kaon splitting ($m_\gamma/\bar{m}_\pi = 1/14$ and $L/a = 24$). Diagonal grid lines have slope $2x$; red/blue points correspond to different sources. Gray bands correspond to statistical and systematic uncertainties on the extracted value for ΔM_{eff} .

$\delta_L M^{NLO} = \alpha Q^2 c_1 / (ML^2)$, where $c_1 = -2.83729\dots$; higher order corrections behave as $\delta_L M^{NNLO} = \mathcal{O}(L^{-3})$, and $\delta_L M^{NNNLO} = \mathcal{O}(L^{-4})$. Note that the leading non-vanishing correction for neutral baryons (mesons) appears at $NNLO$ ($NNNLO$).

LATTICE PARAMETERS AND ENSEMBLES

Electroquenched numerical calculations of the hadron spectrum were performed using a modified version of the Chroma software suite [37]. 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 and three spatial extents: $L \sim 3.48$ fm, 4.64 fm and 6.96 fm. The pion (kaon) and nucleon masses in physical units are $\bar{m}_\pi = \bar{m}_K = 807.0(0.2)(8.9)$ MeV and $\bar{m}_n = 1.634(0)(18)$ MeV, with uncertainties from a combined statistical and fitting systematic and lattice spacing, respectively. The choice of masses ensures that the only appreciable finite-volume corrections to hadron masses are those arising from QED effects. The QCD ensembles used in this work comprise 956 ($L/a = 24$), 515 ($L/a = 32$) and 342 ($L/a = 48$) configurations and are a subset of those described in [?]; further details regarding the ensembles, lattice action and parameters can be found there.

Uncorrelated photon field configurations A_μ were generated using two different lattice actions: a conventional massless Coulomb gauge-fixed action with the zero-mode removed [11], and a naive lattice discretized form of Eq. 1, where 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 $m_\gamma \rightarrow 0$ limit. The photon mass values considered in this work lie on the interval $m_\gamma/\bar{m}_\pi \in [1/14, 1]$, and are provided in Table I. In both cases, we obtain lattice QCD+QED gauge configurations by post-multiplying the QCD configurations by $e^{ieQ_q A_\mu}$, where $Q_u = 2/3$, $Q_d = Q_s = -1/3$. Correlation functions were then estimated on the background QCD+QED gauge fields. For studies of isospin splittings, the electroquenched approximation results in errors that appear at a higher order in isospin breaking.

In the electroquenched theory, the fine structure coupling does not renormalize and therefore we take it to be equal to its experimental value, $\alpha^{-1} = 137.036\dots$, 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 $m_{q\bar{q}}$ obtained from the connected part of the $\bar{q}q$ correlation function is sufficiently close to the pion (kaon) mass \bar{m}_π . 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 [39]. All measurements were performed using valence quark masses $am_u = -0.25501$ and $am_d = am_s = -0.24750$ (the QCD bare quark mass is $am_q = -0.2450$); a summary of the measured values of $\Delta m_{q\bar{q}}/\bar{m}_\pi$ for various $m_\gamma/\bar{m}_\pi \leq 1$ are provided in Table I for $L/a = 48$ ensembles. In all cases, the tuning was achieved with sub-percent precision.

Guided by chiral perturbation theory, we can estimate the induced strong isospin-breaking effects of any mistuning on the spectrum. For the kaon, one finds

$$\frac{\Delta m_{K^+ - K^0}}{\bar{m}_K} \simeq \frac{1}{2} \frac{\Delta m_{uu} - \Delta m_{dd}}{\bar{m}_K} \quad (6)$$

which yields $\Delta m_{K^+ - K^0}/\bar{m}_K \lesssim 0.0004$. In the case of the nucleon, the correction depends upon an unknown low-energy constant

$$\frac{\Delta m_{n-p}}{\bar{m}_n} \simeq \alpha_{d-u} \frac{2(\Delta m_{dd} - \Delta m_{uu})}{\bar{m}_\pi} \frac{\bar{m}_\pi^2}{4\pi f_\pi \bar{m}_n}. \quad (7)$$

We can estimate the parameter α_{d-u} from the LQCD determination of the $m_d - m_u$ contribution to the nucleon mass splitting [2–8] and find $\Delta m_{p-n}/\bar{m}_n \lesssim 0.0002$. In both cases, mistuning is a potentially sizable correction to our results, which affects both the $m_\gamma \neq 0$ and $m_\gamma = 0$ determinations. More precise quark mass tuning is required for practical applications, but is not needed in the present proof-of-principle study.

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 [9], we average observables over $+e$ and $-e$ on a configuration-by-configuration basis in order to exactly cancel off the $\mathcal{O}(e)$ contributions to statistical noise. Mass differences due to electromagnetic effects can be determined from the late-time dependence of single hadron correlation functions $C^A(\tau)$ and $C^B(\tau)$, by studying the plateau region of an *effective mass difference* $\Delta M_{\text{eff}}^{AB}(\tau) = M_{\text{eff}}^A(\tau) - M_{\text{eff}}^B(\tau)$. By exploiting the correlations between A and B , we are able to extract a clear signal for the mass difference. For the nucleons, we consider a generalized effective mass formula of the form:

$$M_{\text{eff,exp}}(\tau) = -\frac{1}{a} \log \frac{C(\tau+a)}{C(\tau)} + 2x\tau + xa, \quad (8)$$

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:

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

where

$$h(\tau, a) = xa(a - T + 2\tau) + \log \frac{C(\tau+a)}{C(\tau)}. \quad (10)$$

Both formulas remove the leading zero-mode contribution to the correlator appearing in Eq. 2, which if left unaccounted for would manifest as linear growth of ΔM_{eff} as a function of τ with slope $2x$. Although this contribution is negligible compared to the hadron masses, for the lattice parameters considered it can be comparable in magnitude to the mass differences we wish to extract. Fig. 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. Note that for neutral hadrons $x = 0$ and the expressions above for the generalized effective mass reduce to their conventional forms.

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

$$\Delta M(\alpha, L, m_\gamma) = \Delta M(\alpha) + \sum_{k=0}^K \Delta M^{N^k LO}(\alpha, m_\gamma)$$

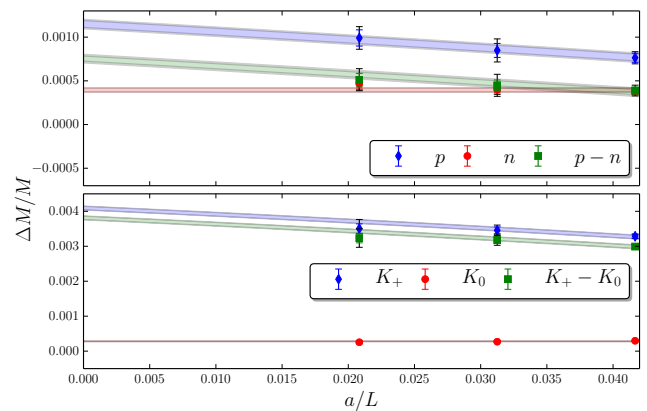


FIG. 2. Mass differences, extrapolated to infinite volume, obtained from Coulomb gauge-fixed ensembles.

$$+ \sum_{k=0}^{K_L} \delta_L M^{N^k LO}(\alpha, m_\gamma, L), \quad (11)$$

where K and K_L indicate the order of each extrapolation. In the case of mass splittings, an appropriate linear combination of mass shift formulas were used. Note that for the infinite volume extrapolations of $m_\gamma = 0$ mass differences, $\Delta M^{N^k LO}(\alpha, m_\gamma) = 0$ for all k .

We carry out two independent analyses to test the viability of our proposal: 1) an infinite volume extrapolation of the $m_\gamma = 0$ mass differences, as is conventionally performed, and 2) a combined $m_\gamma \rightarrow 0$ and $L \rightarrow \infty$ extrapolation of mass differences using data at a *fixed* finite volume. Both types of extrapolation were performed using Eq. 11, noting that many of the lowest-order contributions are fixed by theory. In the case of the m_γ extrapolations, for sufficiently large $m_\gamma L$, the contributions from the second summand become highly suppressed, thus enabling a reliable infinite volume extrapolation for fixed L . The numerical and theoretical volume corrections are in excellent agreement down to at least $m_\gamma L \sim 1$.

Results for the first analysis are provided in Table II and representative fits are shown in Figure 2 (taking $K_L = 1$). Results for the combined extrapolation on 24^3 and 32^3 ensembles (taking $K_L = 1$) are provided in Table III and representative fits are displayed in Figure 3. Corresponding 48^3 extrapolations for the kaon and nucleon mass difference are consistent with these to within 1σ and 2σ , respectively. A global weighted average of all our fits yields the extrapolated electromagnetic splittings

$$\begin{aligned} \Delta m_{K_+ - K_0} &= \begin{cases} 3.08(06)(33) \text{ MeV} & m_\gamma \neq 0 \\ 3.07(06)(33) \text{ MeV} & m_\gamma = 0 \end{cases}, \\ \Delta m_{p-n} &= \begin{cases} 1.18(11)(33) \text{ MeV} & m_\gamma \neq 0 \\ 1.23(10)(33) \text{ MeV} & m_\gamma = 0 \end{cases}, \end{aligned} \quad (12)$$

where the first uncertainty is our combined statistical and systematic fitting uncertainties and the second is our conservative estimate of the mistuning uncertainty.

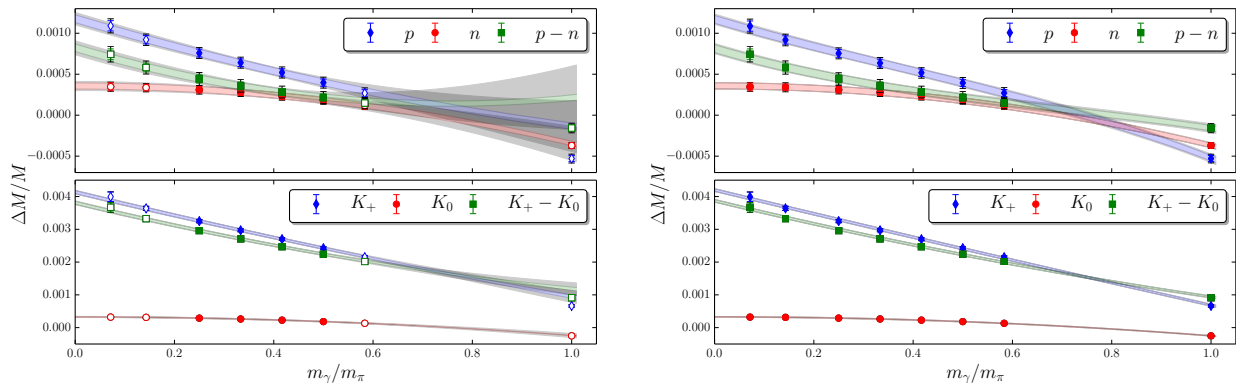


FIG. 3. Volume adjusted ($K_L = 1$) nucleon (top) and kaon (bottom) mass differences, extrapolated to $m_\gamma \rightarrow 0$ at fixed $L/a = 24$. Fits were performed using data at all $m_\gamma \neq 0$ (right) and only the middle four (of eight) values of m_γ (left).

TABLE II. Volume extrapolated mass splittings ($m_\gamma = 0$).

splitting	K_L	χ^2/dof	$\Delta M/M \times 10^3$
$p - n$	1	0.04/2	0.76(05)
	2	0.04/1	0.70(13)
$K^+ - K^0$	1	0.88/2	3.81(06)
	2	0.17/1	3.68(20)

TABLE III. Representative m_γ extrapolated mass splittings.

splitting	L/a	m_γ/m_π range	K	χ^2/dof	$\Delta M/M \times 10^3$
$p - n$	24	1/14 - 1	2	0.09/5	0.79(06)
	24	1/4 - 1/2	1	0.06/2	0.81(08)
	24	1/14 - 1/7	0	0.00/1	0.81(07)
	32	1/14 - 1	2	0.16/5	0.68(08)
	32	1/4 - 1/2	1	0.04/2	0.73(12)
	32	1/14 - 1/7	0	0.05/1	0.69(08)
$K^+ - K^0$	24	1/14 - 1	2	0.42/5	3.77(06)
	24	1/4 - 1/2	1	0.12/2	3.79(06)
	24	1/14 - 1/7	0	0.32/1	3.79(06)
	32	1/14 - 1	2	0.09/5	3.84(06)
	32	1/4 - 1/2	1	0.03/2	3.85(08)
	32	1/14 - 1/7	0	0.03/1	3.86(09)

CONCLUSION

This work demonstrates that reliable infinite volume estimates of hadron mass differences induced by electromagnetic effects are possible with only a single lattice volume of $(3.4 \text{ fm})^3$. On pre-existing 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 [29], our method provides a mass gap

to produce a photon, thus increasing the range of energy for which the standard Lüscher method [40, 41] 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.

We would like to thank R. Edwards, B. Jóó, D. Richards and K. Orginos for the use of the JLab/W&M QCD gauge field configurations used in this work, 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 would like to 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 [42]), 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 the the U. S. Department of Energy Early Career Research Award 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 the U.S. Department of Energy (DOE) contract DE-AC05-06OR23177, under which Jefferson Science Associates, LLC, manages and operates the Jefferson Lab and by the U.S. DOE Early Career Award contract DE-SC0012180.

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