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

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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 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.

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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 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 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, 22] 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 (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] have 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 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 [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 (QFT) [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., [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 $m_\gamma$. 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, $m_\gamma$,
FIG. 1. Zero-mode adjusted (filled) and unadjusted (open) effective mass difference for the kaon splitting ($m_\pi/m_\pi = 1/14$ and $L/a = 24$). Diagonal grid lines have slope 2x; red/blue points correspond to different sinks. Gray bands correspond to uncertainties on the extracted value for $\Delta M_{\text{eff}}$.

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 $R_\xi$ gauge fixed action for the massive photon is given by

$$L_\gamma = \frac{1}{4} F_{\mu\nu}^2 + \frac{1}{2\xi} (\partial_\mu A_\nu)^2 + \frac{1}{2} m_\gamma^2 A_\mu^2$$ (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 $\xi \to 0$. 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 [30]. The BRST symmetry is preserved if one uses a gauge invariant UV cutoff [31], such as a spacetime lattice, thus the renormalizability follows from the power-counting theorems for a lattice regularization [32].

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 FV effects. The analytic forms of these corrections are determined from an EFT for hadrons of mass $M$ ($M = m_\pi$, $m_\rho$, $m_{K^+}$, and $m_{K^0}$) and charge $Q$; the naive expansion is in $m_\gamma/M$ (i.e. $\Delta_{UV} = M$) [29]. The EFT is a generalization of nonrelativistic QED (NRQED) [40] for hadrons that includes a photon mass term, and additional operators that are unconstrained by gauge invariance.

(1) **Zero mode:** For sufficiently small $m_\gamma$, the zero mode of the temporal photon field appearing in Eq. 1 must be treated nonperturbatively [41]. In this regime, the two-point function for single hadrons has the form

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

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

(2) **Photon mass:** The hadrons electromagnetic mass shift can be determined as a function of photon mass, order-by-order in an expansion in powers of $m_\gamma/M$. With the electromagnetic mass written as $M(\alpha, m_\gamma)$, we define the mass shift $\Delta_\gamma M(\alpha, m_\gamma) = M(\alpha, m_\gamma) - M(\alpha, 0)$, which is UV finite. These IR shifts are given by

$$\Delta_\gamma M_{\text{LO}} = \frac{\alpha}{2} Q^2 m_\gamma,$$

$$\Delta_\gamma M_{\text{NLO}} = \left(C e^2 - \frac{\alpha}{4\pi} Q^2\right) \frac{m_\gamma^2}{M}.$$ (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 [42]; the $N^2$LO correction is of order $\Delta_\gamma M^{N^2\text{LO}} = \mathcal{O}(m_\gamma^4/M^2)$. 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 an NRQED approach. This is a finite photon mass generalization of that pursued by [26, 27]. The FV 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 for charged hadrons, are given up to NLO by

$$\delta_L M_{\text{LO}} = 2\pi \alpha Q^2 m_\gamma \left[I_1(m_\gamma L) - \frac{1}{(m_\gamma L)^3}\right],$$

$$\delta_L M_{\text{NLO}} = \pi \alpha Q^2 \frac{m_\gamma^2}{M} \left[2I_{1/2}(m_\gamma L) + I_{3/2}(m_\gamma L)\right].$$ (4)
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 \( m_\gamma \to 0 \) limit. The photon mass values considered in this work are given by \( m_\gamma/m_\pi \in [1/14, 1/7, 1/4, 1/3, 5/12, 1/2, 7/12, 1] \). In both cases, results were obtained by computing correlation functions on QCD+QED gauge configurations generated by post-multiplying each QCD configurations by a single \( e^{-i Q_\alpha A_\mu} \), where \( Q_\alpha = 2/3 \), \( Q_d = Q_s = -1/3 \). In the electroquenched approximation with SU(3) flavor symmetry, isospin splittings have missing contributions that are \( O(\alpha^2) \), and 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, \( \alpha^{-1} = 137.036 \ldots \), measured in the Thomson limit. The presence of electromagnetic interactions demands renormalization of the valence bare quark masses \( m_{q_i} \), 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 \( m_{\pi} \). 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 \( a m_u = -0.25501 \) and \( am_d = am_s = -0.24750 \) (the QCD bare quark mass is \( am_q = -0.2450) \); the resulting mistuning for the charge neutral mesons was \( \Delta m_{\bar{q}q}/m_{\bar{q}q} \lesssim 0.1\% \) for all values of \( m_u/m_s \leq 1 \), where \( \Delta m_{\bar{q}q} = m_{\bar{q}q} - m_{\bar{q}q}^{\text{phys}} \).

The mistuning from strong isospin-breaking can be estimated using chiral symmetry. For the kaon, one finds

\[
\frac{\Delta m_{K^+ - K^0}}{m_{K}} \simeq \frac{1}{2} \frac{\Delta m_{uu} - \Delta m_{dd}}{m_{K}} \lesssim 0.0004 ,
\]

while the nucleon correction is given by

\[
\frac{\Delta m_{n-p}}{m_{n}} \simeq \alpha_{d-u} \frac{2 (\Delta m_{dd} - \Delta m_{uu})}{m_{n}} \frac{m_{n}^2}{4\pi f_{\pi} m_{\pi}} .
\]

We can estimate the parameter \( \alpha_{d-u} \) from the LQCD determination of the \( m_d - m_u \) contribution to the nucleon mass splitting [2,8] and find \( \Delta m_{n-p}/m_n \lesssim 0.0002 \). In both cases, mistuning is a potentially sizable correction to our results, which affects both the QEDTL and QEDM 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 [8], we average observables over \( +e \) and \( -e \) on each configuration in order...
to exactly cancel off the $O(\epsilon)$ 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 $\Delta M^\text{AB}_{\text{eff}}(\tau) = M^\text{A}_{\text{eff}}(\tau) - M^\text{B}_{\text{eff}}(\tau)$. By 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:

$$\Delta M_{\text{eff,exp}}(\tau) = \frac{1}{a} \log \left( \frac{C(\tau + a)}{C(\tau)} \right) + 2\epsilon \tau + xa , \quad (8)$$

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:

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

where $h(\tau,a) = xa(a - T + 2\tau) + \log[C(\tau + a)/C(\tau)]$. Both formulas treat the zero mode of the temporal photon field appearing in Eq. 2 non-perturbatively (for neutral hadrons $x = 0$ and these expressions reduce to their conventional forms). 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.

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 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:

$$\Delta M(\alpha, L, m_\gamma) = \Delta M(\alpha) + \sum_{k=0}^{K_L} \Delta_\gamma M^{N_k \text{LO}}(\alpha, m_\gamma) + \sum_{k=0}^{K_\gamma} \delta L M^{N_k \text{LO}}(\alpha, m_\gamma, L) , \quad (10)$$

where $K_\gamma$ 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 $QED_{TL}$ extrapolations, $K_\gamma = 0$; the appropriate FV formulas for $\delta L M^{N_k \text{LO}}$ retain $T$-dependence, and may be found in [3].

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, $\delta L M$. 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 1 and representative fits are shown in Fig. 2. Results for the second analysis on the smallest volume are provided in Table 1 for comparison, and shown in Fig. 3. Analogous $QED_M$ extrapolations, performed at each of the three volumes, are summarized in Fig. 4 and are consistent not only with each other, but also the $QED_{TL}$ extrapolations. In all cases, we find that the numerical and theoretical mass corrections are in excellent agreement down to at least $m_\gamma L \sim 1$.

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 \text{ times greater. The } L/a = 24 \text{ extrapolations using } m_{\pi}/\bar{m}_{\pi} \in [1/4, 1/2] \text{ data, provided in Table I are consistent with those using all values of } m_{\pi}. \text{ The results are also consistent with the QED 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 calculation of the mass splittings is comparable to or less than that of QED}_{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\textsubscript{M}. Conservatively, the pion-less EFT employed in this work is valid for } m_{\pi} \ll 2m_{\pi} \text{ and } m_{\pi} L \gtrsim 4. \text{ Provided these inequalities are satisfied, the analytic expressions obtained for the mass shift are valid up to } O(m_\gamma^2/M^3, \alpha^2), \text{ 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 \text{ and } m_{\gamma} L \gtrsim 1.

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 \textsuperscript{30}, our method provides a mass gap to produce a photon, thus increasing the range of energy for which the standard Liouville method \textsuperscript{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.

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[39] Dynamical pions must be accounted for when $m_\pi \geq 2m_\sigma$. This can be handled within chiral perturbation theory but is not considered in the present work.
[42] The local operator contributing at $NLO$ is $\phi^+\phi\psi^+\psi$, where the scalar $\phi$ picks up a vacuum expectation value, thereby Higgsing the photon. Whereas the operator $m^2_\sigma A_\mu A_\nu \psi^+\psi$ contributes to masses at $N^3LO$, it is a prime example of a gauge non-invariant operator.
[45] Note that this formulation of $QED$ violates reflection positivity, leading to the ill-behavior of charged particle propagators for $T \rightarrow \infty$ at fixed $L$ [8]. Our $QED_{TL}$ 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 $QED_{TL}$ [8]. Addressing this is required for practical applications, or could be eliminated by using the $QED_{TL}$ formulation.