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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 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 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 straight-forward [24, 25], it presents practical challenges due to the long-range nature of the electromagnetic (QED) interactions. Specifically, such inter-

actions 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_γ . 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_γ ,

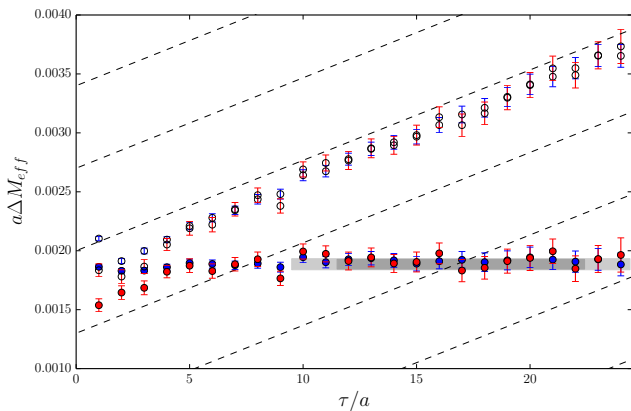


FIG. 1. Zero-mode adjusted (filled) and unadjusted (open) effective mass difference for the kaon splitting ($m_\gamma/\bar{m}_\pi = 1/14$ and $L/a = 24$). Diagonal grid lines have slope $2x$; red/blue points correspond to different sinks. Gray bands correspond to uncertainties on the extracted value for ΔM_{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_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 [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 $\alpha = e^2/(4\pi)$. 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 ($M = m_n, m_p, m_{K^+}$, and m_{K^0}) and charge Q ; the naive expansion is in m_γ/M (i.e. $\Lambda_{UV} = M$) [39]. 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.

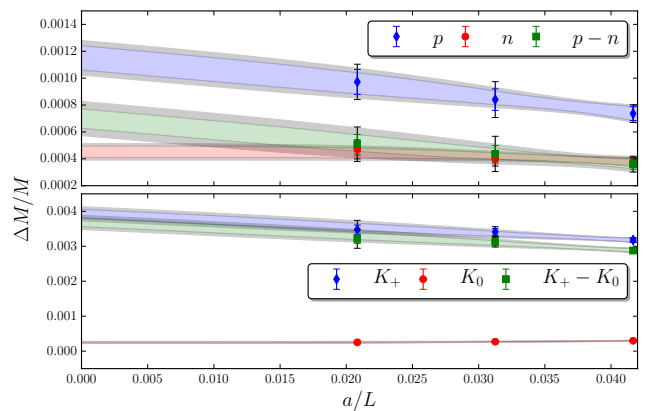


FIG. 2. QED_{TL} induced mass differences, extrapolated to infinite volume (taking $K_L = 2$).

(1) *Zero mode*: For sufficiently small m_γ , 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

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

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 $T \rightarrow \infty$ at fixed L and m_γ .

(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_γ/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

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

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 [42]; the N^2LO correction is of order $\Delta_\gamma M^{N^2LO} = \mathcal{O}(m_\gamma^3/M^2)$. 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 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

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

TABLE I. QED_{TL} induced mass splittings, extrapolated to $L \rightarrow \infty$ ($m_\gamma = 0$, $K_\gamma = 0$).

splitting	K_L	χ^2/dof	$\Delta M/M \times 10^3$
$p - n$	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)

TABLE II. QED_M induced mass splittings, extrapolated to $m_\gamma = 0$ ($L/a = 24$, $K_L = 1$).

splitting	m_γ/m_π range	K_γ	χ^2/dof	$\Delta M/M \times 10^3$
$p - n$	1/14 - 1	2	0.09/5	0.79(06)
	1/4 - 1/2	1	0.06/2	0.81(08)
$K^+ - K^0$	1/14 - 1	2	0.42/5	3.77(06)
	1/4 - 1/2	1	0.12/2	3.79(06)

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 $\boldsymbol{\nu} \in \mathbb{Z}^3$. By contrast, the leading nonvanishing correction for neutral baryons (mesons) appears at N^2LO (N^3LO). 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: $L \sim 3.48$ fm, 4.64 fm and 6.96 fm, and temporal extents $T > L$. The pion (kaon) and nucleon masses in physical units are $\bar{m}_\pi = \bar{m}_K = 807.0(9.1)$ MeV and $\bar{m}_n = 1.634(18)$ 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 ($L/a = 24, T/a = 48$), 515 ($L/a = 32, T/a = 48$) and 342 ($L/a = 48, T/a = 64$) configurations and are a subset of those described in [44]; 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, 24, 25] (QED_{TL}) [45], and a naive lattice discretized form of Eq. 1 (QED_M), 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 are given by $m_\gamma/\bar{m}_\pi \in [1/14, 1/7, 1/4, 1/3, 5/12, 1/2, 7/12, 1]$. 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 $e^{ieQ_q A_\mu}$, where $Q_u = 2/3$, $Q_d = Q_s = -1/3$. In the electroquenched approximation with $SU(3)$ flavor symmetry, isospin splittings have missing contributions that are $\mathcal{O}(\alpha^2)$, 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, $\alpha^{-1} = 137.036\dots$, 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_{qq} 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 [46]. 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 $am_q = -0.2450$); the resulting mistuning for the charge neutral mesons was $\Delta m_{qq}/\bar{m}_\pi \lesssim 0.1\%$ for all values of $m_\gamma/\bar{m}_\pi \leq 1$, where $\Delta m_{qq} \equiv m_{qq} - \bar{m}_\pi$.

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

$$\frac{\Delta m_{K^+ - K^0}}{\bar{m}_K} \simeq \frac{1}{2} \frac{\Delta m_{uu} - \Delta m_{dd}}{\bar{m}_K} \lesssim 0.0004, \quad (6)$$

while the nucleon correction is given by

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

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 QED_{TL} and QED_M 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 [9], we average observables over $+e$ and $-e$ on each configuration in order

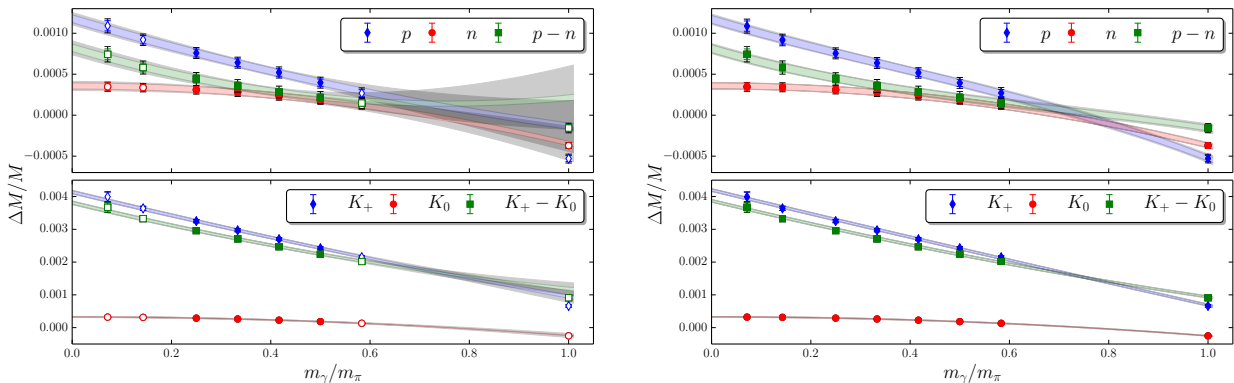


FIG. 3. Volume adjusted ($K_L = 1$) QCD_M induced mass differences, extrapolated to $m_\gamma \rightarrow 0$. Fits were performed using $L/a = 24$ data at all (right) and only the middle four (left) values of m_γ .

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 $h(\tau, a) = xa(a - T + 2\tau) + \log[C(\tau+a)/C(\tau)]$. 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 ΔM_{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:

$$\begin{aligned} \Delta M(\alpha, L, m_\gamma) = \Delta M(\alpha) + \sum_{k=0}^{K_\gamma} \Delta_\gamma M^{N^k LO}(\alpha, m_\gamma) \\ + \sum_{k=0}^{K_L} \delta_L M^{N^k LO}(\alpha, m_\gamma, L), \end{aligned} \quad (10)$$

where K_γ 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 $\delta_L M^{N^k LO}$ retain T -dependence, and may be found in [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 $m_\gamma \rightarrow 0$ 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 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, 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

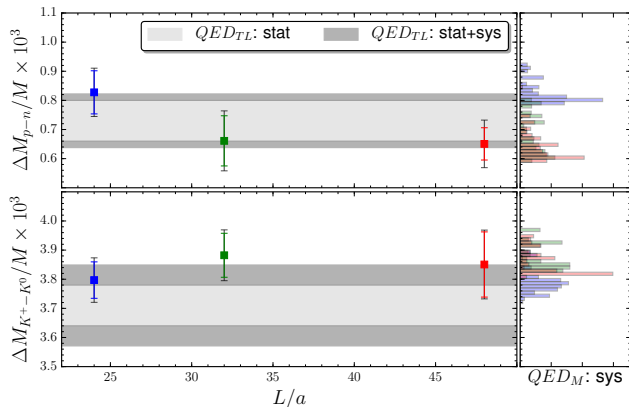


FIG. 4. QED_M extrapolations (points) performed independently at each volume. Systematic errors are estimated by considering fits over multiple ranges of m_γ and orders $K_\gamma \leq 3$ (summarized by the histograms). Summary of QED_{TL} extrapolations are indicated by gray horizontal bands.

is ~ 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_γ . The results are also consistent with the QED_{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_M 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_M . Conservatively, the pion-less 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 $\mathcal{O}(m_\gamma^3/M^3, \alpha^2)$, 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 $m_\gamma L \gtrsim 1$.

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 [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.

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