QED self-energies from lattice QCD without power-law finite-volume errors

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Using the infinite-volume photon propagator, we develop a method which allows us to calculate electromagnetic corrections to stable hadron masses at leading order in α_{QED} with only exponentially suppressed finite-volume effects. The key idea is that the infinite-volume hadronic current-current correlation function with large time separation between the two currents can be reconstructed by its value at modest time separation, which can be evaluated in finite volume with only exponentially suppressed errors. This approach can be extended to other possible applications such as QED corrections to (semi)leptonic decays and some rare decays.

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I. INTRODUCTION

Electromagnetic and strong interactions are two fundamental interactions known to exist in nature. They are described by the first-principle theories of quantum electrodynamics (QED) and quantum chromodynamics (QCD), respectively. In some physical processes, QED and QCD are both present, and both play indispensable roles. A typical example is the neutron-proton mass difference, which is attributed to both electromagnetic and strong isospin-breaking effects. Although this mass difference is only 2.53 times the electron mass, it determines the neutron-proton abundance ratio in the early Universe, which is an important initial condition for big bang nucleosynthesis. This quantity attracts a lot of interest and has motivated a series of lattice QCD studies on the isospin-breaking effects in hadron spectra [1–8].

Generally speaking, QED effects are small due to the suppression of a factor of the fine-structure constant $\alpha_{\mathrm{QED}} \approx 1/137$. However, when the lattice QCD calculations reach the percent or subpercent precision level, the QED correction becomes relevant. It plays a particularly important role in precision flavor physics, where lattice QCD calculations of the semileptonic decay form factors $f_+(0)$ and the leptonic decay constant ratio f_K/f_π have reached a precision of $\lesssim 0.3\%$ [9]. At this precision, the isospin symmetry breakings cannot be neglected. Pioneering works [10–12] have been carried out to include QED corrections to leptonic decay rates.

The conventional approach to include QED in lattice QCD calculations is to introduce an infrared regulator for QED. One popular choice is $\mathrm{QED_L}$, first introduced in Ref. [13], which removes all of the spatial zero modes of the photon field. There are also some other methods: $\mathrm{QED_{TL}}$ [1], massive photon [14], and C^* boundary condition [15]. In general, by including the long-range electromagnetic interaction on a finite-volume lattice, all of these treatments introduce power-law suppressed finite-volume errors. This is different from typical pure QCD lattice calculations where finite-volume errors are suppressed exponentially by the physical size of the lattice. Reference [16] provides an up-to-date systematic analysis of the finite-volume errors for the hadron masses in the presence of QED corrections.

Another approach to incorporate QED with QCD is to evaluate the QED part in infinite volume analytically and completely eliminate the power-law suppressed finite-volume errors. Such an approach, called QED_∞, has been used in the calculation of hadronic vacuum polarization (HVP) and the hadronic light-by-light (HLBL) contribution to muon $g-2$ [17–20]. This approach, when applied to QED corrections to stable hadron masses, does not completely remove the power-law suppressed finite-volume effects. This is mostly because the hadron correlation functions, which one calculates on the lattice to extract hadron masses, are

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exponentially suppressed for a large hadron source and sink separation. Therefore, the finite-volume error of the QED correction to the hadron correlation function evaluated with QED_∞, while its absolute size is still exponentially suppressed by the size of the system, is power-law suppressed only when compared with the correction functions. In this paper, we propose a method to solve this problem. We show that the QED self-energy diagram, at the leading order in α_{QED}, can be calculated on a finite-volume lattice with only exponentially suppressed finite-volume effects.

II. MASTER FORMULA

We first consider the self-energy calculation in an infinite space-time volume. For the case of a stable hadronic state N, the self-energy diagram shown in Fig. 1 can be calculated in Euclidean space from the integral:

$$\Delta M = \mathcal{I} = \frac{1}{2}\int d^4x \mathcal{H}_{\mu,\nu}(x) S^{\gamma}_{\mu,\nu}(x), \tag{1}$$

where the hadronic part $\mathcal{H}_{\mu,\nu}(x) = \mathcal{H}_{\mu,\nu}(t,\vec{x})$ is given by

$$\mathcal{H}_{\mu,\nu}(x) = \frac{1}{2M}\langle N(\vec{0})|T[J_\mu(x)J_\nu(0)]|N(\vec{0})\rangle, \tag{2}$$

where $J_\mu = 2e\bar{u}\gamma_\mu u/3 - e\bar{d}\gamma_\mu d/3 - e\bar{s}\gamma_\mu s/3$ is the hadronic current, $|N(\vec{p})\rangle$ indicates a hadronic state N with the mass M and spatial momentum $\vec{p}$, and $S^{\gamma}_{\mu,\nu}$ is the photon propagator whose form is analytically known. The states $|N(\vec{p})\rangle$ obey the normalization convention $\langle N(\vec{p}')|N(\vec{p})\rangle = (2\pi)^3 2E_{\vec{p}}\delta(\vec{p}'-\vec{p})$. The current operator $J_\mu(t,\vec{x})$ is a standard Euclidean Heisenberg-picture operator $J_\mu(t,\vec{x}) = e^{Ht}J_\mu(0,\vec{x})e^{-Ht}$. A possible short-distance divergence of the integral can be removed by renormalizing the quark mass.

If we examine an L^3 finite-volume system, the main feature of conventional methods such as $\mathrm{QED_L}$ is to design a finite-volume form for the photon propagator, $S^{\gamma,L}_{\mu,\nu}$, and calculate the hadronic correlation function in a finite volume in the presence of finite-volume QED using $S^{\gamma,L}_{\mu,\nu}$. Unfortunately, it results in power-law suppressed finite-volume effects in the mass extracted from the finite-volume hadronic correlation function. For the QED_∞ approach, one may begin with the infinite-volume formula in Eq. (1) to extract the QED self-energy but then limit the range of the integral and replace $\mathcal{H}_{\mu,\nu}(x)$ with a finite-volume version. However, as we will explain later, the result still suffers from power-law finite-volume effects.

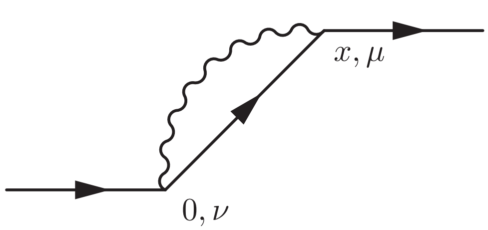

FIG. 1. Self-energy diagram.

To completely solve the problem, we develop a method as follows. We choose a time t_s ($t_s \lesssim L$) that is sufficiently large that the intermediate hadronic states between the two currents are dominated by single hadron states since all of the other states (resonance states, multihadron states, etc.) are exponentially suppressed by t_s:

$$\begin{aligned}
\mathcal{I} &= \mathcal{I}^{(s)} + \mathcal{I}^{(l)},\\
\mathcal{I}^{(s)} &= \frac{1}{2}\int_{-t_s}^{t_s} dt \int d^3\vec{x}\mathcal{H}_{\mu,\nu}(x)S^{\gamma}_{\mu,\nu}(x),\\
\mathcal{I}^{(l)} &= \int_{t_s}^{\infty} dt \int d^3\vec{x}\mathcal{H}_{\mu,\nu}(x)S^{\gamma}_{\mu,\nu}(x).
\end{aligned} \tag{3}$$

We propose approximating $\mathcal{I}^{(s)}$ and $\mathcal{I}^{(l)}$ using the lattice QCD calculable expressions $\mathcal{I}^{(s,L)}$ and $\mathcal{I}^{(l,L)}$,

$$\begin{aligned}
\mathcal{I}^{(s)} \approx \mathcal{I}^{(s,L)} &= \frac{1}{2}\int_{-t_s}^{t_s} dt \int_{-L/2}^{L/2} d^3\vec{x}\mathcal{H}^L_{\mu,\nu}(x)S^{\gamma}_{\mu,\nu}(x),\\
\mathcal{I}^{(l)} \approx \mathcal{I}^{(l,L)} &= \int_{-L/2}^{L/2} d^3\vec{x}\mathcal{H}^L_{\mu,\nu}(t_s,\vec{x})L_{\mu,\nu}(t_s,\vec{x}),
\end{aligned} \tag{4}$$

where $L_{\mu\nu}(t_s,\vec{x})$ is a QED weighting function, defined as

$$\begin{aligned}
L_{\mu,\nu}(t_s,\vec{x}) = &\int \frac{d^3p}{(2\pi)^3} e^{i\vec{p}\cdot\vec{x}} \int_{t_s}^{\infty} dt e^{-(E_{\vec{p}}-M)(t-t_s)}\\
&\times \int d^3\vec{x}' e^{-i\vec{p}\cdot\vec{x}'} S^{\gamma}_{\mu,\nu}(t,\vec{x}').
\end{aligned} \tag{5}$$

Here the energy $E_{\vec{p}}$ is given by the dispersion relation $E_{\vec{p}} = \sqrt{M^2 + \vec{p}^2}$. The integral in $L_{\mu,\nu}(t_s,\vec{x})$ can be calculated in infinite volume (semi)analytically. In Sec. IV, detailed expressions for $L_{\mu,\nu}(t_s,\vec{x})$ are given for both Feynman- and Coulomb-gauge photon propagators.

The finite-volume hadronic part $\mathcal{H}^L_{\mu,\nu}(x)$ is defined through finite-volume lattice correlators (assuming that $t \geq 0$):

$$\mathcal{H}^L_{\mu,\nu}(t,\vec{x}) = L^3 \frac{\langle N(t+\Delta T)J_\mu(t,\vec{x})J_\nu(0)\bar{N}(-\Delta T)\rangle_L}{\langle N(t+\Delta T)\bar{N}(-\Delta T)\rangle_L}, \tag{6}$$

where $\bar{N}(t)/N(t)$ is an interpolating operator which creates/annihilates the zero momentum hadron state N at time t, ΔT is the separation between the source and current operators, which needs only to be large enough to suppress the excited-state effects. The disconnected diagrams, where the vector currents attach to the quark loops instead of the quark lines connected to the interpolating operator of the hadron, should be included in the above matrix elements. Neglecting the disconnected diagrams in the lattice calculation is usually referred to as the QED-quenched approximation.

We will demonstrate below that the quantities $\mathcal{I}^{(s,L)}$ and $\mathcal{I}^{(l,L)}$ defined in the master formula (4) differ from $\mathcal{I}^{(s)}$ and $\mathcal{I}^{(l)}$ only by exponentially suppressed finite-volume effects.

III. PATH TO THE MASTER FORMULA

A. Comparison between $\mathcal{I}^{(s)}$ and $\mathcal{I}^{(s,L)}$

We adopt the conventional expectation (which can be demonstrated in perturbation theory using the Poisson summation formula [21]) that, for a theory such as QCD, with a mass gap a matrix element such as $\mathcal{H}^L_{\mu,\nu}(t,\vec{x})$, evaluated in a finite space-time volume $L^3\times T$ with periodic boundary conditions, will differ from the corresponding matrix element $\mathcal{H}_{\mu,\nu}(t,\vec{x})$ in infinite volume by terms that are exponentially suppressed in the spatial and temporal extents of the volume. In addition, the value of the infinite-volume $\mathcal{H}_{\mu,\nu}(t,\vec{x})$, when $|\vec{x}|\gtrsim t$, is exponentially suppressed in $|\vec{x}|$.

These considerations suggest that the integral for $\mathcal{I}^{(s)}$ is dominated by the region inside the finite-volume lattice and well approximated by the finite-volume integral $\mathcal{I}^{(s,L)}$. We therefore conclude that $\mathcal{I}^{(s,L)}$ differs from its infinite-volume version $\mathcal{I}^{(s)}$ by an exponentially suppressed finite-volume effect.

B. Comparison between $\mathcal{I}^{(l)}$ and $\mathcal{I}^{(l,L)}$

We remind the reader that the value of $\mathcal{H}_{\mu,\nu}(x)$ is not always exponentially suppressed at large $|x|$. In fact, for large $|t|$, we shall have

$$\mathcal{H}_{\mu,\nu}(t,\vec{x})\sim e^{-M(\sqrt{t^2+\vec{x}^2}-t)}\sim e^{-M\frac{\vec{x}^2}{2t}}\sim O(1). \tag{7}$$

Therefore, if we limit the range of the integral for $\mathcal{I}$ in Eq. (1), it will contain an $O(1/L)$ power-law finite-volume effect even if the infinite-volume photon propagator $S^{\gamma}_{\mu,\nu}$ is used instead of $S^{\gamma,L}_{\mu,\nu}$. This is one of the reasons why the traditional QED$_\infty$ method, which works for the cases of HVP and HLBL, does not work for the QED self-energy diagram. As both ends of the photon propagator couple to the quark current, one can perform the intergral over a finite time window only. Even if we could create an infinite time-extent lattice and use the integral

$$\int_{-\infty}^{\infty}dt\int_{-L/2}^{L/2}d^3\vec{x}\mathcal{H}^L_{\mu,\nu}(t,\vec{x})S^{\gamma}_{\mu,\nu}(t,\vec{x}), \tag{8}$$

the result would still carry an $O(1/L^4)$ finite-volume effect, due to the fact that $\mathcal{H}^L_{\mu,\nu}(t,\vec{x})-\mathcal{H}_{\mu,\nu}(t,\vec{x})$ is not exponentially suppressed at large $|t|$.

Instead of using $\mathcal{H}^L_{\mu,\nu}(t,\vec{x})$ at large $|t|$ directly, we study the t dependence of the infinite-volume $\mathcal{H}_{\mu,\nu}(t,\vec{x})$ for $|t|>t_s$. By inserting a complete set of intermediate states, we can rewrite $\mathcal{H}_{\mu,\nu}(t,\vec{x})$ as

$$\mathcal{H}_{\mu,\nu}(t,\vec{x})=\sum_n\int\frac{d^3\vec{p}}{(2\pi)^3}\frac{1}{2E_{n,\vec{p}}}e^{i\vec{p}\cdot\vec{x}}e^{-(E_{n,\vec{p}}-M)t}\times\frac{1}{2M}\langle N(\vec{0})|J_\mu(0)|n(\vec{p})\rangle\langle n(\vec{p})|J_\nu(0)|N(\vec{0})\rangle. \tag{9}$$

Without losing generality, positive t is assumed in the above equation. In Euclidean space with large t, the contribution from excited states is exponentially suppressed. The following approximation, where only the lowest energy states' contributions are kept, is then valid for $t>t_s$:

$$\mathcal{H}_{\mu,\nu}(t,\vec{x})\approx\int\frac{d^3\vec{p}}{(2\pi)^3}\frac{1}{2E_{\vec{p}}}e^{i\vec{p}\cdot\vec{x}}e^{-(E_{\vec{p}}-M)t}\times\frac{1}{2M}\langle N(\vec{0})|J_\mu(0)|N(\vec{p})\rangle\langle N(\vec{p})|J_\nu(0)|N(\vec{0})\rangle, \tag{10}$$

where $E_{\vec{p}}=\sqrt{M^2+\vec{p}^2}$. On the one hand, Eq. (10) suggests that we can calculate $\mathcal{H}_{\mu,\nu}(t,\vec{x})$, for large t, via the matrix element $\langle M(\vec{p})|J_\mu(0)|M\rangle$. On the other hand, it indicates that the Fourier transformation of $\mathcal{H}_{\mu,\nu}(t,\vec{x})$ at fixed $t=t_s$ gives the relevant matrix element:

$$\int d^3\vec{x}\mathcal{H}_{\mu,\nu}(t_s,\vec{x})e^{-i\vec{p}\cdot\vec{x}}=\frac{1}{2E_{\vec{p}}}e^{-(E_{\vec{p}}-M)t_s}\times\frac{1}{2M}\langle N(\vec{0})|J_\mu(0)|N(\vec{p})\rangle\langle N(\vec{p})|J_\nu(0)|N(\vec{0})\rangle. \tag{11}$$

Putting Eq. (11) into Eq. (10), we are able to reconstruct the needed infinite-volume hadronic matrix element at large t from its value at modest t_s:

$$\mathcal{H}_{\mu,\nu}(t,\vec{x}')\approx\int d^3\vec{x}\mathcal{H}_{\mu,\nu}(t_s,\vec{x})\times\int\frac{d^3\vec{p}}{(2\pi)^3}e^{i\vec{p}\cdot\vec{x}}e^{-(E_{\vec{p}}-M)(t-t_s)}e^{-i\vec{p}\cdot\vec{x}'}. \tag{12}$$

We will refer to this relation, which is the crucial step in the derivation, as the "infinite-volume reconstruction" (IVR) method. Here the $\approx$ symbol reminds us that the excited-state contributions in $\mathcal{H}_{\mu,\nu}(t,\vec{x})$ and $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$ are exponentially suppressed and have been neglected. This relation allows us to express all of the long-distance contributions $\mathcal{I}^{(l)}$ in terms of the matrix elements evaluated with a fixed time separation, $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$, as

$$\begin{aligned}\mathcal{I}^{(l)} &= \int_{t_s}^{\infty} dt \int d^3\vec{x}' \mathcal{H}_{\mu,\nu}(t,\vec{x}') S^{\gamma}_{\mu,\nu}(t,\vec{x}') \\ &\approx \int d^3\vec{x} \mathcal{H}_{\mu,\nu}(t_s,\vec{x}) \int_{t_s}^{\infty} dt \int d^3\vec{x}' \\ &\quad \times \int \frac{d^3\vec{p}}{(2\pi)^3} e^{i\vec{p}\cdot\vec{x}} e^{-(E_{\vec{p}}-M)(t-t_s)} e^{-i\vec{p}\cdot\vec{x}'} S^{\gamma}_{\mu,\nu}(t,\vec{x}') \\ &= \int d^3\vec{x} \mathcal{H}_{\mu,\nu}(t_s,\vec{x}) L_{\mu,\nu}(t_s,\vec{x}). \end{aligned} \tag{13}$$

On the second line, we have used relation (12) to convert $\mathcal{H}_{\mu,\nu}(t,\vec{x})$ to $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$. Note that all of the integrals except the first can be performed (semi)analytically and independently of the hadronic function. We name it as the weighting function $L_{\mu,\nu}(t_s,\vec{x})$ on the last line. As a preview, the definition of $L_{\mu,\nu}(t_s,\vec{x})$ is already given in Eq. (5). It can be seen that the only information needed to calculate $L_{\mu,\nu}(t_s,\vec{x})$ is the mass of the target hadron. We then approximate $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$ by a lattice calculable quantity $\mathcal{H}^{L}_{\mu,\nu}(t_s,\vec{x})$ up to the exponentially suppressed finite-volume effects

$$\mathcal{I}^{(l)} \approx \int_{-L/2}^{L/2} d^3\vec{x} \mathcal{H}^{L}_{\mu,\nu}(t_s,\vec{x}) L_{\mu,\nu}(t_s,\vec{x}) = \mathcal{I}^{(l,L)}. \tag{14}$$

Note that integral runs over a finite-volume box with $\vec{x} \in [-L/2, L/2]$. Outside the box, the contribution from $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$ is exponentially suppressed by the lattice size L. By reaching Eq. (14), we complete the derivation of the master formula.

IV. QED WEIGHTING FUNCTION $L_{\mu,\nu}(t_s,\vec{x})$

Detailed expressions for the QED weighting function $L_{\mu,\nu}(t_s,\vec{x})$ defined in Eq. (5) can be evaluated for the following Feynman- and Coulomb-gauge photon propagators:

(a) Feynman gauge,

$$S^{\gamma}_{\mu,\nu}(x) = \frac{\delta_{\mu,\nu}}{4\pi^2 x^2} = \delta_{\mu,\nu} \int \frac{d^4 p}{(2\pi)^4} \frac{e^{ipx}}{p^2}, \tag{15}$$

$$L_{\mu,\nu}(t_s,\vec{x}) = \frac{\delta_{\mu,\nu}}{2\pi^2} \int_0^{\infty} dp \frac{\sin(p|\vec{x}|)}{2(p+E_p-M)|\vec{x}|} e^{-pt_s}. \tag{16}$$

(b) Coulomb gauge,

$$S^{\gamma}_{\mu,\nu}(t,\vec{x}) = \begin{cases} \frac{1}{4\pi|\vec{x}|}\delta(t) & \mu=\nu=0 \\ \int \frac{d^3\vec{p}}{(2\pi)^3}\frac{1}{2|\vec{p}|}(\delta_{i,j} - \frac{p_i p_j}{\vec{p}^2}) e^{-|\vec{p}|t + i\vec{p}\cdot\vec{x}} & \mu=i, \nu=j \cdot \\ 0 & \text{otherwise} \end{cases} \tag{17}$$

$$\begin{aligned} L_{i,j}(t_s,\vec{x}) &= \left(\delta_{i,j} - \frac{x_i x_j}{\vec{x}^2}\right)\frac{1}{(2\pi)^2}\int_0^{\infty} dp \frac{\sin(p|\vec{x}|)}{2(p+E_p-M)|\vec{x}|} e^{-pt_s} \\ &\quad + \left(\delta_{i,j} - 3\frac{x_i x_j}{\vec{x}^2}\right)\frac{1}{(2\pi)^2} \\ &\quad \times \int_0^{\infty} dp \frac{p|\vec{x}|\cos(p|\vec{x}|) - \sin(p|\vec{x}|)}{2(p+E_p-M)|\vec{x}|^3} e^{-pt_s}. \end{aligned} \tag{18}$$

Only the spatial polarization components are needed for the large time expression in Coulomb gauge. All other components of L are zero.

V. EXTENDED DISCUSSIONS

Equation (12) tells us that the large time hadronic matrix elements $\mathcal{H}_{\mu,\nu}(t,\vec{x})$ can be determined using $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$, while $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$ can be calculated using the lattice. Before reaching Eq. (12), we explored other methods to determine $\langle N(\vec{0})|J_\mu(0)|N(\vec{0})\rangle$. We recognized that by using the Coulomb-gauge photon propagator and assuming that $|N(\vec{0})\rangle$ is a spin-0 charged particle, the corresponding matrix element can be determined easily. Our discussion follows.

The infinite-volume photon propagator in Coulomb gauge is given in Eq. (17). This implies, for $\mathcal{I}^{(l)}$, that only $S^{\gamma}_{i,j}$ is relevant. For a spin-0 charged particle, we have

$$\langle N(\vec{p}_1)|J_\mu(0)|N(\vec{p}_2)\rangle = -ie(p_1+p_2)_\mu F(q^2), \tag{19}$$

where the matrix element is expressed in terms of the form factor $F(q^2)$ with $q = p_1 - p_2$. If the initial or the final state has zero momentum, as is the case in Eq. (10), we have

$$\langle N(\vec{0})|J_i(0)|N(\vec{p})\rangle = -iep_i F(q^2). \tag{20}$$

Therefore, we can obtain the result that $\mathcal{I}^{(l)} = 0$ simply because of the Coulomb-gauge condition. Thus

$$\mathcal{I} \approx \mathcal{I}^{(s,L)} = \frac{1}{2}\int_{-t_s}^{t_s} dt \int_{-L/2}^{L/2} d^3\vec{x} \mathcal{H}^{L}_{\mu,\nu}(t,\vec{x}) S^{\gamma}_{\mu,\nu}(t,\vec{x}) \tag{21}$$

for a spin-0 charged particle and a Coulomb-gauge photon propagator, and all of the finite-volume errors are exponentially suppressed by the lattice size L or the integration range in the time direction t_s. Note that $t_s \lesssim L$ is required for the above statement to be valid.

VI. CONCLUSION

We have demonstrated that the QED self-energy for a stable hadron can be calculated on a finite-volume lattice with only exponentially suppressed finite-volume effects.

The power-law finite-volume effects, which are common in QCD + QED calculations, are completely eliminated. This is achieved using the following three ideas.

(1) QED_∞: We start with an integral $\mathcal{I}$, where the QED part in the integrand can be calculated in infinite volume analytically, and the hadronic part is purely a QCD matrix element and enjoys an exponential suppressed long-distance behavior because of the mass gap, as is familiar from pure QCD lattice calculations.

(2) Window method: We introduce a cut in the time extent of the integral t_s to separate the integral into the short-distance part, which can be calculated within finite volume directly, and the remaining long-distance part.

(3) Infinite-volume reconstruction (IVR) method: We use the fact that the long-distance hadronic function is dominated by the lowest isolated pole (the hadron whose QED mass shift is under study) in the spectral representation to express the infinite-volume hadronic function at large t in terms of its value at modest t_s, which can be evaluated in finite volume.

The first idea, QED_∞, has already been employed in some QED + QCD calculations, e.g., HVP [17], HLBL [18,19], and the QED correction to HVP [20]. For these calculations, this idea is able by itself to remove all of the power-law suppressed finite-volume errors. The second idea used in this work, the window method, is relatively new. The name of the method comes from Ref. [20], where the integrand is also divided into parts, and different treatments are applied to different parts. The third idea, the infinite-volume reconstruction method, combined with the window method, is the essential part of our framework. It should be emphasized that it is the *infinite-volume* hadronic function, $\mathcal{H}_{\mu,\nu}(t,\vec{x})$, at large t, expressed in terms of $\mathcal{H}_{\mu,\nu}(t_s,\vec{x})$ at modest t_s, which helps eliminate the power-law finite-volume errors.

In additional to QED self-energy, the framework developed here can also be applied to other QED + QCD problems. One example is the QED corrections to (semi) leptonic decays, which can be used to determine some important Cabibbo-Kobayashi-Maskawa matrix elements like V_{ud} and V_{us} [10–12]. Another example is rare kaon decays [22–26], where the light electron propagator can be treated in a way similar to the photon discussed in this paper to reduce the finite-volume error. In these QED + QCD problems, just like the self-energy case studied here, the finite-volume errors for QED_L can arise from two sources: the short time separation region, which can be fixed by using the QED_∞ photon propagator, the long time separation region, which can be fixed by the IVR method. For problems like HVP or HLBL, the finite-volume errors for QED_L are only from the short-distance region. Therefore, QED_∞ can be successfully applied for these problems, and the IVR method is not needed.

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APPENDIX A: NUMERICAL TEST

As a simple demonstration of the method, we shall apply the method in scalar QED, where we shall refer to the charged scalar particle as π and present some numerical results in this section.

In scalar QED, Eq. (10) is valid for any $t > 0$. Therefore, the hadronic correlation function takes the following form:

$$\begin{aligned}
&H_{\mu,\nu}(t,\vec{x}) \\
&= \int \frac{d^3\vec{p}}{(2\pi)^3}\frac{1}{2E_{\pi,\vec{p}}} e^{i\vec{p}\cdot\vec{x}} e^{-(E_{\pi,\vec{p}}-m_\pi)t} \\
&\quad\times \frac{1}{2m_\pi}\langle\pi(\vec{0})|J_\mu(0)|\pi(\vec{p})\rangle\langle\pi(\vec{p})|J_\nu(0)|\pi(\vec{0})\rangle \\
&= e^2\int\frac{d^3\vec{p}}{(2\pi)^3}\frac{-(im_\pi\delta_{\mu,t}+p_\mu)(im_\pi\delta_{\nu,t}+p_\nu)}{4m_\pi E_{\pi,\vec{p}}}, \\
&\quad\times e^{i\vec{p}\cdot\vec{x}}e^{-(E_{\pi,\vec{p}}-m_\pi)t}
\end{aligned} \tag{A1}$$

where $p_t = iE_{\pi,\vec{p}}$. In the above derivation, we have already applied Eq. (19) with $F(q^2) = 1$, the form factor for the charged particle in scalar QED. In the Feynman gauge, only $H_{\mu,\mu}$ contributes to the self-energy, which can be written as

$$\begin{aligned}
&H_{\mu,\mu}(t,\vec{x}) \\
&= e^2\int\frac{d^3\vec{p}}{(2\pi)^3}\frac{m_\pi+E_{\pi,\vec{p}}}{2E_{\pi,\vec{p}}}e^{i\vec{p}\cdot\vec{x}}e^{-(E_{\pi,\vec{p}}-m_\pi)t}.
\end{aligned} \tag{A2}$$

To study the finite-volume effects numerically, we use the lattice version of $\mathcal{H}_{\mu,\mu}$ with

$$\mathcal{H}^{L,a}_{\mu,\mu}(t,\vec{x}) = \frac{e^2}{L^3}\sum_{\vec{p}}\frac{m_\pi+E_{\pi,\vec{p}}}{2E_{\pi,\vec{p}}}e^{i\vec{p}\cdot\vec{x}}e^{-(E_{\pi,\vec{p}}-m_\pi)t}, \tag{A3}$$

where the standard discretization of $\vec{p} = 2\pi\vec{n}/L$ ($n_k \in (-L/2a, L/2a)$) indicates the finite-volume momenta summation, and the upper bound of momenta π/a indicates the hard cutoff. Here L is the linear lattice size in the spatial direction. We can apply this lattice version function $\mathcal{H}^{L,a}_{\mu,\mu}(t,\vec{x})$ to master formula equation (4). This allows us to test the size of the finite-volume error and how it depends on the lattice volume. Feynman-gauge equation (15) is used in this numerical test.

In the numerical test, we choose the scalar QED parameter m_π close to the charged pion mass, with $m_\pi = 140$ MeV. We choose the lattice spacing to be $a = 1\ \mathrm{GeV}^{-1}$ and vary the lattice size to test the finite-volume

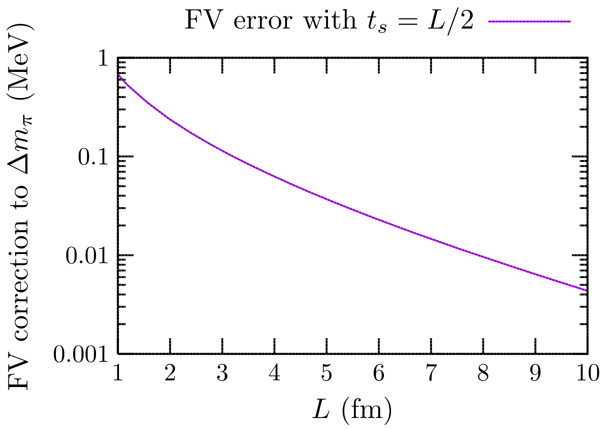

FIG. 2. Exponential dependence of the finite-volume (FV) error.

effects. We calculate with $L/a = 6, 8, \ldots, 96$. The infinite-volume value is approximated by the $L/a = 96$ ($L \approx 19$ fm) calculation. The finite-volume corrections on the QED self-energy are plotted in Fig. 2. As denoted in the plot, we always use $t_s = L/2$, mimicking the situation in a real lattice QCD calculation where large t_s is needed to suppress the excited-state effects.

We also plot the t_s dependence for two specific volumes, $L/a = 24$, 32, in Fig. 3. It should be noted that $t_s \lesssim L$ is required to guarantee the small exponentially suppressed finite-volume effects. Taking the $t_s \to \infty$ limit will introduce new power-law suppressed finite-volume effects.

Finally, as we have studied the exponentially suppressed finite-volume effects using scalar QED, we can make the corresponding correction to lattice results from infinite-volume reconstruction if necessary. Such a correction has been applied to our recent calculation on the $\pi^- \to \pi^+ ee$ transition [27].

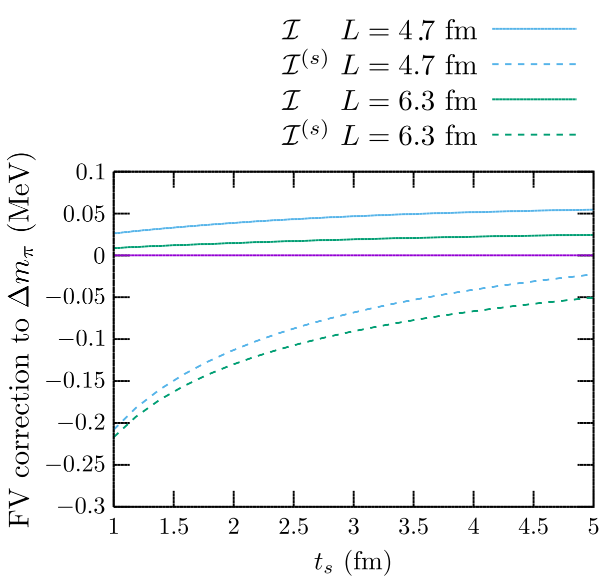

FIG. 3. Fixing $L = 4.7$ and 6.3 fm, we display the finite-volume correction to QED self-energy as a function of t_s.

APPENDIX B: POSSIBLE STRATEGY FOR LATTICE QCD CALCULATIONS AND COST ESTIMATION

In lattice calculations, there are two popular computational strategies to include QED effects.

(a) QCD + QED: Generate QCD + QED ensembles (fully dynamical or quenched QED), and perform the lattice calculation in the presence of both QCD and QED gauge fields. This method is usually referred to as the nonperturbative method, as both the QCD and QED effects are included to all orders. This strategy was used in the very early era of including QED in lattice QCD calculations [1,2].

(b) Perturbative: Express the QED effects perturbatively in terms of the photon propagator and the hadronic matrix elements. The hadronic matrix elements shall be calculated on pure QCD ensembles. The final results are obtained by integrating over the QED photon quark vertex locations, possibly with some stochastic integration techniques. This strategy allows various ways to calculate the hadronic matrix elements and perform the integrations. For example, in Ref. [6], the leading QED and strong isospin-breaking effects on the lattice are studied following a perturbative strategy.

There is no sharp boundary between the two strategies in the quenched QED calculations at leading order in α_{QED}. In particular, the QCD + quenched QED calculation is effectively identical to a perturbative approach where the quenched QED fields are used for the stochastic method to include the photon propagators [8]. The two strategies differ on how unquenched QED effects are included in the calculation. In the QED + QCD simulation, the unquenched QED effects are included in the distribution of the QCD and QED gauge configurations, which are generated by a Markov chain process. In the perturbative approach, these unquenched QED effects are described by the contributions of disconnected diagrams The cost comparison between the two strategies for the unquenched QED effects is not clear.

The IVR method introduced in this paper fits naturally within the perturbative strategy, as we explicitly work with the QED corrections of masses and express the correction in terms of integration of the hadronic matrix elements which can be calculated with Eq. (6).

However, it should be noted that for both the IVR method and QED_L, at leading order, the mass shift can be expressed as an integral of the following form:

$$\Delta M = \frac{1}{2} \int d^4x \mathcal{H}_{\mu,\nu}(x) W_{\mu,\nu}(x). \tag{B1}$$

The only difference is in the function $W_{\mu,\nu}(x)$. For QED_L, the function $W_{\mu,\nu}(x)$ is the photon propagator in finite volume with all of the spatial zero modes removed. For the IVR method, the function $W_{\mu,\nu}(x)$ can be extracted via the master formula equation (4). In both cases, the function $W_{\mu,\nu}(x)$ is defined within a finite-volume lattice and can be evaluated (semi)analytically with very little computational cost. Therefore, we can use basically any existing computational strategy for which QED_L can be used, with only the function form of the photon propagator needing to be changed.

As an extreme example, the IVR method can be used even with the QCD + QED strategy. We can set up a nonlocal "IVR gauge action" whose inverse is the function $W_{\mu,\nu}(x)$ for the IVR method. We can then perform a dynamical QCD + IVR simulation to include the unquenched QED contributions for QED corrections to hadron masses. Although the cost of the dynamical QCD + IVR lattice simulation is similar to the corresponding QCD + QED_L lattice simulation, the ensemble generated with the IVR method is less useful for applications other than the leading QED corrections to the hadron mass. In addition, the nonlocal IVR gauge action depends on the mass of the target hadron; therefore, the QCD + IVR ensemble is useful only for hadrons with a similar mass as the target hadron. These drawbacks do not apply if we adopt a perturbative computational strategy.

If the perturbative strategy is used instead, as the only difference between the IVR method and QED_L (and many other schemes) is the function $W_{\mu,\nu}(x)$, the computational cost for the IVR method is the same as QED_L for the same statistics. On the other hand, there are two advantages for the IVR method:

(a) Smaller finite-volume errors. For the IVR method, the finite-volume error is exponentially suppressed by the lattice size, while QED_L has finite-volume errors suppressed only by some power of the lattice size.

(b) Shorter source sink separation. For QED_L, the source sink separation needs to be large enough to suppress the hadron + one photon excited-state effects. This becomes very difficult, as the gap between ground and excited states vanishes in the infinite-volume limit. However, for the IVR method, t_s needs only to be large enough to suppress the QCD excited-state effects, rather than the hadron + photon effects; thus only modest values of t_s are required.

For applications with a signal-to-noise-ratio problem, i.e., a nucleon or π^0 disconnected diagram, the second advantage can dramatically reduce the statistical error.

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