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

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Using the infinite-volume photon propagator, we developed a method which allows us to calculate electromagnetic corrections to stable hadron masses 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.

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 [1–7].

Generally speaking, QED effects are small due to the suppression of a factor of the fine-structure constant $\alpha_{\text{QED}} \approx 1/137$. However, when the lattice QCD calculations reach the percent or sub-percent precision level, the QED correction becomes relevant. It plays a particularly important role in precision flavor physics, where lattice QCD calculations of the semi-leptonic decay form factors $f_+(0)$ and the leptonic decay constant ratio $f_K/f_\pi$ have reached the precision of $\lesssim 0.3\%$ [8]. At this precision the isospin symmetry breakings cannot be neglected. Pioneering works [9–11] 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 QED$_L$, first introduced in Ref. [12], which removes all the spatial zero modes of the photon field. There are also some other methods: QED$_{TL}$ [6], massive photon [13], $C^*$ boundary condition [14]. In general, by including the long-range electromagnetic interaction on a finite-volume lattice, all 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. Ref. [15] 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$_\infty$, has been used in the calculation of hadronic vacuum polarization (HVP) and the hadronic light-by-light (HLbL) contribution to muon $g-2$ [16–19]. 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 exponentially suppressed for large hadron source and sink separation. Therefore, the finite volume error of the QED correction to the hadron correlation function evaluated with QED$_\infty$, while its absolute size is still exponentially suppressed by the size of the system, is only power-law suppressed compared with the correction functions. In this paper, we propose a method to solve this problem. We show that the QED self-energy diagram can be calculated on a finite volume lattice with only exponentially suppressed finite-volume effects.

FIG. 1. Self-energy diagrams
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. I can be calculated in Euclidean space from the integral:

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

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

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

where $J_{\mu} = 2e \bar{u} \gamma_{\mu} u/3 - e \bar{u} \gamma_{\mu} u/3 - e \bar{s} \gamma_{\mu} s/3$ is the hadronic current, $\langle N(\bar{p})\rangle$ indicates a hadronic state $N$ with the mass $M$ and spatial momentum $\bar{p}$, and $S_{\mu,\nu}$ is the photon propagator whose form is analytically known. The states $|N(\bar{p})\rangle$ obey the normalization convention $\langle N(\bar{p})|N(\bar{p})\rangle = (2\pi)^3/2 E_{\bar{p}}\delta(\bar{p} - \bar{p})$. 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 the conventional methods such as QED is to design a finite-volume form for photon propagator, $S_{\mu,\nu}^{L}$, and calculate the hadron correlation function in a finite volume in the presence of finite-volume QED using $S_{\mu,\nu}^{L}$. Unfortunately, it results in power-law suppressed finite-volume effects in the mass extracted from the finite-volume hadron correlation function. For the QED$_{\infty}$ 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 $H_{\mu,\nu}(x)$ by a finite volume version. However, as we will explain later, the result still suffers from power-law finite-volume effects.

To completely solve the problem, we develop a method as follows. We choose a time $t_{s}$, such that the intermediate hadronic states between the two currents are dominated by single hadron states since all the other states (resonance states, multi-hadron states, etc.) are exponentially suppressed by $t_{s}$.

$$\mathcal{I} = \mathcal{I}^{(s)} + \mathcal{I}^{(l)},$$

$$\mathcal{I}^{(s)} = \frac{1}{2} \int_{t_{s}}^{t_{t}} dt \int d^3 \vec{x} \mathcal{H}_{\mu,\nu}(x) S_{\mu,\nu}^{L}(x),$$

$$\mathcal{I}^{(l)} = \int_{t_{s}}^{\infty} dt \int d^3 \vec{x} \mathcal{H}_{\mu,\nu}(x) S_{\mu,\nu}^{L}(x).$$

We propose to approximate $\mathcal{I}^{(s)}$ and $\mathcal{I}^{(l)}$ using the lattice-QCD calculable expressions $\mathcal{I}^{(s,L)}$ and $\mathcal{I}^{(l,L)}$, which are defined as

$$\mathcal{I}^{(s,L)} = \frac{1}{2} \int_{-t_{s}}^{t_{s}} dt \int d^3 \vec{x} \mathcal{H}_{\mu,\nu}^{L}(x) S_{\mu,\nu}^{L}(x),$$

$$\mathcal{I}^{(l,L)} = \int_{-t_{s}/2}^{t_{s}/2} d^3 \vec{x} \mathcal{H}_{\mu,\nu}^{L}(x_{s}, \vec{x}) L_{\mu,\nu}(t_{s}, \vec{x}),$$

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

$$L_{\mu,\nu}(t_{s}, \vec{x}) = \int d^3 p \, \frac{e^{i \vec{p} \cdot \vec{x}}}{(2\pi)^3} \int_{t_{s}}^{\infty} dt \, e^{-(E_{\vec{p}} - M)(t - t_{s})} \times \int d^3 \vec{x} \, e^{-i \vec{p} \cdot \vec{x}} S_{\mu,\nu}^{L}(t, \vec{x}).$$

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 section 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 $\mathcal{H}_{\mu,\nu}^{L}(x)$ is defined through finite-volume lattice correlators (assuming $t \geq 0$):

$$\mathcal{H}_{\mu,\nu}^{L}(t, \vec{x}) = \mathcal{I}^{L} \langle N(t + \Delta T)J_{\mu}(t, \vec{x})J_{\nu}(0)\bar{N}(-\Delta T)\rangle_L,$$

where $\bar{N}(t)/N(t)$ is an interpolating operator which creates/annihilates the zero momentum hadron state $N$ at time $t$, $\Delta T$ is the separation between the source and current operators, which only needs to be large enough to suppress the excited states effects.

We will demonstrate below the quantities $\mathcal{I}^{(s,L)}$ and $\mathcal{I}^{(l,L)}$ defined in the master formula (4) only differ from $\mathcal{I}^{(s)}$ and $\mathcal{I}^{(l)}$ 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 [29]) that for a theory such as QCD with a mass gap a matrix element such as $\mathcal{H}_{\mu,\nu}(t, \vec{x})$, 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:

$$H_{\mu,\nu}(t, \vec{x}) \sim e^{-M(\sqrt{t^2 + \vec{x}^2} - t)} \sim e^{-M \frac{2t}{\pi}} \sim O(1). \quad (7)$$

Therefore if we limit the range of the integral for $T$ in Eq. (11), it will contain an $O(1/L^4)$ power-law finite volume effect even if the infinite-volume photon propagator $S_{\mu,\nu}^\gamma$ is used instead of $S_{\mu,\nu}^\gamma_L$. 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 only perform the integral over a finite time window. Even if we could create an infinite-time-extent lattice and use the integral

$$\int_{-\infty}^{\infty} dt \int_{-L/2}^{L/2} d^3 \vec{x} H_{\mu,\nu}(t, \vec{x}) S_{\mu,\nu}^\gamma(t, \vec{x}), \quad (8)$$

the result would still carry an $O(1/L^4)$ finite-volume effect, due to the fact that $H_{\mu,\nu}(t, \vec{x}) - H_{\mu,\nu}(t, \vec{x})$ is not exponentially suppressed at large $|t|$. Instead of using $H_{\mu,\nu}(t, \vec{x})$ at large $|t|$ directly, we study the $t$-dependence of the infinite-volume $H_{\mu,\nu}(t, \vec{x})$ for $|t| > t_s$. By inserting a complete set of intermediate states, we can rewrite $H_{\mu,\nu}(t, \vec{x})$ as

$$H_{\mu,\nu}(t, \vec{x}) = \sum_n \int \frac{d^3 \vec{p}}{(2\pi)^3} \frac{1}{2E_{\mu,\nu}} \eta_{\mu,\nu} e^{-\langle E_n - M \rangle t} \left( \frac{1}{2M} \langle N(\vec{0})|J_\mu(0)|n(\vec{p})\rangle\langle n(\vec{p})|J_\nu(0)|N(\vec{0})\rangle \right) e^{i\vec{p}\cdot\vec{x}}. \quad (9)$$

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

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

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

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

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 $t_s$:

$$H_{\mu,\nu}(t, \vec{x}) \approx \int d^3 \vec{x} H_{\mu,\nu}(t_s, \vec{x}) \times \int \frac{d^3 \vec{p}}{(2\pi)^3} \eta_{\mu,\nu} e^{-\langle E_\mu - M \rangle t} e^{-i\vec{p}\cdot\vec{x}}. \quad (12)$$

We will refer this relation, which is the crucial step in the derivation, as the “infinite volume reconstruction method”. Here the $\approx$ symbol reminds us that the excited-state contributions in $H_{\mu,\nu}(t, \vec{x})$ and $H_{\mu,\nu}(t_s, \vec{x})$ are exponentially suppressed and have been neglected.

In the previous section, we have confirmed that $H_{\mu,\nu}(t_s, \vec{x})$ is equal to $H_{\mu,\nu}^L(t_s, \vec{x})$ up to some exponentially suppressed corrections if $\vec{x} \in [-L/2, L/2]$, and is exponentially suppressed itself otherwise. We therefore conclude that $T^{(l)}$ can be well approximated by $T^{(l,L)}$ through

$$T^{(l)} = \int_{t_s}^{\infty} dt \int d^3 \vec{x} H_{\mu,\nu}(t, \vec{x}) S_{\mu,\nu}^\gamma(t, \vec{x}) \approx \int d^3 \vec{x} H_{\mu,\nu}(t_s, \vec{x}) L_{\mu,\nu}(t_s, \vec{x}) \approx \int_{-L/2}^{L/2} d^3 \vec{x} H_{\mu,\nu}^L(t_s, \vec{x}) L_{\mu,\nu}(t_s, \vec{x}) = T^{(l,L)} \quad (13)$$

where the weighting function $L_{\mu,\nu}(t_s, \vec{x})$ has been given in Eq. (5) and will be discussed in the following section.

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 Feynman- and Coulomb- gauge photon propagators:

- Feynman gauge

$$S_{\mu,\nu}^\gamma(x) = \frac{\delta_{\mu,\nu}}{4\pi^2 x^2} = \delta_{\mu,\nu} \int \frac{d^4 p}{(2\pi)^4} \eta_{\mu,\nu} e^{i\vec{p}\cdot\vec{x}}. \quad (14)$$

$$L_{\mu,\nu}(t_s, \vec{x}) = \frac{\delta_{\mu,\nu}}{2\pi^2} \int_0^{\infty} dp \frac{\sin(p|x|)}{2(p + E_p - M)|\vec{x}|} e^{-p t_s}. \quad (15)$$

- Coulomb gauge

$$S_{\mu,\nu}^\gamma(t) = \frac{1}{4\pi |\vec{r}|} \delta(t) \quad \mu = \nu = 0$$

$$= \left\{ \begin{array}{ll} \frac{1}{4\pi |\vec{r}|} \delta(t) & \mu = \nu = 0 \\ \frac{1}{2|\vec{r}|^2} \delta_1(i, \vec{r}) \cos(p |\vec{r}|) e^{-p t_s} & \mu = i, \nu = j \\ 0 & \text{otherwise} \end{array} \right.$$

$$L_{i,j}(t_s, \vec{x}) = \left( \delta_{i,j} - \frac{x_i x_j}{\vec{x}^2} \right) \frac{1}{(2\pi)^2} \int_0^{\infty} dp \frac{\sin(p|x|)}{2(p + E_p - M)|\vec{x}|} e^{-p t_s}$$

$$+ \left( \delta_{i,j} - 3 \frac{x_i x_j}{\vec{x}^2} \right) \frac{1}{(2\pi)^2} \int_0^{\infty} dp \frac{p|x| \cos(p |\vec{r}|) - \sin(p |\vec{r}|)}{2(p + E_p - M)|\vec{x}|^3} e^{-p t_s}. \quad (17)$$

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

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

The infinite volume photon propagator in Coulomb gauge is given in Eq. (16). This implies, for $\mathcal{I}^{(0)}$, only $S_{i,j}^{0}$ is relevant. For a spin-0 charged particle, we have

$$\langle N(\vec{p}_1)|J_{\mu}(0)|N(\vec{p}_2)\rangle = (p_1 + p_2)_{\mu} F(q^2), \quad (18)$$

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

$$\langle N(\bar{0})|J_{\mu}(0)|N(\bar{p})\rangle = p_\mu F(p^2). \quad (19)$$

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

$$\mathcal{I} \approx \mathcal{I}^{(s,L)} = \frac{1}{2} \int_{-t_s}^{t_s} dt \int_{-L/2}^{L/2} d^3 \vec{x} H_{\mu,\nu}^{L}(t, \vec{x}) S_{i,j}^{0}(t, \vec{x}) \quad (20)$$

for a spin-0 charged particle and a Coulomb-gauge photon propagator, and all 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 with the following three ideas:

1. QED$_{\infty}$: 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 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$_{\infty}$, has already been employed in some QED+QCD calculations, e.g. HVP [16], HLbL [17, 18] and the QED correction to HVP [19]. For these calculations, this idea by itself is able to remove all 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. [19], 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, $H_{\mu,\nu}(t, \vec{x})$, at large $t$, being expressed in terms of $H_{\mu,\nu}(t_s, \vec{x})$ at modest $t_s$, which helps eliminate the power-law finite-volume errors.

In addition 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 CKM matrix elements like $V_{ud}$ and $V_{us}$ [9–11]. Another example is the rare kaon decays [21–25], where the light electron propagator can be treated in a similar way as the photon discussed in this paper to reduce the finite-volume error.

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