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Two-Particle Elastic Scattering in a Finite Volume Including QED

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Abstract

The presence of long-range interactions violates a condition necessary to relate the energy of two particles in a finite volume to their S-matrix elements in the manner of Lüscher. While in infinite volume, QED contributions to low-energy charged particle scattering must be resummed to all orders in perturbation theory (the Coulomb ladder diagrams), in a finite volume the momentum operator is gapped, allowing for a perturbative treatment. The leading QED corrections to the two-particle finite-volume energy quantization condition below the inelastic threshold, as well as approximate formulas for energy eigenvalues, are obtained. In particular, we focus on two spinless hadrons in the A_1^+ irreducible representation of the cubic group, and truncate the strong interactions to the s-wave. These results are necessary for the analysis of Lattice QCD+QED calculations of charged-hadron interactions, and can be straightforwardly generalized to other representations of the cubic group, to hadrons with spin, and to include higher partial waves.

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I. INTRODUCTION

Lattice QCD (LQCD) calculations of the properties of the lowest-lying mesons are reaching the level of accuracy where it is necessary to consider the strong interactions in the context of the full Standard Model. In particular, hadronic spectra and other hadronic observables are now being calculated in the presence of both isospin violation from the light-quark masses and Quantum Electrodynamics (QED) [1–11]. QED plays a critical role in the stability and structure of nuclei, and therefore first principles calculations of nuclear structure require the inclusion of the electromagnetic (EM) interactions among quarks. Due to computational resource limitations, LQCD calculations of nuclei remain at an early stage, with calculations of the binding energies of systems with up to five nucleons and hyperons currently being performed at unphysical light-quark masses [12–21]. While the time is not yet ripe for the inclusion of QED in nuclear calculations, there are two-body scattering processes that can now be calculated with high accuracy in LQCD and where Coulomb corrections are relevant, for instance $\pi^+\pi^+$. Therefore, formalism that allows for the systematic calculation of electromagnetic corrections to two-body interactions in a finite volume (FV) is required.

The extraction of hadronic interactions from Lattice QCD calculations is more complicated than determining the spectrum of stable hadrons. The Maiani-Testa theorem [22] demonstrates that S-matrix elements cannot be directly extracted from infinite-volume Euclidean-space Green's functions except at kinematic thresholds. While discouraging from the viewpoint of nuclear physics, where a central objective is determining the forces between nucleons, hyperons and other hadrons, it is clear from its statement that the theorem can be evaded with FV calculations. The essential formalism that enables extraction of continuum S-matrix elements describing two-body elastic scattering from measurements of two-body energies in a finite spatial volume has been known for decades in the context of non-relativistic quantum mechanics [23] and, for two spinless particles, was extended to quantum field theory by Lüscher [24, 25]. The energy of two particles in a FV depends in a calculable way upon their elastic scattering amplitudes, and their masses, for energies below the inelastic threshold. A fundamental assumption in this formalism is that the two particles experience only finite-range interactions, such that the typical interaction length scale is well-contained within the spatial volume. Recently, Lüscher's formalism has been extended to coupled-channels systems (i.e. channels that are coupled in infinite-volume), and to systems comprised of particles with non-zero spin [26–38]. Further, the FV formalism describing nucleon-nucleon (NN) systems with arbitrary CM momenta, spin, angular momentum, isospin and twisted boundary conditions has been developed, providing the quantization conditions (QCs) for the energy eigenvalues in irreducible representations (irreps) of the FV symmetry groups [39]. Efforts to account for the exponentially-suppressed effects of the finite range of the interactions have also been made [40, 41].

At a fundamental level, the inclusion of QED into LQCD calculations poses a theoretical challenge, as the long-range nature of the interaction is truncated and modified by the boundary of the volume. In particular, Ampere's law and Gauss's law cannot be satisfied with a QED gauge field subject to periodic boundary conditions (PBCs) [42–45]. A uniform background charge density can be introduced to circumvent this problem, a procedure which is equivalent to removing the zero modes of the photon. That is, the Coulomb potential energy between charges, e, in a cubic spatial volume with the zero modes removed, is

$$U(\mathbf{r}, L) \ = \ \frac{\alpha}{\pi L} \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{|\mathbf{n}|^2} e^{\frac{i 2\pi \mathbf{n} \cdot \mathbf{r}}{L}} \tag{1}$$

where $\alpha = e^2/4\pi$, $\mathbf{n}$ are triplets of integers and L is the spatial extent of the cubic volume. The FV Coulomb potential can be seen in comparison with the infinite-volume potential in Fig. 1 (left panel). A cross section of the FV electric field due to a point charge in the center of the volume is show in Fig. 1 (right panel). Given the large density of momentum states in typical lattice volumes, the removal of the zero modes will not change the desired infinite-volume values of calculated observables [1].

In the absence of QED, there is a clear separation of the FV artifacts into those that behave as power laws in L, and those that are exponentially suppressed in L. The latter are governed by the longest correlation length in the volume, which, in chiral perturbation theory (χPT) and nucleon-nucleon effective field theory (NNEFT), is the pion Compton wavelength. In contrast, the QED FV effects behave as a power law, which means that the energy eigenvalues of two charged hadrons will be modified in the same way by their self interactions and by their interactions with each other. Therefore, unlike the case with only short-range forces, in the presence of photons, the kinematics of "scattering processes" in lattice calculations also receive power-law modifications in the FV.

[1] The FV modifications to the values of counterterms in a low-energy effective field theory of QCD will scale as $\sim e^{-L/r}$, where r is the typical scale of the strong interactions.

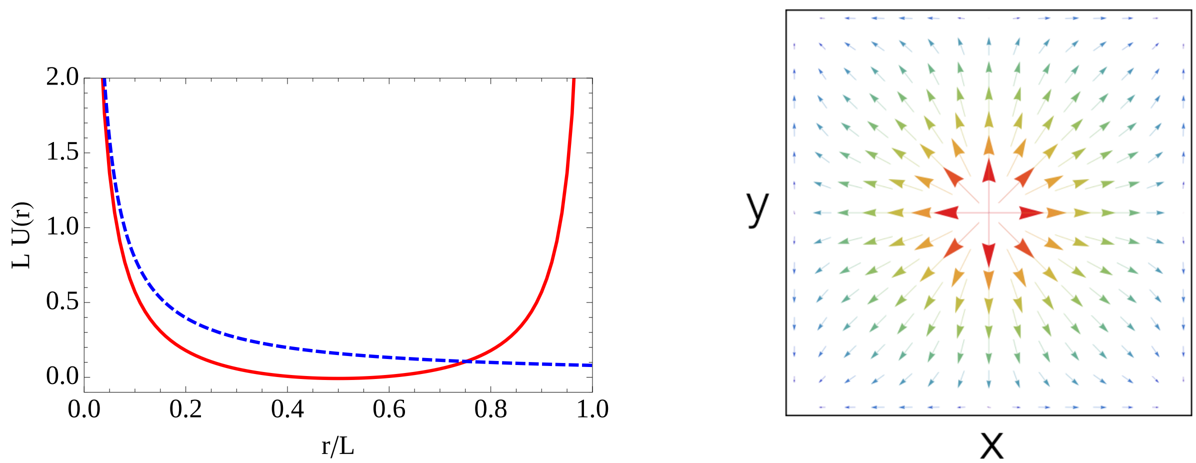

FIG. 1: The left panel shows the FV Coulomb potential energy between unit charges along an axis of a cubic volume (solid red curve) obtained from Eq. (1), and the infinite-volume Coulomb potential (dashed blue curve) [45]. The right panel shows the FV electric field in the $z = 0$ plane due to a point charge located at the center of the cube.

The separation of QED effects from strong interaction effects in scattering processes has a long history. However, it is convenient to use effective field theory (EFT) technology, and its associated power-counting, in deriving the QED corrections to the FV QCs, the solution of which provides the energy eigenvalues. Generally, for low-energy charged-particle scattering processes, the Coulomb interaction is included nonperturbatively through a resummation of ladder diagrams. In an infinite volume this is necessary because the scale of the Coulomb bound state is set by the "Bohr" radius, $(\alpha M)^{-1}$, and interactions with momenta that probe the binding energy of the system are nonperturbative in α. In FV, the non-perturbative treatment would appear to be quite involved due to the proliferation of increasingly complex integer sums. However, in the spatial lattice volume, L^3, the momentum operator is gapped, with a scale that is set by $1/L$, and not by the inverse Bohr radius. Therefore, there is a range of volumes in which the QED interactions can be treated in perturbation theory in a loop expansion, leading to a significant simplification in the corrections to Lüscher's QCs. Another energy scale that must be considered is the inelastic threshold, set by the lowest photon energy in the FV, $E = 2\pi/L$. Given that there are no zero-modes in the FV, by construction, some of the infrared (IR) issues that are usually encountered in QED are absent. As expected, this threshold dictates the kinematical region of validity of the truncation of the QC to two-body states.

This paper is organized as follows. In Section II, we review the basic EFT results that allow for a separation of the QCD and QED interactions in the elastic scattering of two charged hadrons in the continuum. These results form the basis of the FV generalization. QED modifications to the FV QCs that provide the energy eigenvalues of the A_1^+ cubic irrep, truncated to s-wave interactions, are the subject of Section III. First, the modifications to the scattering process kinematics due to FV self-energy shifts is considered, then the truncated QC is determined. In the limit of small scattering lengths compared to L, perturbative expressions for the energy eigenvalues are derived. Furthermore, the QED corrections to the energy of a bound state (when one exists) are determined. Requisite integer sums are provided in the Appendix.

II. COULOMB SCATTERING

QED contributions to two-particle interactions in a FV will be considered in the context of the pionless EFT [46–53]. The effective range expansion (ERE), which describes the low-energy strong interactions between two hadrons, emerges naturally from the pionless EFT, and it was shown by Bethe [54] how the ERE is modified in the presence of Coulomb interactions. Bethe's analysis was reformulated in EFT by Kong and Ravndal [55], and as this formalism plays a central role in the calculations that follow, it is helpful to review its salient features.

The T-matrix describing the QED interactions of two spinless charged particles of mass M, charge e, carrying equal but opposite momentum $\mathbf{p}$, and in the absence of strong interactions, has a partial-wave expansion of the form

$$T_C \;=\; -\frac{4\pi}{M}\sum_l \,(2l+1)\,\frac{e^{i2\sigma_l}-1}{2ip}\,P_l(\cos\theta) \quad , \tag{2}$$

where $p = |\mathbf{p}|$ and $\sigma_l = \arg\,\Gamma(1+l+i\eta)$. l is the angular momentum of the scattering channel, $\eta = \alpha M/(2p)$, and θ is the center-of-mass (CoM) scattering angle. The strong interactions between two hadrons below the t-channel cut in an s-wave can be described by an EFT of four-hadron operators. The effects of these operators can be encapsulated, for the purposes of this work, by a single interaction (a pseudo-potential) with a coefficient $C(E^*)$, which is an analytic function of the CoM energy E^* [2].

[2] At the level of the non-relativistic Lagrange density, expressed as a gradient expansion of local operators

Treating $C(E^*)$ nonperturbatively by summing all bubble diagrams with a $C(E^*)$ insertion at each vertex, and using dimensional regularization (DR) to regulate ultraviolet divergences, the T-matrix including the strong and the leading QED interactions is

$$T_{SC} \;=\; C^2_{\eta(p)}\, \frac{C(E^*)e^{i2\sigma_0}}{1 - C(E^*)J_0^\infty(E^*)} \;=\; -\frac{4\pi}{M}\frac{e^{2i\sigma_0}}{p\cot\delta - ip} \quad , \tag{4}$$

where δ is the s-wave phase shift. $J_0^\infty(E^*)$ is the $\mathbf{r} = \mathbf{0}$ to $\mathbf{r} = \mathbf{0}$ Green's function including QED interactions, and can be written as

$$J_0^\infty(E^*) \;=\; M\int \frac{d^3q}{(2\pi)^3}\frac{C^2_{\eta(q)}}{p^2 - q^2 + i\epsilon} \ , \tag{5}$$

and $C_{\eta(p)}$ is the Coulomb corrected vertex resulting from the resummation of Coulomb ladder diagrams, with a square given by

$$C^2_{\eta(p)} \;=\; \frac{2\pi\eta(p)}{e^{2\pi\eta(p)} - 1} \quad . \tag{6}$$

The parameter $\eta \sim \alpha/v$, where v is the relative velocity of the two hadrons, governs the viability of QED perturbation theory and therefore, as pointed out above, for momenta of order αM, $\eta \sim 1$ and Coulomb ladders must be treated to all orders in α and resummed.

Decomposing J_0^∞ into finite and divergent parts, $J_0^{fin} + J_0^{div}$, leads to [55]

$$J_0^{fin} \;=\; M\int \frac{d^3q}{(2\pi)^3}\frac{C^2_{\eta(q)}}{q^2}\frac{p^2}{p^2 - q^2 + i\epsilon} \;=\; -\frac{\alpha M^2}{4\pi}\ H(\eta) \ , \tag{7}$$

where

$$H(\eta) \;=\; \psi(i\eta) + \frac{1}{2i\eta} - \ln(i\eta) \ , \tag{8}$$

with ψ the logarithmic derivative of the Gamma function. Using DR with modified minimal subtraction ($\overline{MS}$) in $n = 4 - 2\epsilon$ dimensions, [3] the divergent part becomes

$$J_0^{div} \;=\; -M\int \frac{d^3q}{(2\pi)^3}\frac{C_{\eta(q)}}{q^2} \;=\; \frac{\alpha M^2}{4\pi}\left[\frac{1}{\epsilon} + \ln\left(\frac{\mu\sqrt{\pi}}{\alpha M}\right) + 1 - \frac{3}{2}\gamma_E\right] \ , \tag{9}$$

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built out of a field ψ, it is straightforward to show, using equations of motion and integrating by parts, that [52, 56]

$$-\hat\theta\ \psi^T(\overleftarrow{\nabla} - \overrightarrow{\nabla})^2\psi \;=\; 4M\ \hat\theta\ \left[i\partial_0 + \frac{\nabla^2}{4M}\right]\psi^T\psi \equiv 4M\ \hat\theta\ \mathcal{O}_{E^*}\psi^T\psi \quad , \tag{3}$$

where $\hat\theta$ is an arbitrary operator, and terms that are total derivatives are not shown. The operator $\mathcal{O}_{E^*}$ when acting on the two-particle operator simply yields the non-relativistic center-of-mass energy, E^*.

[3] The power counting in the EFT is manifest in the PDS scheme [46, 47]. Here for simplicity we use $\overline{MS}$, which obscures the strong power counting, but does not change it.

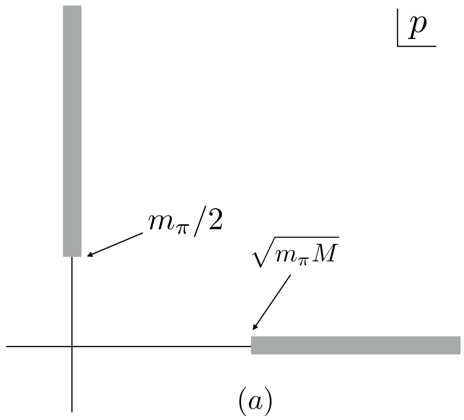

FIG. 2: The analytic structure of the scattering amplitude in the complex p plane (a) without QED and (b) with QED. The imaginary axis exhibits the QCD t-channel cut with its threshold at $m_\pi/2$, while the real axis gives the inelastic pion-production cut with its threshold at $\sqrt{m_\pi M}$. In the presence of QED, both the t-channel cut (dark blue) and the inelastic cut (yellow) begin at the origin.

where μ is the renormalization scale introduced in n dimensions, and γ_E is Euler's constant. The expression for T_{SC} in Eq. (4) then leads to

$$C^2_{\eta(p)}\, p\cot\delta + \alpha M h(\eta) \;=\; -\frac{4\pi}{MC(E^*)} \;+\; \alpha M\left[\frac{1}{\epsilon} + \ln\left(\frac{\mu\sqrt{\pi}}{\alpha M}\right) + 1 - \frac{3}{2}\gamma_E\right] \tag{10}$$

where

$$\mathrm{Im}H(\eta) \;=\; \frac{C^2_{\eta(p)}}{2\eta} \quad \text{and} \quad \mathrm{Re}H(\eta) \;\equiv\; h(\eta)\ , \tag{11}$$

have been used. As Bethe showed, the left-hand side of Eq. (10) admits an ERE of the form

$$C^2_{\eta(p)}\, p\cot\delta + \alpha M h(\eta) \;=\; -\frac{1}{a_C} \;+\; \frac{1}{2}r_0 p^2 \;+\; \ldots \tag{12}$$

where a_C is the Coulomb-corrected scattering length and r_0 is the effective range. The presence of the extra term on the left-hand side can be understood based on the analytic structure of the scattering amplitude (see Fig. 2). As the t-channel cut begins at the origin when photons are present, this term removes this cut from the scattering amplitude, thus leaving an expression that is analytic in p^2 (neglecting radiation) and which consequently admits an ERE [4]. While the inelastic threshold is at $p = 0$, this cut is suppressed by powers of α compared to the t-channel cut.

[4] At higher orders in α, other functions will have to be subtracted to allow an ERE.

Matching the right-hand sides of Eq. (10) and Eq. (12) is achieved through renormalization [46, 47, 55]. Rather than use $\overline{MS}$ to subtract the $1/\epsilon$ pole, a slightly modified scheme, denoted $\overline{MS}_{FV}$, is used, which corresponds to subtracting

$$\frac{\alpha M^2}{4\pi}\left[\frac{1}{\epsilon}-\frac{\gamma_E}{2}+1+\ln\frac{\sqrt{\pi}}{2}\right] \ . \tag{13}$$

In this scheme, which is convenient for the FV calculations to follow, the ERE can be described by renormalized coefficients,

$$-\frac{4\pi}{MC(p;\mu)} \ + \ \alpha M\left[\ln\left(\frac{2\mu}{\alpha M}\right)-\gamma_E\right] \ = \ \frac{1}{a_C} \ + \ \frac{1}{2}r_0 p^2 \ + \ \ldots \ , \tag{14}$$

where $C(p;\mu)=C_0(\mu)+C_2(\mu)p^2+\ldots$ is the renormalized strong-interaction pseudo-potential coefficient.

The analysis of this section is appropriate for the interactions of like-charged hadrons, such as proton-proton scattering. In the case of hadrons with opposite charges, the kinematic factor η changes sign, $\eta=-\alpha M/(2p)$, and $H(\eta)$ becomes

$$\overline{H}(\eta) \ = \ \psi(i\eta)+\frac{1}{2i\eta}-\ln(-i\eta) \ , \tag{15}$$

III. FINITE VOLUME COULOMB SCATTERING

A. Power Counting and Kinematics

In a cubic spatial volume with PBCs, a free particle can carry momentum $\mathbf{p}=2\pi\mathbf{n}/L$, where $\mathbf{n}$ is a triplet of integers. In the absence of zero modes, the momentum carried by a photon is restricted to $k\geq 2\pi/L$ and the relevant size of η in the FV is $\eta\sim\alpha ML$, which implies that for $ML\ll 1/\alpha$, QED interactions can be treated perturbatively in α. Of course, η grows with the spatial volume and, for a given M, there is a critical value of L at which perturbation theory breaks down and the Coulomb ladders must be resummed to all orders, as in the continuum. In addition, LQCD calculations have volumes large enough so that $M\gg 1/L$, and this limit will also be assumed throughout this analysis. Note that due to the absence of the zero mode, the inelastic threshold of the two-hadron state, which is set by the two hadrons recoiling against a photon, is at $\sqrt{2\pi M/L}+\mathcal{O}(1/M)$.

The power-law nature of the expansion parameter leads to various subtleties. In the absence of QED, hadron self energies contain FV corrections that are exponentially suppressed by the dimensionless parameter $m_\pi L$, and therefore, neglecting these corrections, the kinematics in the FV are the same as in the continuum. This is no longer the case in the presence of QED as the hadron masses have power-law volume dependencies [42–45].

The total CoM energy of the two-hadron system can be written as $E^* = 2M^L + T^{*L}$, where T^{*L} is the CoM kinetic energy, and M^L is the mass of the single hadron, in the FV. The ERE, while usually written in terms of an expansion in square of the hadron three momentum, is an analytic function of E^* below the inelastic threshold, and with the FV shift in the hadron mass(es), is evaluated at a shifted value of the kinetic energy in the FV,

$$\begin{aligned} p\cot\delta \;&=\; -\frac{1}{a_C}+\frac{1}{2}r_0p^2+r_1p^4\;+\;...\;=\;-\frac{1}{a_C}+\frac{1}{2}r_0MT^*+r_1M^2T^{*2}\;+\;... \\ &=\; -\frac{1}{a_C}+\frac{1}{2}r_0M(E^*-2M)+r_1M^2(E^*-2M)^2\;+\;... \\ &\to\; -\frac{1}{a'_C}+\frac{1}{2}r'_0MT^{*L}+r'_1M^2(T^{*L})^2\;+\;...\quad , \end{aligned} \tag{16}$$

where r_1 is the shape parameter. The primed scattering parameters, that are required to describe the FV two-point function, are defined by

$$\frac{1}{a'_C} \;=\; \frac{1}{a_C}-\frac{\alpha\; r_0 M\,\mathcal{I}}{2\pi L}\;+\;\mathcal{O}(\alpha^2;\alpha/L^2)\;\;,\;\; r'_0 \;=\; r_0+\frac{4\;\alpha\; r_1 M\;\mathcal{I}}{\pi L}\;+\;\mathcal{O}(\alpha^2;\alpha/L^2)\,, \tag{17}$$

with similar modifications to the terms that are higher order in the ERE. In these shifted ERE parameters, the single-particle FV corrections of Refs. [44, 45] have been used, and $\mathcal{I} \sim -8.913632$ is an integer sum detailed in the Appendix.

Up to this point, the discussion has been focused on the dynamics of point-like particles, but as this work is relevant to LQCD calculations, the effect of compositeness must be considered. In Ref. [45], the EFT describing the low-energy dynamics of hadrons was used to determine the FV corrections to hadron masses in LQCD calculations, in which the effect of compositeness, manifesting itself through a hierarchy of electromagnetic multipole interactions and other multi-photon gauge-invariant interactions, was made explicit. These one-body QED interactions, beyond the electric charge, will also contribute to energy eigenvalues of two hadrons, electrically charged or neutral. For spinless hadrons, the leading interaction beyond the charge is from its charge radius. Given that the charge radius is proportional to the square of the momentum carried by the photon, the leading effect of the charge radius is to provide an constant additive renormalization of $C(E^*)$, which is the same in finite and infinite volume. Further, this contribution cannot be isolated from the experimental scattering data without a model dependent subtraction, or with an explicit

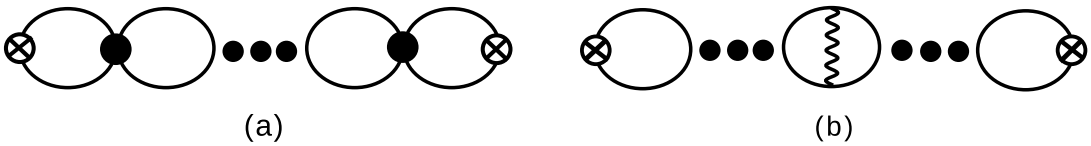

FIG. 3: Feynman diagrams contributing to the FV two-point function. Diagram (a) is one of the bubble diagrams resulting from the strong interactions, while diagram (b) is one of the diagrams at $\mathcal{O}(\alpha)$ from the exchange of a Coulomb photon (that becomes one of the Coulomb ladder diagrams in infinite-volume).

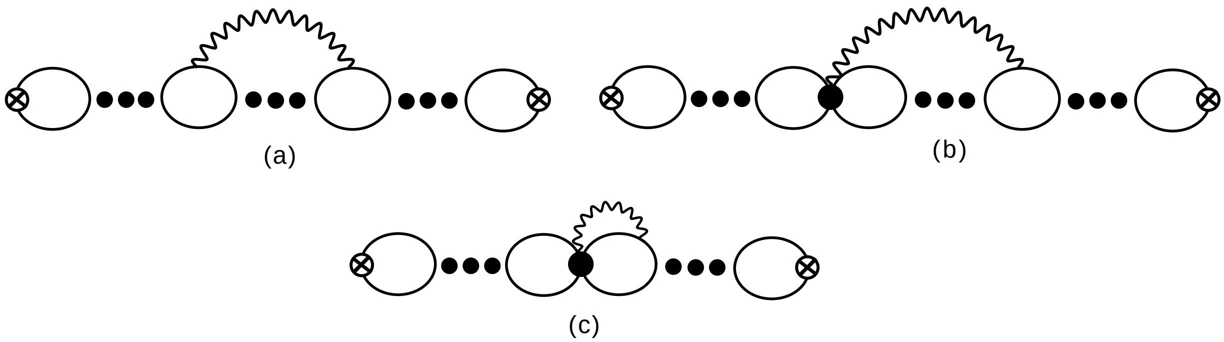

FIG. 4: Feynman diagrams contributing to the FV two-point function but which are suppressed in the IR compared to the Coulomb ladder diagrams.

calculation of the low-momentum transfer contribution using EFT. Therefore, in what follows, the leading contribution from the structure of spinless hadrons is already included in the definition of the scattering parameters, and the comparison with experiment should not remove this contribution from the experimental data prior to comparing. The analysis that follows does not make explicit the contribution from the hadron charge radius, but one should keep in mind that it is implicit.

B. Quantization Condition including QED

The truncated QC that determines the A_1^+ FV energy eigenvalues can be determined by the singularities of the FV two-point function. In general, the $\mathcal{O}(\alpha)$ corrections to the two-point function result from the sum of all diagrams with a single insertion of a photon and the related counterterms, examples of which are shown in Fig. 3 and Fig. 4. Consider the correlation function between a source, $S^\dagger$ and a sink, S, where $S^\dagger, S$ couple to two hadrons in an s-wave. Denoting the contribution to this two-point function from the sums of bubbles shown in Fig. 3 as $J_0^L(E^*)$, and the (generally) energy-dependent FV strong interaction as $C^L(E^*)$, this correlation function is

$$S^\dagger \left[J_0^L(E^*) \ + \ C^L(E^*) \left(J_0^L(E^*)\right)^2 \ + \ C^L(E^*)^2 \left(J_0^L(E^*)\right)^3 \ + \ ... \right] S$$
$$= \ S^\dagger \frac{J_0^L(E^*)}{1 - C^L(E^*) J_0^L(E^*)} S \ = \ S^\dagger \frac{1}{1/J_0^L(E^*) - C^L(E^*)} S \quad . \tag{18}$$

Therefore, the FV QC that determines the A_1^+ energy eigenvalues is simply

$$\frac{1}{C^L(E^*)} \ = \ J_0^L(E^*) \ . \tag{19}$$

In the infinite volume limit, the Feynman diagrams represented in Fig. 3 (given to all orders in Eq. (5)), after performing the energy integrations, give

$$J_0^\infty(E^*) \ = \ -M \int \frac{d^3q}{(2\pi)^3} \frac{1}{q^2 - p^2}$$
$$+ \ 4\pi\alpha M^2 \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \frac{1}{q^2 - p^2} \frac{1}{k^2 - p^2} \frac{1}{|\mathbf{q} - \mathbf{k}|^2} \ + \ \ldots , \tag{20}$$

which in a FV, and using a momentum cut off, takes the form

$$J_0^L(E^*) \ = \ -\frac{M}{4\pi^2 L} \sum_{\mathbf{n}}^{\Lambda_n} \frac{1}{|\mathbf{n}|^2 - \tilde{p}^2}$$
$$+ \ \frac{\alpha M^2}{16\pi^5} \sum_{\mathbf{n}}^{\Lambda_n} \sum_{\mathbf{m} \neq \mathbf{n}}^{\infty} \frac{1}{|\mathbf{n}|^2 - \tilde{p}^2} \frac{1}{|\mathbf{m}|^2 - \tilde{p}^2} \frac{1}{|\mathbf{n} - \mathbf{m}|^2} \ + \ \ldots , \tag{21}$$

where $\tilde{p} = Lp/2\pi$ and $\Lambda_n = L\Lambda/2\pi$ with Λ a momentum cutoff, and the ellipses signify omitted $\mathcal{O}(\alpha^2)$ effects. Note that the zero mode has been removed from the photon propagator by the condition $\mathbf{m} \neq \mathbf{n}$. As the FV does not alter the ultraviolet (UV) behavior of the sums from that of the infinite-volume integrals, the renormalization of divergences in FV is the same as in infinite volume. In Eq. (21), the infinite volume hadron mass, M, has been used, rather than M^L. As the present analysis assumes $ML \gg 1$, and the mass does not explicitly appear in the leading QC, this difference represents a higher order effect. In order to regulate the divergent sums for numerical evaluation, while maintaining the mass-independent renormalization scheme, Eq. (19) becomes [57]

$$\frac{1}{C^L(E^*)} \ - \ \mathrm{Re}(J_0^{\infty\{DR\}}(E^*)) \ = \ J_0^L(E^*) \ - \ \mathrm{Re}(J_0^{\infty\{\Lambda\}}(E^*)) \ , \tag{22}$$

where the {} superscript indicates regularization scheme, and it is straightforward to show that

$$\mathrm{Re}(J_0^{\infty\{\Lambda\}}(E^*)) \;=\; -\frac{M\Lambda}{2\pi^2} - \frac{\alpha M^2}{4\pi}\ln\left(\frac{2p}{\Lambda}\right) \;+\; \ldots, \tag{23}$$

and

$$\mathrm{Re}(J_0^{\infty\{DR\}}(E^*)) \;=\; -\frac{\alpha M^2}{4\pi}\left[\frac{1}{2}\gamma_E - \frac{1}{\epsilon} - 1 + \ln\left(\frac{2p}{\mu}\right) - \ln\sqrt{\pi}\right] \;+\; \ldots, \tag{24}$$

which matches the perturbative expansion of the all-orders propagator given in Sec. II. The remaining task is to relate the FV interactions, $C^L(E^*)$, to their infinite volume counterparts, $C(E^*)$, which define the scattering matrix in Eq. (4), and hence to the scattering parameters.

In general, the FV interactions, $C^L(E^*)$, result from a summation of all bubble diagrams of the type shown in Fig. 4, in which the photon is exchanged between bubbles, or between an interaction and a bubble, or between interactions, or produces a loop from the same interaction. Consider a generic diagram with a photon across bubbles, as in Fig. 4. As a single bubble with CoM kinetic energy T^* scales as $\sim M\sqrt{MT^*}$, the contribution from the photon pole is $\sim \sqrt{|\mathbf{p}|} \sim \sqrt{M/L}$. Therefore, diagrams with photons across n-bubbles are suppressed by $\sim (\sqrt{M/L})^n$ [5]. To determine the parametric contributions from these diagrams, it is sufficient to evaluate the diagram without bubbles between the insertions of the photon vertices, i.e. the photon across a single $C(E^*)$ vertex. Analogous arguments apply to the diagrams with photons emerging from the strong interaction (by gauge invariance) and connecting to bubbles, as in Fig. 4(c), or other interactions. It follows that $C^L(E^*)$ differs from $C(E^*)$ by $\delta C^{(FV)}(E^*) = C^L(E^*) - C(E^*)$,

$$\delta C^{(FV)}(E^*) \;=\; -\alpha\left(\frac{2a_C}{\pi M}\,\alpha_{3/2} \;+\; \frac{4a_C^2 r_0}{L}\,\mathcal{I} \;+\; \ldots.\right)\;, \tag{25}$$

where $\alpha_{3/2}$ is a numerical constant given in the Appendix. As these contributions depend explicitly on the scattering parameters and do not constitute a simple multiplicative renormalization of $p\cot\delta$, they explicitly preclude a direct extraction of T-matrix elements. This should come as no surprise, as the QED interactions of systems containing two or more hadrons (or interactions of such systems with other types of probes) are not described by

[5] The diagrams in Fig. 4 are analogous to those involving radiation pions in NNEFT [46, 47], which were analyzed in detail in Ref. [58].

the two-body scattering parameters alone. For instance, in the case of two nucleons, there will be contributions from the gauge-invariant two-body operators that contribute to the deuteron quadrupole moment, and from the operators contributing to the electric and magnetic polarizabilities.

It follows from Eq. (12) that, at $\mathcal{O}(\alpha)$, the truncated A_1^+ FV QC for fields subject to spatial PBCs is

$$-\frac{1}{a_C'} \ + \ \frac{1}{2}r_0'p^2 \ + \ ... \ = \ \frac{1}{\pi L}\mathcal{S}^C\left(\tilde{p}\right) \ + \ \alpha M\left[\ln\left(\frac{4\pi}{\alpha M \mathrm{L}}\right) - \gamma_E\right] \ + \ ... \ , \tag{26}$$

where the single sum over integer triplets, which determines the effects of the strong interactions in the absence of QED interactions, is modified to

$$\mathcal{S}^C\left(\, x\, \right) \ \equiv \ \mathcal{S}\left(\, x\, \right) \ - \ \frac{\alpha M L}{4\pi^3}\,\mathcal{S}_2\left(\, x\, \right) \ + \ \frac{\alpha\ M a_C^2 r_0}{\pi^2 L^2}\mathcal{I}\left[\mathcal{S}\left(\, x\, \right)\right]^2 \ + \ ... \ , \tag{27}$$

with

$$\mathcal{S}\left(\, x\, \right) \ \equiv \ \sum_{\mathbf{n}}^{\Lambda_n} \frac{1}{|\mathbf{n}|^2 - x^2} \ - \ 4\pi\Lambda_n \ ;$$

$$\mathcal{S}_2\left(\, x\, \right) \ \equiv \ \sum_{\mathbf{n}}^{\Lambda_n}\sum_{\mathbf{m}\neq\mathbf{n}}^{\infty} \frac{1}{|\mathbf{n}|^2 - x^2}\frac{1}{|\mathbf{m}|^2 - x^2}\frac{1}{|\mathbf{n}-\mathbf{m}|^2} \ - \ 4\pi^4\ln\Lambda_n \ . \tag{28}$$

The scattering parameters in Eq. (27) are unprimed and the ellipses denote terms that are higher order in the α, $1/L$ and $1/M$ expansions and in the ERE. Eq. (26) is the main result of this paper.

The numerical evaluation of the function $\mathcal{S}(x)$ through exponential acceleration techniques is well known [24, 25], and it is convenient to express the $\mathcal{O}(\alpha)$ regulated double sum as

$$\begin{aligned}\mathcal{S}_2\left(x\right) \ = \ & \mathcal{R} - \frac{2}{x^2}\sum_{\mathbf{n}\neq\mathbf{0}}\frac{1}{|\mathbf{n}|^2}\frac{1}{|\mathbf{n}|^2 - x^2} \\ & + \sum_{\mathbf{n}\neq 0}\ \sum_{\mathbf{m}\neq 0,\mathbf{n}}\left[\frac{1}{|\mathbf{n}|^2 - x^2}\frac{1}{|\mathbf{m}|^2 - x^2} - \frac{1}{|\mathbf{n}|^2}\frac{1}{|\mathbf{m}|^2}\right]\frac{1}{|\mathbf{n}-\mathbf{m}|^2} \quad ,\end{aligned} \tag{29}$$

where

$$\mathcal{R} \ \equiv \ \sum_{\mathbf{n}\neq 0}^{\Lambda_n}\ \sum_{\mathbf{m}\neq 0,\mathbf{n}}^{\infty}\frac{1}{|\mathbf{n}|^2|\mathbf{m}|^2}\frac{1}{|\mathbf{n}-\mathbf{m}|^2} \ - \ 4\pi^4\ln\Lambda_n \ = \ -178.42(01) \ . \tag{30}$$

The evaluation of this geometric constant, $\mathcal{R}$, is presented in the Appendix.

The QC given in Eq. (26) determines the FV energy eigenvalues of two like-charged hadrons. The analogous QC for oppositely-charged hadrons can be determined from Eq. (26) by the substitution $\alpha \to -\alpha$ except in the argument of the logarithm where $\alpha \to +\alpha$.

C. Renormalization Group Evolution

It is tempting to combine the terms in brackets on the left and right hand sides of Eq. (26), however, it is only this particular decomposition that allows an ERE of the left hand side [54]. Indeed, the appearance of the logarithm on the right-hand side is essential to the physical interpretation of the QC, and can be understood with the aid of the renormalization group (RG). In the $\overline{MS}_{FV}$ scheme, a running scattering length can be defined,

$$\frac{1}{a(\mu)} \equiv \frac{4\pi}{MC(0;\mu)} = \frac{1}{a_C} + \alpha M \left[\ln\left(\frac{2\mu}{\alpha M}\right) - \gamma_E \right] , \tag{31}$$

which, by construction, satisfies

$$\frac{1}{a(\mu)} = \frac{1}{a(\nu)} + \alpha M \ln\left(\frac{\mu}{\nu}\right) . \tag{32}$$

This (scheme-dependent) running scattering length can be interpreted as the scattering length with the leading QED effects from distance scales $> 1/\mu$ removed [55].

With this running scattering length in mind, it is convenient to give alternate forms of the QC, Eq. (26). For instance, the QC can be expressed in terms of the $\overline{MS}_{FV}$ scattering length with the leading QED effects from length scales outside of the spatial volume removed. To this end, a renormalization-scale dependent function, $\bar{\delta}(p,\mu)$, can be defined such that

$$p \cot \bar{\delta}(p,\mu) \equiv -\frac{1}{a(\mu)} + \frac{1}{2} r_0 p^2 + \ldots , \tag{33}$$

leading to

$$p \cot \bar{\delta}'(p, 2\pi/L) \equiv -\frac{1}{a'(2\pi/L)} + \frac{1}{2} r_0' p^2 + \ldots = \frac{1}{\pi L} \mathcal{S}^C(\tilde{p}) , \tag{34}$$

where the primes denote the modified kinematics. Despite the presence of the scheme-dependent scattering length, this form of the QC is the most physical, as it is written only in terms of quantities which have support within the boundaries of the FV. The price that is paid for expressing the QC directly in terms of the physical scattering length is the presence of the extra term (in brackets) on the right side of Eq. (26), which removes contributions to the scattering length from length scales outside of the FV [6]. Working with the running scattering length, this logarithm can be absorbed, and the QC can be expressed in terms of

[6] Similar considerations apply to the analogous QC (without EM) in two spatial dimensions [59].

quantities that have support only within the FV, i.e. $a(2\pi/L)$. When working directly with physical quantities, the infrared scale $\bar{\mu} = \alpha M e^{\gamma_E}/2$ can be chosen, which implies $a(\bar{\mu}) = a_C$ and the function $p\cot\bar{\delta}(p) \equiv p\cot\bar{\delta}(p,\bar{\mu})$ can be used in the QC,

$$p\cot\bar{\delta}'(p) \;=\; -\frac{1}{a'_C} \;+\; \frac{1}{2}r'_0 p^2 \;+\; \ldots \;=\; \frac{1}{\pi L}\mathcal{S}^C(\tilde{p}) \;+\; \alpha M\left[\ln\left(\frac{4\pi}{\alpha M L}\right) - \gamma_E\right]\;. \qquad (35)$$

D. Approximate Energy Eigenvalues

Ideally, the QC in Eq. (26) is solved numerically to determine the FV energy eigenvalues. However, the smallness of αML in present day calculations, and those of the foreseeable future, implies that the QED FV shifts in the two-hadron energy eigenvalues are small, and the numerics will not be particularly enlightening. However, considering the $\mathcal{O}(\alpha)$ perturbative corrections to the eigenvalues is informative. It is worth emphasizing the somewhat peculiar nature of the expansions in the approximate formulas that follow, which suggest a somewhat narrow range of validity. While the expansions are formally perturbative in $1/L$ times the length scale which characterizes the strength of the interaction, and are also nonrelativistic, it is further assumed that $ML \ll 1/\alpha$ so that the QED interactions can be treated perturbatively.

1. The Ground State

In a perturbative expansion around the non-interacting ground state, with energy $E = 2M^L$, there is no contribution from the QED interactions at $\mathcal{O}(\alpha)$ in the absence of strong interactions. This is due to the absence of the photon zero mode, with the uniform background charge density in the unperturbed state exactly canceling the particle charge density [7]. Using standard methods, it is straightforward to find the ground-state energy shift for scattering parameters that are small compared to L,

$$\begin{aligned}\Delta E_0^C =&\; \Delta E_0 + \Delta E_0^{(\alpha)} \\ =&\; \frac{4\pi\, a'}{M\, L^3}\left\{1 - \left(\frac{a'}{\pi\, L}\right)\mathcal{I} + \left(\frac{a'}{\pi\, L}\right)^2\left[\mathcal{I}^2 - \mathcal{J}\right] + \ldots\right\}\end{aligned}$$

[7] Note that the ground-state energy of boosted systems will have pure Coulomb corrections as the charge density is no longer uniformly zero.

$$
\begin{aligned}
& - \frac{2\alpha\, a'}{L^2\pi^2}\Bigg\{\mathcal{J} + \left(\frac{a'}{\pi\, L}\right)\left[\mathcal{K} - \mathcal{I}\mathcal{J} - \mathcal{R}/2\right] \\
& \qquad + \left(\frac{a'}{\pi\, L}\right)^2 \left[\mathcal{R}\mathcal{I} + \mathcal{I}^2\mathcal{J} - 2\mathcal{J}^2 - 2\mathcal{I}\mathcal{K} + \mathcal{L} - \mathcal{R}_{24}\right] \\
& \qquad + \frac{2a' r_0' \pi^2}{L^2}\mathcal{I} + \ldots \Bigg\} ,
\end{aligned} \tag{36}
$$

where $a' \equiv a'(2\pi/L)$ is the $\overline{MS}_{FV}$ scattering length and the geometric constants, $\mathcal{I}$, $\mathcal{J}$, $\mathcal{K}$, $\mathcal{L}$, $\mathcal{R}$ and $\mathcal{R}_{24}$ are defined and evaluated in the Appendix. The first term in braces is the well-known energy shift due to QCD interactions, while the second term is the shift due to the combined QCD and QED interactions. This can also be expressed in terms of the kinematically-shifted scattering parameters,

$$
\begin{aligned}
\Delta E_0^C \;&= \frac{4\pi\, a_C'}{M\, L^3}\Bigg\{1 - \left(\frac{a_C'}{\pi\, L}\right)\mathcal{I} + \left(\frac{a_C'}{\pi\, L}\right)^2 \left[\mathcal{I}^2 - \mathcal{J}\right] + \ldots\Bigg\} \\
& - \frac{2\alpha\, a_C'}{L^2\pi^2}\Bigg\{\mathcal{J} + \left(\frac{a_C'}{\pi\, L}\right)\left[\mathcal{K} - \mathcal{I}\mathcal{J} - \tilde{\mathcal{R}}/2\right] \\
& \qquad + \left(\frac{a_C'}{\pi\, L}\right)^2 \left[\tilde{\mathcal{R}}\mathcal{I} + \mathcal{I}^2\mathcal{J} - 2\mathcal{J}^2 - 2\mathcal{I}\mathcal{K} + \mathcal{L} - \mathcal{R}_{24}\right] \\
& \qquad + \frac{2a_C' r_0' \pi^2}{L^2}\mathcal{I} + \ldots \Bigg\} ,
\end{aligned} \tag{37}
$$

where

$$
\tilde{\mathcal{R}} \;\equiv\; \mathcal{R} \;-\; 4\pi^4 \left[\ln\left(\frac{4\pi}{\alpha M L}\right) - \gamma_E\right] . \tag{38}
$$

The ellipsis denote terms that are higher order in $1/M$, $1/L$ and α. In terms of the physical scattering parameters, the energy shift of the ground state is

$$
\begin{aligned}
\Delta E_0^C \;&= \frac{4\pi\, a_C}{M\, L^3}\Bigg\{1 - \left(\frac{a_C}{\pi\, L}\right)\mathcal{I} + \left(\frac{a_C}{\pi\, L}\right)^2 \left[\mathcal{I}^2 - \mathcal{J}\right] + \ldots\Bigg\} \\
& - \frac{2\alpha\, a_C}{L^2\pi^2}\Bigg\{\mathcal{J} + \left(\frac{a_C}{\pi\, L}\right)\left[\mathcal{K} - \mathcal{I}\mathcal{J} - \tilde{\mathcal{R}}/2\right] \\
& \qquad + \left(\frac{a_C}{\pi\, L}\right)^2 \left[\tilde{\mathcal{R}}\mathcal{I} + \mathcal{I}^2\mathcal{J} - 2\mathcal{J}^2 - 2\mathcal{I}\mathcal{K} + \mathcal{L} - \mathcal{R}_{24}\right] \\
& \qquad + \frac{a_C r_0 \pi^2}{L^2}\mathcal{I} + \ldots \Bigg\} ,
\end{aligned} \tag{39}
$$

The only difference between Eq. (37) and Eq. (39) is the coefficient of the last term, as other differences are higher order in the expansion.

2. *The First Excited State*

In contrast to the ground state, the energy shift of the first excited state in the FV receives a contribution from the exchange of a single Coulomb photon as the uniform background charge density does not cancel against the $|\mathbf{n}| = 1$ unperturbed two-hadron charge density. Following Lüscher [24, 25] and expanding [8] the energy shift in terms of $\tan\overline{\delta}'$ evaluated at the unperturbed energy, the energy shift of the first excited state is

$$\begin{aligned} \Delta E_1^C = & \ \Delta E_1 + \Delta E_1^{(\alpha)} \\ = & \ \frac{4\pi^2}{ML^2} - \frac{12\tan\overline{\delta}'}{ML^2}\left(1 + c_1'\tan\overline{\delta}' + c_2'\tan^2\overline{\delta}' + ...\right) \\ & + \frac{9\alpha}{4\pi \mathrm{L}}\left(1 + c_{1\alpha}'\tan\overline{\delta}' + \left(c_{2\alpha}' + \frac{8}{3}\log\left(\alpha ML\right)\right)\tan^2\overline{\delta}' + ...\right) \quad , \end{aligned} \tag{40}$$

where $c_1' = -0.061365$, $c_2' = -0.35415$ and $c_{1\alpha}' = 3.83582$, $c_{2\alpha}' = -7.12197$, The strong coefficients, $c_{1,2}'$ were first computed by Lüscher [24, 25], and we do not repeat their determination here. The leading QED contribution arises from the exchange of a single Coulomb photon between $|\mathbf{n}| = 1$ two-hadron states, and is simply given by

$$\frac{\alpha}{6\pi L}\sum_{\substack{|\mathbf{m}|,|\mathbf{n}|=1 \\ \mathbf{n}\neq\mathbf{m}}} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} = \frac{9\alpha}{4\pi L} \quad , \tag{41}$$

while the remaining QED contributions are of the form

$$\begin{aligned} c_{1\alpha}' &= -\frac{4}{9\pi^2}\left(6 - \mathcal{X}_2\right) \quad ; \\ c_{2\alpha}' &= -\frac{2}{3\pi^4}\Big[\frac{1}{3}\left(6 - \mathcal{X}_2\right)\mathcal{I}^{(1)} + \frac{1}{6}\mathcal{X}_1\mathcal{J}^{(1)} - \mathcal{R} + 12 \\ & \qquad +2\left(\mathcal{X}_3 + \mathcal{X}_4 + \mathcal{X}_5\right) + \mathcal{X}_1 - \mathcal{X}_6 - 4\pi^4\left(\gamma_E - \log 4\pi\right)\Big] \quad , \end{aligned} \tag{42}$$

where the geometric constants, $\mathcal{I}^{(1)}$, $\mathcal{J}^{(1)}$, and $\mathcal{X}_1$-$\mathcal{X}_6$ are defined and evaluated in the Appendix. Terms higher order in $1/L$, such as the leading contribution from r_0 at $1/L^2$, e.g. $+\frac{9\alpha}{4\pi L}\frac{3r_0}{\pi L}\tan^2\overline{\delta}$, are not shown. Further, at this order, $\tan\overline{\delta}'$ can be replaced with $\tan\overline{\delta}$ without modifying the form of Eq. (40). To give some perspective, in a L = 10 fm volume, the leading $\mathcal{O}(\alpha)$ energy shift from the exchange of a single Coulomb photon is ~ 100 keV.

[8] Note that this expansion requires special care due to the singular, purely Coulombic, contribution.

3. The (Possible) Bound State

In nature, there are no bound doubly-charged two hadron systems, however such systems do exist at unphysical pion masses, as determined with Lattice QCD calculations [17, 19, 21, 60]. The bound-state energy in the FV is determined from the large-x limit of $\mathcal{S}^C(x)$ in Eq. (26) and Eq. (27), and, in particular, the sums contributing to $\mathcal{S}^C(x)$ are

$$\sum_{\mathbf{n}}^{\Lambda_n} \frac{1}{|\mathbf{n}|^2+\tilde{\kappa}^2} \ \rightarrow\ 4\pi\Lambda_n \ -\ 2\pi^2\tilde{\kappa} \ \ ; \tag{43}$$

$$\sum_{\mathbf{n}}^{\Lambda_n}\sum_{\mathbf{m}\neq\mathbf{n}} \frac{1}{|\mathbf{m}|^2+\tilde{\kappa}^2}\frac{1}{|\mathbf{n}|^2+\tilde{\kappa}^2}\frac{1}{|\mathbf{n}-\mathbf{m}|^2} \ \rightarrow\ 4\pi^4\ \left(\log\Lambda_n \ -\ \log\left(2\tilde{\kappa}\right)\ \right) \ +\ \frac{\pi^2}{\tilde{\kappa}}\mathcal{I} \quad , \tag{44}$$

in the large volume limit, $\tilde{\kappa}\rightarrow\infty$, where only the leading power-law corrections are shown [9]. At the order to which we are working, these limits lead to a FV QC for the bound state of

$$-\frac{1}{a_C} - \frac{1}{2}r_0\kappa^2 \ =\ -\kappa - \alpha M\left(\gamma_E + \log\left(\frac{\alpha M}{4\kappa}\right)\right) \ -\ \frac{\alpha M}{2\pi\kappa L}(1-\kappa r_0)\mathcal{I} \quad , \tag{45}$$

which determines the leading Coulomb corrections to the bound-state binding energy. Performing a perturbative expansion of $\kappa=\kappa_0+\kappa_1+...$ leads to a binding energy of

$$B^C \ =\ \frac{\kappa_0^2}{M} \ -\ \frac{2\alpha\kappa_0}{1-\kappa_0 r_0}\ \left[\ \gamma_E \ +\ \log\left(\frac{\alpha M}{4\kappa_0}\right)\right] \ -\ \frac{\alpha}{\pi L}\mathcal{I} \ +\ ... \quad , \tag{46}$$

where κ_0 is the binding momentum resulting from the strong interactions alone. The leading QED contribution to the infinite-volume binding energy is consistent with a direct perturbative calculation in the ER theory. Further, the leading FV correction to the binding is given [10], which vanishes as $1/L$, as expected.

In the limit in which the bound state is compact compared to the lattice volume, the leading corrections to its total mass should be that of a charge-2 system, as calculated in Ref. [45]. There are two contributions to the mass shift of the bound state, one from the shifts of the individual constituent hadrons, and one from the shift in the binding energy.

[9] Eq. (44) is obtained by first shifting $\mathbf{m}\rightarrow\mathbf{n}+\mathbf{p}$, performing the sum over $\mathbf{n}$ using the Poisson summation formula, and then dividing the sum over $\mathbf{p}$ into two regions. The first region generates the power law correction, and the second region is again evaluated using Poisson summation to give the logarithmic contributions.

[10] The relation between the scattering parameters and the binding momentum has been used, with terms higher order in the scattering parameters neglected.

We find that in the deep-binding limit, the total mass of the bound state is shifted by

$$\delta M_{BS}^{(FV)} \ = \ 2\delta M^{(FV)} - \delta B^C \ = \ 2\left(\frac{\alpha}{2\pi L}\mathcal{I}\right) + \frac{\alpha}{\pi L}\mathcal{I} \ + \ ... \ = \ \frac{2\alpha}{\pi L}\mathcal{I} \ + \ ... \quad , \tag{47}$$

consistent with expectations [44, 45].

Above we have considered the case of a system bound by the strong interaction, and shown how the quantization condition, Eq. (26), gives the correct compact limit. If the system is bound in the continuum by the electromagnetic interaction, then the compact limit cannot be explicitly taken, as this would require moving through a region of parameter space where the Coulomb interaction becomes non-perturbative in the finite volume. Of course, the compact result will necessarily coincide with the results of Ref. [44, 45].

IV. SUMMARY AND DISCUSSION

Lattice QCD has reached the point where QED is being included in calculations of some of the simplest hadronic properties, such as the masses of the lowest lying hadrons. Naively, the inclusion of QED should be problematic for calculations in a finite volume due to its long range nature. However, by simply omitting the zero-modes of the photon field, which lead to the violation of both Gauss's and Ampere's laws, Lattice QCD+QED calculations can be performed in meaningful ways to reliably extract important quantities without corrupting the infinite-volume limit. Recently, the relation between the single hadron masses calculated in a finite volume and their infinite-volume values has been established [44, 45]. Given the nonperturbative nature of the Coulomb interaction in low-energy scattering, extending this work to relate two-hadron energy eigenvalues to their corresponding S-matrix elements had the potential to be quite involved. In this work, we have shown that there is a large range of volumes, satisfying $ML \ll 1/\alpha$, for which the non-relativistic relation between the finite-volume energy of two hadrons in the A_1^+ representation of the cubic group and their s-wave phase shift receives calculable perturbative QED corrections. Our results will straightforwardly generalize to the relations between the energies of two hadrons in other representations of the cubic group and the phase shifts and mixing parameters in all relevant scattering channels.

The confining nature of QCD simplifies the evaluation of hadronic correlation functions using Lattice QCD, as it dictates that the interactions among hadrons are contained within a volume set by the longest correlation length, which is the pion Compton wavelength. As long as the size of the spatial lattice is significantly larger than the inverse pion mass, there is a hierarchy of length scales and finite-volume artifacts can be removed, as in the case of single-particle properties, or exploited, as in the calculation of two-particle interactions. The presence of an infinite-range force destroys this hierarchy. With no zero modes and a gap in the spectrum of the momentum operator, there is a region of parameter space for the calculation of the energy of two non-relativistic hadrons of mass M. In particular, if the lattice volume satisfies $ML \ll 1/\alpha$, Coulomb ladders are perturbative, and their contribution to the two-particle energy, along with other contributions that are absent in infinite volume, can be computed perturbatively in α. Furthermore, in the absence of zero modes, the gap in the spectrum sets the scale of the contribution due to inelastic processes. It is essential that such a gap exist in order to derive the quantization conditions that relate the energies computed in LQCD and relevant S-matrix elements - those dictating the two-hadron scattering amplitude, and those which determine electromagnetic processes [11]. In the absence of QED, the low-energy EFT, which is valid up to the start of the QCD t-channel cut, gives a QC in a form that is valid up to the QCD inelastic threshold when expressed in terms of $p \cot \delta$ (see Fig. 2). However, it is important to stress that in the presence of QED, the expressions we have derived are valid up to the QED inelastic threshold when this lies below the QCD t-channel cut, or otherwise up to the QCD t-channel cut.

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[11] In the case of a light scalar with no gauge or chiral symmetry present that gives rise to nonperturbative interactions in the continuum, one can still remove the zero mode without affecting physics, and in principle find a region of parameter space where perturbation theory is valid. If there is no such region, then formalism beyond what has been developed here will be necessary.

APPENDIX: Integer Sums

Single Sums

The single sums over integer triplets that are required for the modified kinematics in a finite volume and for the approximate two-hadron energy eigenvalues are:

$$
\begin{aligned}
\mathcal{I} &= \sum_{\mathbf{n}\neq 0}^{\Lambda_n} \frac{1}{|\mathbf{n}|^2} - 4\pi\Lambda_n = -8.9136 \quad , & \mathcal{J} &= \sum_{\mathbf{n}\neq 0} \frac{1}{|\mathbf{n}|^4} = 16.5323 \ ; \\
\mathcal{K} &= \sum_{\mathbf{n}\neq 0} \frac{1}{|\mathbf{n}|^6} = 8.4019 \quad , & \mathcal{L} &= \sum_{\mathbf{n}\neq 0} \frac{1}{|\mathbf{n}|^8} = 6.9458 \ ; \\
\mathcal{I}^{(1)} &= \sum_{|\mathbf{n}|\neq 1} \frac{1}{|\mathbf{n}|^2 - 1} = -1.2113 \quad , & \mathcal{J}^{(1)} &= \sum_{|\mathbf{n}|\neq 1} \frac{1}{(|\mathbf{n}|^2 - 1)^2} = 23.2430 \ ; \\
\mathcal{X}_1 &= \sum_{\substack{|\mathbf{m}|,|\mathbf{n}|=1 \\ \mathbf{n}\neq\mathbf{m}}} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} = \frac{27}{2} \quad , & \mathcal{X}_2 &= \sum_{\substack{|\mathbf{n}|=1 \\ |\mathbf{m}|>1}} \frac{1}{|\mathbf{m}|^2 - 1} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} = 91.1806 \ ; \\
\mathcal{X}_3 &= \sum_{|\mathbf{n}|>1} \frac{1}{|\mathbf{n}|^2(|\mathbf{n}|^2 - 1)} = 14.7022 \quad , & \mathcal{X}_4 &= \sum_{\substack{|\mathbf{m}|=1 \\ |\mathbf{n}|>1}} \frac{1}{|\mathbf{n}|^2} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} = 65.3498 \ ; \\
\mathcal{X}_5 &= \sum_{\substack{|\mathbf{n}|=1 \\ |\mathbf{m}|>1}} \frac{1}{(|\mathbf{m}|^2 - 1)^2} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} = 46.5687 \quad . & & \qquad\qquad \text{(A-1)}
\end{aligned}
$$

Double Sums

Unlike the situation in large volumes when only strong interactions contribute, and explicit two-loop sums are not required, the leading QED contributions resulting from the exchange of Coulomb photons require non-trivial two-loop sums over triplets of integers. Consider the finite double sum:

$$
\begin{aligned}
\mathcal{R} &\equiv \sum_{\mathbf{n}\neq 0}^{\Lambda_n} \sum_{\mathbf{m}\neq 0,\mathbf{n}}^{\infty} \frac{1}{|\mathbf{n}|^2|\mathbf{m}|^2} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} - 4\pi^4 \ln\Lambda_n \\
&= \sum_{\mathbf{n}\neq 0}^{\Lambda_n} \frac{1}{|\mathbf{n}|^2} \mathcal{R}_{sub}(\mathbf{n}) - 4\pi^4 \ln\Lambda_n \ . \qquad \text{(A-2)}
\end{aligned}
$$

It is regulated asymmetrically, by first evaluating the inner sum without a cut off,

$$
\mathcal{R}_{sub}(\mathbf{n}) \equiv \sum_{\mathbf{m}\neq 0,\mathbf{n}}^{\infty} \frac{1}{|\mathbf{m}|^2} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} \ , \qquad \text{(A-3)}
$$

and then straightforwardly evaluated using the methods described in Ref. [61]. It is found to be

$$\mathcal{R}_{sub}(\mathbf{n}) \;=\; -2\eta\left(1-e^{-\eta|\mathbf{n}|^2}\right)\frac{1}{|\mathbf{n}|^2} \;+\; \sum_{\mathbf{m}\neq 0,\mathbf{n}}^{\infty}\left(e^{-\eta D_{\mathbf{nm}}}+e^{-\eta|\mathbf{m}|^2}-e^{-\eta(D_{\mathbf{nm}}+|\mathbf{m}|^2)}\right)\frac{1}{|\mathbf{m}|^2 D_{\mathbf{nm}}}$$
$$+\int d^3\mathbf{m}\left(1-e^{-\eta D_{\mathbf{nm}}}\right)\left(1-e^{-\eta m^2}\right)\frac{1}{|\mathbf{m}|^2 D_{\mathbf{nm}}}\;, \qquad \text{(A-4)}$$

where $D_{\mathbf{nm}} \equiv |\mathbf{n}-\mathbf{m}|^2$, and η is a small number introduced to provide a clean way to separate sums into UV and IR contributions where the UV sums can be replaced by integrals. The η used here should not be confused with the kinematic variable used in the main body of the paper. The η-independent piece (in the integral) is readily evaluated, giving

$$\mathcal{R}_{sub}(\mathbf{n}) \;=\; \frac{\pi^3}{|\mathbf{n}|} - 2\eta\left(1-e^{-\eta|\mathbf{n}|^2}\right)\frac{1}{|\mathbf{n}|^2}$$
$$+\sum_{\mathbf{m}\neq 0,\mathbf{n}}^{\infty}\left(e^{-\eta D_{\mathbf{nm}}}+e^{-\eta|\mathbf{m}|^2}\;-\;e^{-\eta(D_{\mathbf{nm}}+|\mathbf{m}|^2)}\right)\frac{1}{|\mathbf{m}|^2 D_{\mathbf{nm}}}$$
$$-2\pi\int_0^{\infty}dm\int_{-1}^{1}dc\left(e^{-\eta D_{nmc}}+e^{-\eta m^2}-e^{-\eta(D_{nmc}+m^2)}\right)\frac{1}{D_{nmc}}\;. \qquad \text{(A-5)}$$

where $D_{nmc} \equiv |\mathbf{n}|^2 - 2|\mathbf{n}||\mathbf{m}|c + |\mathbf{m}|^2$, from which Eq. (A-2) becomes

$$\mathcal{R} \;=\; \pi^3\,\alpha_{3/2} \;-\; 2\eta\,\mathcal{J} \;+\; 2\eta\,\mathcal{J}^{\eta} \;+\; \mathcal{T}_1 \;-\; 2\pi\,\mathcal{T}_2 \;=\; -178.42(01)\;. \qquad \text{(A-6)}$$

where [61]

$$\alpha_{3/2} \;\equiv\; \sum_{\mathbf{n}\neq 0}^{\Lambda_n}\frac{1}{|\mathbf{n}|^3} \;-\; 4\pi\ln\Lambda_n \;=\; 3.8219\;, \qquad \text{(A-7)}$$

The η-dependent sums are

$$\mathcal{J}^{\eta} \;\equiv\; \sum_{\mathbf{n}\neq 0}^{\infty}\frac{e^{-\eta|\mathbf{n}|^2}}{|\mathbf{n}|^4}\;;$$
$$\mathcal{T}_1 \;\equiv\; \sum_{\mathbf{n}\neq 0}^{\infty}\sum_{\mathbf{m}\neq 0,\mathbf{n}}^{\infty}\left(e^{-\eta D_{\mathbf{nm}}}+e^{-\eta|\mathbf{m}|^2}-e^{-\eta(D_{\mathbf{nm}}+|\mathbf{m}|^2)}\right)\frac{1}{|\mathbf{n}|^2|\mathbf{m}|^2 D_{\mathbf{nm}}}\;;$$
$$\mathcal{T}_2 \equiv \sum_{\mathbf{n}\neq 0}^{\infty}\frac{1}{|\mathbf{n}|^2}\int_0^{\infty}dm\int_{-1}^{1}dc\left(e^{-\eta D_{nmc}}+e^{-\eta m^2}-e^{-\eta(D_{nmc}+m^2)}\right)\frac{1}{D_{nmc}}\;, \qquad \text{(A-8)}$$

where are all evaluated numerically for a range of values of η that provide stable results for each.

Evaluation of the perturbative expansion of the ground-state energy requires sums of the form

$$\mathcal{R}_{st} \equiv \sum_{\mathbf{n}\neq 0}^{\infty} \sum_{\mathbf{m}\neq 0,\mathbf{n}}^{\infty} \frac{1}{|\mathbf{n}|^s |\mathbf{m}|^t} \frac{1}{|\mathbf{n}-\mathbf{m}|^2} \ , \tag{A-9}$$

but at the order to which we have worked, only $\mathcal{R}_{24} = 170.97(01)$ is required. Further, in the perturbative expansion of the energy of the first excited states, the two-loop sum

$$\mathcal{X}_6 = \sum_{\substack{|\mathbf{m}|,|\mathbf{n}|>1 \\ \mathbf{n}\neq\mathbf{m}}} \left(\frac{1}{|\mathbf{n}|^2-1} \frac{1}{|\mathbf{m}|^2-1} - \frac{1}{|\mathbf{n}|^2} \frac{1}{|\mathbf{m}|^2} \right) \frac{1}{|\mathbf{n}-\mathbf{m}|^2} = 264.508 \quad , \tag{A-10}$$

is required, and it is evaluated with techniques similar to those used previously.

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