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Charged hadrons in local finite-volume QED+QCD with C^* boundary conditions

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ABSTRACT: In order to calculate QED corrections to hadronic physical quantities by means of lattice simulations, a coherent description of electrically-charged states in finite volume is needed. In the usual periodic setup, Gauss’s law and large gauge transformations forbid the propagation of electrically-charged states. A possible solution to this problem, which does not violate the axioms of local quantum field theory, has been proposed by Wiese and Polley, and is based on the use of C^* boundary conditions. We present a thorough analysis of the properties and symmetries of QED in isolation and QED coupled to QCD, with C^* boundary conditions. In particular we learn that a certain class of electrically-charged states can be constructed in a fully consistent fashion without relying on gauge fixing and without peculiar complications. This class includes single particle states of most stable hadrons. We also calculate finite-volume corrections to the mass of stable charged particles and show that these are much smaller than in non-local formulations of QED.

KEYWORDS: Gauge Symmetry, Nonperturbative Effects, Discrete and Finite Symmetries, Lattice Quantum Field Theory

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1 Introduction

Electromagnetic interactions contribute at the order of a few percentage points to masses, decay rates and scattering cross-sections of hadrons. Nevertheless these small contributions cannot be ignored if one is interested in quantifying isospin breaking effects like the charged-neutral mass splittings of baryons and mesons, or when one aims at percent accuracy in the calculation of hadronic matrix elements. In these cases first-principle theoretical predictions can be obtained only by means of lattice techniques, which require a consistent formulation of QCD+QED in finite volume.

The problem addressed in this paper arises every time one needs to produce an electrically-charged state in a finite periodic box, as for instance in the calculation of the proton mass, and is intrinsically related to the dynamics of the zero-modes of the gauge field. In a torus with periodic boundary conditions for the gauge fields, Gauss's law

implies that only neutral states belong to the physical Hilbert space of the theory. One might think to overcome this limitation by gauge-fixing. For instance in Coulomb gauge the Gauss's law is locally solved and the Hilbert space splits in sectors labeled by the total electric charge. However states generated by electrically-charged local operators in Coulomb gauge are also charged under large gauge transformations which survive a local gauge-fixing procedure. Because of this, even after gauge-fixing, the two-point function $\langle \psi(x) \bar{\psi}(y) \rangle$ vanishes if x and y are separated in a periodic box. In practice large gauge transformations act on the gauge field by shifting the global zero-modes $\int_{TL^3} d^4x A_\mu(x)$. Therefore the obstructions to the propagation of charged particles on a periodic torus can be traced back to the functional integration over the global zero-modes.

A possible solution to this problem can be found in ref. [1] where the first lattice calculation of the electromagnetic mass splitting of nucleons and light pseudoscalar mesons has been attempted. The proposed solution consists in *quenching* a particular set of Fourier modes of the gauge field, in such a way that the global zero-modes decouple from the dynamics. A lot of theoretical and algorithmic progress has been made after the pioneering work of ref. [1], particularly in the past few years, leading to recent determinations of the electromagnetic mass splitting of light pseudoscalar mesons and light baryons, see refs. [2–9] for recent works on the subject. All these works rely on finite-volume formulations of QED obtained by quenching some Fourier modes of the gauge field.¹

The particular formulation called QED_L is obtained by quenching the spatial zero-modes of the gauge field at any time, i.e. by enforcing the constraint $\tilde{A}_\mu(t, \mathbf{0}) = \int_{L^3} d^3x A_\mu(t, \mathbf{x}) = 0$. As opposed to other formulations, QED_L has a well defined transfer matrix. However the constraint $\tilde{A}_\mu(t, \mathbf{0}) = 0$ is *non-local*. Even though one can argue that the modification generated by the constraint is a finite-volume effect, many properties of local quantum field theories are not automatically guaranteed for QED_L. Among these we mention renormalizability, volume-independence of renormalization constants, the validity of the operator product expansion and of the Symanzik improvement program. Mild violations of locality may preserve some of these properties but this needs to be shown explicitly case by case.

QED_L has been studied at one-loop in perturbation theory in refs. [2, 4, 17]. The quenching of the zero-modes does not generate ultraviolet divergences at one loop, other than the infinite-volume ones. However it does generate unusual phenomena, for instance particles and antiparticles do not decouple in the non-relativistic limit [18, 19]. This can be seen as a failure of the effective-theory description which is not surprising if the underlying microscopic theory is non-local. On the other hand the numerical results of lattice simulations of QED_L performed in refs. [2, 5] might be viewed as reassuring evidence that the

¹Recently other approaches have been proposed. In ref. [11] the zero modes of the gauge field are lifted by adding a mass term for the photon. The proposal of refs. [12, 13] consists in combining QCD matrix elements extracted from finite volume simulations with infinite volume QED kernels. In refs. [14, 15], see also ref. [16], the global zero modes of the gauge field are treated as compact dynamical variables. The massive photon provides a local formulation of the finite-volume theory. Nevertheless we believe that the interplay between the $m_\gamma \rightarrow 0$ and the $L \rightarrow \infty$ limits requires deeper investigation. The other two approaches rely on non-local constructions at finite volume.

non-localities of QED_L have only mild effects on the hadronic spectrum. Nevertheless we believe that QED_L is not sufficiently well understood at all orders in perturbation theory. Our approach is to eliminate any potential problems at the root, by seeking a consistent formulation of the finite volume theory that does not require quenching dynamical degrees of freedom.

In this paper we consider a *local* solution to the problem of charged particles in finite volume. This solution is not new, it has been proposed in [20–23] and consists in enforcing C^* boundary conditions for all fields along the spatial directions, i.e. in requiring that the fields are periodic up to charge conjugation. In this theory, which we refer to as QED_C , the zero-modes of the gauge field are absent by construction because $A_\mu(x)$ is anti-periodic in space, and the classical problems of the periodic setup are avoided from the very beginning. We show that a complete description of a certain class of electrically-charged states can be obtained without relying either on perturbation theory or on gauge-fixing. As we shall discuss in detail, this class of states covers most of the relevant spectroscopic applications and includes the proton, the neutron, the charged pions, the charged kaons, the charged D and B mesons and the Σ^\pm baryons. The proposed construction is based on the fact that C^* boundary conditions break the global gauge symmetry group $U(1)$ down to its discrete subgroup \mathbb{Z}_2 . In other words charge conservation is partially violated by the boundary conditions. The full group of gauge transformations splits in two disconnected components: the subgroup of local gauge transformations which are connected to the identity, and the set resulting by the composition of local gauge transformations with the nontrivial global gauge transformation. In this setup one can construct states that are invariant under local gauge transformations but not under global gauge transformations, and these can be identified as electrically-charged states.

Along with charge conservation, C^* boundary conditions partially violate flavour conservation. This happens because flavour-charged particles traveling once around the torus turn into their antiparticles, and therefore change their flavour content. Being associated with the propagation of massive colorless particles, these effects are exponentially suppressed with the volume. We study in detail the pattern of flavour violation in QED_C , particularly in the case when electromagnetic interactions are coupled to QCD, and quantify these effects in the framework of a generic effective theory of hadrons. In particular we show that, although the Ω^- and Ξ^- baryons can mix with lighter states because of the boundary conditions, the exponential suppression is so strong that these mixings can hardly represent a problem in numerical simulations.

Finite-volume effects on the masses of charged particles are considerably smaller in QED_C than in QED_L . When these corrections are expanded in a power series in $1/L$, at order α_{em} in both theories the $1/L$ and $1/L^2$ finite-volume corrections to the mass of a charged particle are universal, i.e. they do not depend on the spin and on the internal structure of the particle (for QED_L see refs. [2, 4, 18, 19, 24]). We show that these universal corrections are always appreciably larger in QED_L than in QED_C . For instance at $mL = 4$ we gain a factor of about 2 with three C^* -periodic spatial directions and a factor of about 5 with a single C^* -periodic spatial direction, see figure 4. More importantly, the spin and structure-dependent corrections are $\mathcal{O}(1/L^3)$ in QED_L , while they are only $\mathcal{O}(1/L^4)$ in QED_C . This extra suppression can be seen as a direct effect of locality.

The calculation of decay rates and cross sections in presence of electromagnetic interactions requires a consistent procedure to deal with soft photons. When electromagnetic interactions are treated perturbatively, these degrees of freedom are at the origin of the well-known problem of infrared divergences. A discussion of these issues in the framework of lattice simulations can be found in ref. [10] where a method to calculate QED radiative corrections to the leptonic decay rates of pseudoscalar mesons has been recently proposed. The calculation of hadronic matrix elements in QCD+QED_C will be the subject of future works. Here we just want to notice that the renormalization of any operator, in particular of the weak effective Hamiltonian, is not affected by the fact that flavour is partially violated in QCD+QED_C. This is because QCD+QED_C is a local theory and flavour is violated only by the boundary conditions.

The paper is organized as follows. In section 2 we introduce C* boundary conditions and study the symmetries of QED_C. In section 3 we introduce the gauge invariant interpolating operators for charged particles and study their properties. In section 4 we couple electromagnetic and strong interactions and study the symmetries of QCD+QED_C. In section 5 we discuss the finite volume corrections to the masses of charged hadrons. In section 6 we discuss the details of the lattice implementation of C* boundary conditions and of the proposed gauge invariant interpolating operators. We draw our conclusions in section 7.

The paper contains four appendices with the explicit derivation of some of the results presented in the main body of the paper. The material discussed in the appendices is technical and some of it is, we believe, original. Appendix A presents a detailed study of some flavour-violation processes in QCD+QED_C, in the context of a generic effective theory of hadrons. This analysis requires an extension of the techniques developed to study finite-volume effects in [25], and it is complicated by the need to keep track of flavour flow and violations through all possible Feynman diagrams. In appendix B we give an *ab-initio* derivation (i.e. without using an effective description of hadrons) of the power-law finite-volume corrections on the mass of charged hadrons in QCD+QED_C. The coefficients of the expansion in powers of $1/L$ are expressed in terms of physical quantities, i.e. derivatives of the forward Compton amplitude for the scattering of a soft photon on the charged hadron. The authors are convinced that the technology developed in these appendices will find other uses in the field.

2 QED_C

In this section we introduce the finite-volume theory QED_C and study its symmetries. For simplicity, we consider the case of a maximally symmetric torus with linear size equal to L , with fields obeying C* boundary conditions in all space directions. The Euclidean time direction can be either infinite or compact with linear size T . In the latter case the corresponding boundary conditions for the fields will be left unspecified. Common choices are periodic, Schrödinger Functional (SF), open or open-SF boundary conditions.

The action of QED_C is given by

$$S[A, \psi] = \int_{L^3T} d^4x \left\{ \frac{1}{4e^2} F_{\mu\nu} F_{\mu\nu} + \sum_{f=1}^{N_f} \bar{\psi}_f \left(\gamma_\mu D_\mu^{\vec{f}} + m_f \right) \psi_f \right\}. \quad (2.1)$$

The field strength and covariant derivative are defined as

$$\begin{aligned} F_{\mu\nu}(x) &= \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x), \\ D_\mu^{\vec{f}} &= \partial_\mu^{\leftrightarrow} - iq_f A_\mu, \end{aligned} \quad (2.2)$$

where the left-right derivative $\partial_\mu^{\leftrightarrow} = \frac{1}{2}(\partial_\mu^{\rightarrow} - \partial_\mu^{\leftarrow})$ is defined in terms of the partial derivative $\partial_\mu^{\rightarrow}$ acting to the right and the partial derivative $\partial_\mu^{\leftarrow}$ acting to the left. In our notation q_f is the electric charge of the f -th flavour normalized to the electric charge of the positron (i.e. q_f does not include the coupling constant e). Throughout the paper we use this normalization for the electric charge.

Fields obey C* boundary conditions under translations in the three space directions,

$$\begin{aligned} A_\mu(x + \hat{L}_i) &= A_\mu^C(x) = -A_\mu(x), \\ \psi_f(x + \hat{L}_i) &= \psi_f^C(x) = C^{-1} \bar{\psi}_f^T(x), \\ \bar{\psi}_f(x + \hat{L}_i) &= \bar{\psi}_f^C(x) = -\psi_f^T(x) C, \end{aligned} \quad (2.3)$$

where \hat{L}_i is L times the unit vector in direction i . The charge conjugation matrix can be taken to be any invertible matrix C with unit determinant such that

$$C^{-1} \gamma_\mu^T C = -\gamma_\mu, \quad (2.4)$$

where γ_μ are the Euclidean gamma matrices. In four dimensions such a matrix exists and satisfies

$$C^T = -C, \quad C^\dagger = C^{-1}, \quad (2.5)$$

independently of the particular representation of the gamma matrices.

Notice that the action density eq. (2.1) is the same as in infinite volume and it is therefore invariant under charge conjugation. Since a shift of a period in space corresponds to charge conjugation, the action density is periodic in space.

We are now going to study the symmetries of QED_C, in turn gauge transformations, spatial translations, parity and flavour symmetries.

2.1 Gauge transformations

Gauge transformations are defined in the usual way

$$\begin{aligned} A_\mu^{[\alpha]}(x) &= A_\mu(x) + \partial_\mu \alpha(x), \\ \psi_f^{[\alpha]}(x) &= e^{iq_f \alpha(x)} \psi_f(x), \\ \bar{\psi}_f^{[\alpha]}(x) &= e^{-iq_f \alpha(x)} \bar{\psi}_f(x). \end{aligned} \quad (2.6)$$

Only gauge transformations that do not change the boundary conditions of the fields are admissible. Translating the transformed field by a period along a spatial direction yields

$$\begin{aligned} A_\mu^{[\alpha]}(x + \hat{L}_i) &= A_\mu(x + \hat{L}_i) + \partial_\mu \alpha(x + \hat{L}_i) \\ &= -A_\mu(x) + \partial_\mu \alpha(x + \hat{L}_i) = -A_\mu^{[\alpha]}(x) + \partial_\mu [\alpha(x + \hat{L}_i) + \alpha(x)]. \end{aligned} \quad (2.7)$$

The transformed field $A_\mu^{[\alpha]}(x)$ is anti-periodic if and only if the gauge transformation satisfies

$$\partial_\mu \alpha(x + \hat{L}_i) = -\partial_\mu \alpha(x), \quad (2.8)$$

i.e. $\alpha(x)$ can be decomposed into an anti-periodic function plus a generic constant. The boundary conditions for fermions constrain this constant. Translating a fermion field by a period along a spatial direction yields

$$\begin{aligned} \psi_f^{[\alpha]}(x + \hat{L}_i) &= e^{iq_f \alpha(x + \hat{L}_i)} \psi_f(x + \hat{L}_i) \\ &= e^{iq_f \alpha(x + \hat{L}_i)} C^{-1} \bar{\psi}_f^T(x) = e^{iq_f [\alpha(x + \hat{L}_i) + \alpha(x)]} C^{-1} [\bar{\psi}^{[\alpha]}]_f^T(x). \end{aligned} \quad (2.9)$$

The transformed field $\psi_f^{[\alpha]}(x)$ satisfies C^* boundary conditions if and only if an integer n_f exists such that

$$\alpha(x) = \beta(x) + \frac{n_f \pi}{q_f}, \quad \beta(x + \hat{L}_i) = -\beta(x). \quad (2.10)$$

Notice that this equation has to be satisfied for all fermion fields and for any pair of charges. In the physically relevant case² all charges q_f are integer multiples of an elementary charge q_{el} , therefore the gauge transformation $\alpha(x)$ preserves the boundary conditions of all fields if and only if an integer n exists such that

$$\alpha(x) = \beta(x) + \frac{n\pi}{q_{el}}. \quad (2.11)$$

Quantization of the electric charge can be seen as a consequence of the fact that the gauge group is the compact $U(1)$. A generic gauge transformation is assigned by choosing a phase factor $\Lambda(x) = e^{iq_{el}\alpha(x)}$ in each point of spacetime. A matter field with charge q_f transforms with $\Lambda(x)^{\hat{q}_f}$ where $\hat{q}_f = q_f/q_{el}$ is an integer, i.e. accordingly to some irreducible representation of the gauge group $U(1)$. This analysis can be restated in terms of operators: given the electric-charge operator Q , the generator of global gauge transformations is

$$\hat{Q} = \frac{Q}{q_{el}}, \quad (2.12)$$

and has only integer eigenvalues. C^* boundary conditions break the $U(1)$ group of global gauge transformations. In fact eq. (2.11) implies that the only allowed global gauge transformations are $\Lambda = \pm 1$, i.e. the global $U(1)$ is broken down to \mathbb{Z}_2 . Breaking of the global $U(1)$ implies a partial violation in electric-charge conservation: Q is not conserved but the quantum number $(-1)^{\hat{Q}}$ is. The origin and consequences of this violation will be discussed

²If two of the charges have irrational ratio, then one of the n_f has to be zero and consequently $\alpha(x)$ has to be anti-periodic.

in more details in subsection 2.4 for the case of QED_C in isolation, and in section 4 for the case of QCD+QED_C.

Eq. (2.11) implies that the group of gauge transformations is disconnected. Only gauge transformations with $n = 0$, i.e. with $\alpha(x)$ anti-periodic in space, are continuously connected to the identity. We will refer to these gauge transformations as *local gauge transformations*. Note that the large gauge transformations have a very simple structure (they are just the composition of a global gauge transformation and a local gauge transformation). This contrasts with the case of periodic boundary conditions in space, where large gauge transformations are linear in the coordinates (i.e. $\alpha(x) = 2\pi n x_i / L$ with some integer n).

2.2 Translations

C* boundary conditions preserve translational invariance and charge conjugation. Even though in infinite volume the momentum and the C quantum number are unrelated, this is not true in QED_C. Eqs. (2.3) imply that the translation of a generic (elementary or composite) field $\phi(x)$ by \hat{L}_i is equivalent to a charge conjugation

$$\phi(x + \hat{L}_i) = \phi^C(x). \tag{2.13}$$

The C-even and C-odd components of the field $\phi(x)$ are

$$\phi_{\pm}(x) = \frac{\phi(x) \pm \phi^C(x)}{\sqrt{2}}. \tag{2.14}$$

$\phi_+(x)$ is periodic in space while $\phi_-(x)$ is anti-periodic. The two components have different Fourier representations. Since we want to leave the time boundary conditions unspecified, we expand our fields in the time-momentum representation,

$$\phi_{\pm}(x) = \frac{1}{L^3} \sum_{\mathbf{p} \in \Pi_{\pm}} \tilde{\phi}_{\pm}(x_0, \mathbf{p}) e^{i\mathbf{p}\mathbf{x}}, \tag{2.15}$$

where Π_+ is the set of periodic momenta and Π_- is the set of anti-periodic momenta,

$$\begin{aligned} \Pi_+ &= \left\{ \frac{2\pi}{L} \mathbf{n} \mid \mathbf{n} \in \mathbb{Z}^3 \right\}, \\ \Pi_- &= \left\{ \frac{\pi}{L} (2\mathbf{n} + \bar{\mathbf{n}}) \mid \mathbf{n} \in \mathbb{Z}^3, \bar{\mathbf{n}} = (1, 1, 1) \right\}. \end{aligned} \tag{2.16}$$

Notice that the $A_{\mu}(x)$ field is C-odd and it has only the anti-periodic component, while the fields $\psi_f(x)$ contain both,

$$\begin{aligned} A_{\mu}(x) &= \frac{1}{L^3} \sum_{\mathbf{p} \in \Pi_-} \tilde{A}_{\mu}(x_0, \mathbf{p}) e^{i\mathbf{p}\mathbf{x}}, \\ \psi_{f,\pm}(x) &= \frac{1}{L^3} \sum_{\mathbf{p} \in \Pi_{\pm}} \tilde{\psi}_{f,\pm}(x_0, \mathbf{p}) e^{i\mathbf{p}\mathbf{x}}. \end{aligned} \tag{2.17}$$

The two $\psi_{f,\pm}$ components of the fermion fields satisfy the (anti) Majorana condition

$$\psi_{f,\pm}(x) = \pm C^{-1} [\bar{\psi}_{f,\pm}]^T(x). \tag{2.18}$$

2.3 Parity

Even though not in a trivial fashion, parity is conserved by C^* boundary conditions. Under parity the fields transform like

$$\begin{aligned} A_0(x) &\rightarrow A_0(x_P), & \psi_f(x) &\rightarrow \eta_P \gamma_0 \psi_f(x_P), \\ A_k(x) &\rightarrow -A_k(x_P), & \bar{\psi}_f(x) &\rightarrow \eta_P^* \bar{\psi}_f(x_P) \gamma_0, \end{aligned} \quad (2.19)$$

where $x_P = (x_0, -\mathbf{x})$. In infinite volume η_P is a generic complex phase. For each choice of η_P one obtains a different but equally good parity operator. A customary choice amounts to $\eta_P = 1$. However the parity operator defined in this way does not commute with the charge conjugation operator that we have used to define the C^* boundary conditions. A more natural choice is $\eta_P = i$. The corresponding parity transformation \mathcal{P} commutes with the charge conjugation operator. This can be shown explicitly by acting on the elementary fields with charge conjugation \mathcal{C} first and parity \mathcal{P} after, and by comparing the result with the same operations applied in reversed order. For example, in the case of the fermion field we have

$$\psi_f(x) \xrightarrow{\mathcal{C}} C^{-1} \bar{\psi}_f^T(x) \xrightarrow{\mathcal{P}} -i C^{-1} \gamma_0^T \bar{\psi}_f^T(x_P), \quad (2.20)$$

and

$$\psi_f(x) \xrightarrow{\mathcal{P}} i \gamma_0 \psi_f(x_P) \xrightarrow{\mathcal{C}} i \gamma_0 C^{-1} \bar{\psi}_f^T(x_P). \quad (2.21)$$

The results of the two transformations are shown to be equal by using $C^{-1} \gamma_0^T C = -\gamma_0$. The reader can check that this conclusion applies to the other fields.

Since \mathcal{P} leaves the action and the C^* boundary conditions unchanged, it is an exact symmetry in finite volume. Even though parity will play no special role in this paper, we notice that the parity transformations can be easily used to construct operators that have definite parity.

2.4 Flavour symmetries

C^* boundary conditions violate flavour (and consequently electric charge) conservation. The violation arises because a flavour-charged particle flips the sign of its flavour content by turning into its antiparticle when it travels once around the torus. We are now going to show that flavour is violated by two units at the time in this process and that this effect is exponentially suppressed with the volume. In this subsection and in section 4 we will argue that flavour violation does not represent a limitation to the use of C^* boundary conditions in most of the relevant applications.

We start by considering the theory with a single species of charged particles with unit charge, e.g. the electron. In this case flavour coincides with the electric charge Q and with the generator \hat{Q} of global gauge transformations. The detailed way charge conservation is violated by finite-volume effects can be easily understood by means of Feynman diagrams. We assume here some gauge fixing that we do not need to specify at this level. The theory in finite volume has the same interaction vertex as the infinite-volume one which, in particular, conserves electric charge. The violation of charge conservation is visible in those terms in the action that are sensitive to the C^* boundary conditions, i.e. the ones containing

spatial derivatives. In other words, charge violation is generated by the propagators, which we will discuss in detail.

In order to write down the free propagators, one needs to keep into account the fact that a free particle is able to travel around the torus. If it travels once around a direction with C^* boundary conditions, the particle turns into its antiparticle. The winding numbers of the particle world-line around each spatial direction can be organized into a vector $\mathbf{n} \in \mathbb{Z}^3$. By defining

$$\langle \mathbf{n} \rangle = \sum_{i=1}^3 n_i \pmod{2} \quad (2.22)$$

we can separate those winding numbers characterised by $\langle \mathbf{n} \rangle = 1$ that flip the electric charge of the particle from the winding numbers characterised by $\langle \mathbf{n} \rangle = 0$ that do not. We do not need the explicit expression of the gauge field propagator as the photon carries neither electric nor flavour charge. Concerning the matter field, in coordinate space we have

$$\langle \psi(x) \bar{\psi}(y) \rangle = x \xrightarrow{\quad} y = \sum_{\langle \mathbf{n} \rangle=0} S(x-y + \hat{L}_i n_i), \quad (2.23)$$

$$\langle \psi(x) \psi^T(y) \rangle = x \xrightarrow{\quad} \leftarrow y = - \sum_{\langle \mathbf{n} \rangle=1} S(x-y + \hat{L}_i n_i) C^{-1}, \quad (2.24)$$

$$\langle \bar{\psi}^T(x) \bar{\psi}(y) \rangle = x \xleftarrow{\quad} y = \sum_{\langle \mathbf{n} \rangle=1} C S(x-y + \hat{L}_i n_i), \quad (2.25)$$

where $S(x)$ is the infinite-volume fermion propagator. Notice that the $\psi\psi^T$ and $\bar{\psi}^T\bar{\psi}$ propagators vanish in infinite spatial volume as the sums in eqs. (2.24) and (2.25) do not include $\mathbf{n} = 0$. They are precisely the source of violation of charge conservation. The violation is not arbitrary, but amounts to a $\Delta Q = \pm 2$ every time one of these propagator is inserted. This shows explicitly that the electric charge Q is not conserved, but the quantum number $(-1)^{\hat{Q}}$ is, which means

$$\Delta \hat{Q} = 0 \pmod{2}. \quad (2.26)$$

Time evolution mixes all sectors with odd electric charge among each other, and all sectors with even electric charge among each other. For example a single-electron state can mix with a three-electron state but not with the vacuum, see figure 1. This in particular means that, chosen some suitable interpolating operator as we will discuss in section 3, single-electron states can be selected by looking at the leading decaying exponential in two-point functions. However two-electron states cannot be extracted in the same way, as the leading decaying exponential in a two-point function constructed with an operator with charge equal to 2 will select always the vacuum. As we will discuss in section 4 this is sufficient in most of the interesting low-energy applications in QCD+QED_C.

From the discussion above it is obvious that the violation arises only from the charged particle that travels at least once around the torus. If the fermion is massive we have

$$\langle \psi(x) \psi^T(y) \rangle \sim \langle \bar{\psi}^T(x) \bar{\psi}(y) \rangle \sim \left(\frac{m}{L} \right)^{\frac{3}{2}} e^{-mL}, \quad (2.27)$$

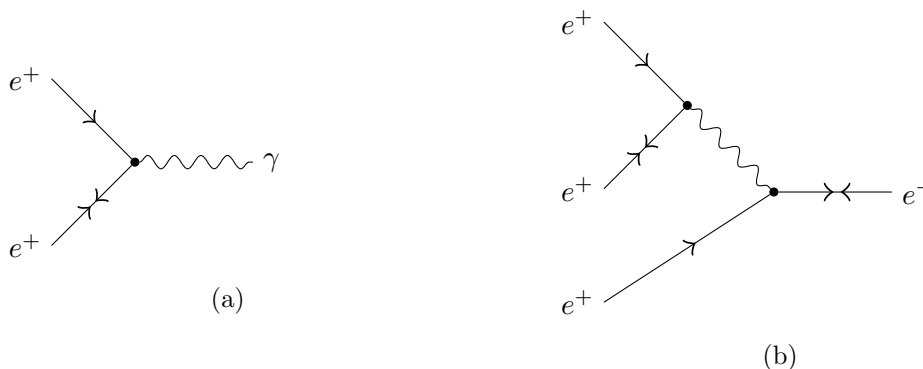


Figure 1. (a) Diagram contributing to the $e^+e^+ \rightarrow \gamma$ process, which involves one e^+ traveling around the torus and flipping charge. (b) Diagram contributing to the $e^+e^+e^+ \rightarrow e^-$ process.

for $L \rightarrow \infty$, and charge-violating diagrams are exponentially suppressed.

In the case of N_f flavours the infinite-volume theory has a $U(1)^{N_f}$ flavour symmetry corresponding to independent phase rotations of each flavour. We will denote the generator of the f -th $U(1)$ by F_f . Notice that the electric charge is a linear combination of the flavour-symmetry generators,

$$Q = \sum_{f=1}^{N_f} q_f F_f, \tag{2.28}$$

where q_f is the electric charge of the f -th flavour. In infinite volume each F_f is conserved independently. C^* boundary conditions break the flavour symmetry group down to a $\mathbb{Z}_2^{N_f}$,³ and this implies that only each $(-1)^{F_f}$ is conserved, i.e. violations can occur only in multiples of two,

$$\Delta F_f = 0 \pmod{2}. \tag{2.29}$$

Notice that the ΔQ has to be a multiple of 2 only if all flavours have equal electric charge. In the general case it is replaced by eqs. (2.26), (2.28) and (2.29). This observation will play an important role in section 4 where we will discuss QCD coupled to QED.

3 Gauge-invariant interpolating operators

We are concerned with physical observables, i.e. observables that are invariant under local gauge transformations. Often these observables are extracted from intermediate quantities defined in a particular gauge. For instance masses of charged particles are usually extracted from the long-distance behaviour of two-point functions after the photon field has been gauge-fixed. Although this is a necessary step in perturbation theory it can be completely avoided non-perturbatively without adding any particular complication. Keeping in mind that no issue arises with gauge fixing for QED and that a particular gauge can be chosen at any time, we think that it is more natural to rely on a completely gauge-invariant

³If n_f out of the N_f flavours are degenerate (i.e. same mass and same electric charge), the $U(1)^{n_f}$ flavour subgroup is lifted to a $U(n_f)$ flavour symmetry. C^* boundary conditions break this down to its natural $O(n_f)$ subgroup. We mention this special case for completeness, but it is not relevant for the purpose of this paper.

formulation. In this section we show how to construct states that are invariant under local gauge transformations and electrically charged at the same time, i.e. they have $(-1)^{\hat{Q}} = -1$. This will be achieved by acting with suitably-constructed interpolating operators on the vacuum. Even though we discuss primarily how to apply this construction to the calculation of charged-particle masses from two-point functions, the same interpolating operators can be used to extract other physical quantities, e.g. decay rates, in a completely gauge-invariant fashion.

To simplify the notation in this section we consider a single matter field with charge q . The generalization of the following discussion to the case of several flavours with different charges is completely straightforward. Consider the operator [26]

$$\Psi_J(x) = e^{iq \int d^4y A_\mu(y) J_\mu(y-x)} \psi(x), \tag{3.1}$$

where $\psi(x)$ is the matter field and $J_\mu(x)$ is a generic function or distribution that satisfies

$$\partial_\mu J_\mu(x) = \delta^4(x), \quad J_\mu(x + \hat{L}_i) = -J_\mu(x). \tag{3.2}$$

In case of periodic boundary conditions in time $J_\mu(x)$ is chosen to be periodic as well. Under a global transformation $\psi(x) \rightarrow e^{iq\alpha} \psi(x)$, the above operator transforms like $\Psi_J(x) \rightarrow e^{iq\alpha} \Psi_J(x)$, which implies that in infinite volume $\Psi_J(x)$ would have electric charge equal to q . In finite volume we have already noticed that α can be only 0 or π/q , which implies that the operator $\Psi_J(x)$ has quantum number $(-1)^{\hat{Q}} = -1$. The non-local factor

$$\Theta(x) = e^{iq \int d^4y A_\mu(y) J_\mu(y-x)} \tag{3.3}$$

transforms under a local gauge transformation that is anti-periodic in space as

$$\begin{aligned} \Theta(x) &\rightarrow \Theta(x) e^{iq \int d^4y \partial_\mu \alpha(y) J_\mu(y-x)} = \Theta(x) e^{-iq \int d^4y \alpha(y) \partial_\mu J_\mu(y-x)} \\ &= \Theta(x) e^{-iq\alpha(x)}. \end{aligned} \tag{3.4}$$

Notice that the product $\alpha(y) J_\mu(y-x)$ is periodic with respect to \mathbf{y} . Given also the boundary conditions in time, no boundary terms arise from the integration by parts. The extra factor $e^{-iq\alpha(x)}$ obtained by gauge-transforming $\Theta(x)$ cancels the analogous factor coming from the transformation of $\psi(x)$, making $\Psi_J(x)$ invariant.

Summarising, the non-local operator $\Psi_J(x)$ has $(-1)^{\hat{Q}} = -1$ and is invariant under local gauge transformations. It also satisfies the same boundary conditions as the field $\psi(x)$, and therefore operators with definite momentum can be easily constructed by considering the C-even and C-odd components of $\Psi_J(x)$ as done in eqs. (2.14) for a generic operator $\phi(x)$.

If the function $J_\mu(x)$ is chosen to be proportional to $\delta(x-x_0)$, then the operator $\Psi_J(x)$ is local in time, i.e. it is a function of the elementary fields at the time x_0 only. In this case $\Psi_J(x)$ maps naturally to an operator acting on the Hilbert space. The state $\Psi_J(x)|0\rangle$ obtained acting with the interpolating operator on the vacuum is invariant under local gauge transformations and has electric charge $(-1)^{\hat{Q}} = -1$. By decomposing the Euclidean two-point function $\langle \Psi_J(x) \bar{\Psi}_J(0) \rangle$ in decaying exponentials in x_0 , one can extract the spectrum

of the gauge-invariant Hamiltonian. The energy levels are gauge-invariant by construction and they do not depend on the particular choice of $J_\mu(x)$, as they are a property of the Hamiltonian rather than of the interpolating operator (as long as this is local in time). We will refer to the energy of the lightest state propagating in the Euclidean two-point function as the finite-volume mass of the charged particle. We assume that this quantity has an infinite-volume limit which can be interpreted as the mass of the charged particle.⁴

The whole construction presented above is based on the assumption that solutions of eq. (3.2) exist. If periodic boundary conditions were employed in all spatial directions eq. (3.2) would have no solutions. In the case of C^* boundary conditions we will construct explicitly some possible choices for the function $J_\mu(x)$. The first one is defined by the equations

$$J_0(x) = 0, \quad J_k(x) = \delta(x_0)\partial_k\Phi(\mathbf{x}), \quad \partial_k\partial_k\Phi(\mathbf{x}) = \delta^3(\mathbf{x}), \quad (3.5)$$

where $x = (x_0, \mathbf{x})$ and $\Phi(\mathbf{x})$ is anti-periodic. An explicit (convergent) representation for $\Phi(\mathbf{x})$ is given in terms of the heat-kernel

$$\Phi(\mathbf{x}) = -\frac{1}{L^3} \int_0^\infty du \sum_{\mathbf{p} \in \Pi_-} e^{-u\mathbf{p}^2 + i\mathbf{p}\mathbf{x}}. \quad (3.6)$$

With this choice the operator $\Psi_J(x)$ can be written like

$$\Psi_{\mathbf{c}}(x) = e^{-iq \int d^3y \partial_k A_k(x_0, \mathbf{y}) \Phi(\mathbf{y} - \mathbf{x})} \psi(x). \quad (3.7)$$

Notice that in Coulomb gauge $\Psi_{\mathbf{c}}(x) = \psi(x)$, and therefore the gauge invariant correlator $\langle \Psi_{\mathbf{c}}(x) \bar{\Psi}_{\mathbf{c}}(y) \rangle$ is identical to usual correlator $\langle \psi(x) \bar{\psi}(y) \rangle$ in Coulomb gauge. In other words, $\Psi_{\mathbf{c}}(x)$ is the unique gauge-invariant extension of the operator $\psi(x)$ defined in Coulomb gauge. This in particular shows explicitly the gauge-invariance of the mass extracted in Coulomb gauge.

Another possible choice is given by

$$J_\mu(x) = \frac{1}{2} \delta_{\mu,k} \operatorname{sgn}(x_k) \prod_{\nu \neq k} \delta(x_\nu). \quad (3.8)$$

Once this equation is inserted in eq. (3.1), it yields the following interpolating operator

$$\Psi_{\mathbf{s}}(x) = e^{-\frac{iq}{2} \int_{-x_k}^0 ds A_k(x+s\hat{k})} \psi(x) e^{\frac{iq}{2} \int_0^{L-x_k} ds A_k(x+s\hat{k})}. \quad (3.9)$$

This choice generates a string wrapping around the torus along the direction k , chosen among the ones with C^* boundary conditions (see figure 2). The operator $\Psi_{\mathbf{s}}(x)$ is less symmetric with respect to $\Psi_{\mathbf{c}}(x)$ but, as discussed in section 6, it might be more practical to use in numerical simulations, especially in the framework of compact QED_C.

Another choice that might look more convenient because of its explicit $O(4)$ covariance is given by

$$J_\mu(x) = \partial_\mu\Phi(x), \quad \partial_\mu\partial_\mu\Phi(x) = \delta^4(x), \quad (3.10)$$

⁴This issue is not trivial in QED because of the absence of a mass gap. See for instance the discussion in chapter 6 of [27] or chapter 6 of [28], and references therein.

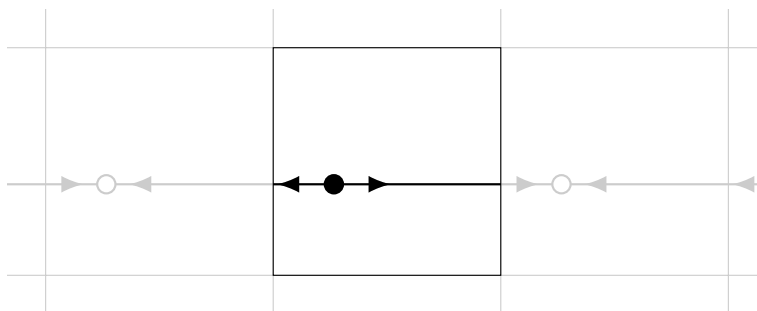


Figure 2. Graphical representation of the interpolating operator $\Psi_{\mathfrak{s}}$ defined in eq. (3.9). The black circle represents the electric charge, and the white circles are the image anti-charges. The lines with arrows represent the electric flux (i.e. the Wilson lines), which has to escape the box in a symmetric way through the two opposite planes because of the boundary conditions.

where $\Phi(x)$ is anti-periodic in space and has appropriate boundary conditions in time. With this choice the operator $\Psi_J(x)$ can be written as

$$\Psi_{\ell}(x) = e^{-iq \int d^4y \partial_{\rho} A_{\rho}(y) \Phi(y-x)} \psi(x). \tag{3.11}$$

In Landau gauge we get $\Psi_{\ell}(x) = \psi(x)$, and the operator $\Psi_{\ell}(x)$ is the unique gauge-invariant extension of the operator $\psi(x)$ defined in Landau gauge. Even though the Landau and other covariant gauges are often used in perturbative calculations, notice that the operator $\Psi_{\ell}(x)$ is non-local in time and interferes with the dynamics by effectively generating a time-dependent contribution to the Hamiltonian. One can show that this contribution vanishes at large time separations, and therefore the same masses will be obtained, but in practical situations the asymptotic behavior could be reached very slowly. These complications can be avoided in the first place by sticking to a gauge-invariant formalism with the local-in-time interpolating operators introduced before.

4 Flavour symmetry in QCD+QED_C

QCD is coupled to QED in the standard way

$$S[A, \psi] = \int_{L^3T} d^4x \left\{ \frac{1}{4e^2} F_{\mu\nu} F_{\mu\nu} + \frac{1}{2g^2} \text{tr} G_{\mu\nu} G_{\mu\nu} + \sum_{i=f}^{N_f} \bar{\psi}_f (\gamma_{\mu} D_{\mu}^{\vec{f}\rightarrow} + m_f) \psi_f \right\}, \tag{4.1}$$

where the chromo-magnetic field strength and the covariant derivative are

$$\begin{aligned} G_{\mu\nu}(x) &= \partial_{\mu} B_{\nu}(x) - \partial_{\nu} B_{\mu}(x) - i[B_{\mu}(x), B_{\nu}(x)], \\ D_{\mu}^{\vec{f}\rightarrow} &= \partial_{\mu}^{\leftrightarrow} - iq_f A_{\mu} - iB_{\mu}, \end{aligned} \tag{4.2}$$

and $B_{\mu}(x)$ denotes the colour gauge field. $B_{\mu}(x)$ is defined to be a traceless hermitian 3×3 matrix. Up-type and down-type quarks have electric charge $q_f = 2/3$ and $q_f = -1/3$

respectively. Since quark fields obey C^* boundary conditions, the colour gauge field must obey C^* boundary conditions as well in order to ensure periodicity of the action density,

$$B_\rho(x + \hat{L}_i) = -B_\rho(x)^* . \tag{4.3}$$

Let us now focus on the violation of flavour and electric-charge conservation, since they are substantially different from the case of QED_C alone.

Since the elementary charge is $1/3$, from the discussion in section 2 it might seem that processes with a $\Delta Q = \pm 2/3$ violation are allowed by the boundary conditions. However fractional charges are confined in hadrons which have integer electric charge. *If the box size is large enough* only colourless particles can travel around the torus, implying that charge violation can be produced only in multiples of $\Delta Q = \pm 2$. Consequently a proton state can mix with an antiproton state, or with a $p\pi^+\pi^+$ state.

One might wonder whether C^* boundary conditions can induce a spurious mixing of the proton with some lighter state. This issue is surely relevant if one wants to extract the proton properties from the long-distance behaviour of two-point functions from lattice simulations. It is also not entirely trivial, considering that C^* boundary conditions produce a violation of the baryon-number conservation. When a hadron travels around the torus its baryon number changes sign, which in turn implies that baryon-number violation can be produced only in multiples of 2. A proton state cannot mix with states with zero baryon number, i.e. with lighter states.

Both charge and baryon number are linear combinations of the individual species numbers, which we refer to as flavour numbers,

$$Q = \sum_f q_f F_f , \quad B = \frac{1}{3} \sum_f F_f . \tag{4.4}$$

Since each flavour-number conservation law is violated by the C^* boundary conditions, one might wonder for instance whether a pion state can mix with a kaon state. This is not the case, as individual flavour conservation can be violated again only in multiples of two,

$$\Delta F_f = 0 \pmod{2} . \tag{4.5}$$

Also notice that ΔB being a multiple of 2 implies that total-flavour $F = \sum_f F_f$ violation is produced only in multiples of six,

$$\Delta F = 0 \pmod{6} . \tag{4.6}$$

For instance, if only strangeness conservation is violated in a given process, this violation must be produced in multiples of 6. If strangeness violation amounts to a multiple of 2 which is not a multiple of 6, then it must be accompanied by violation in the conservation of some other flavour. For example the $\Omega^- = sss$ will mix, via a $K^- = s\bar{u}$ traveling around the torus, with $\Sigma^+ + 2\gamma$ where $\Sigma^+ = suu$ and with other two particle states like $\Lambda^0\pi^+$. This process has $\Delta F_s = -2$ and $\Delta F_u = +2$. In particular this implies that the Ω^- mass cannot be extracted from the long-distance behaviour of a two-point function at finite volume. In

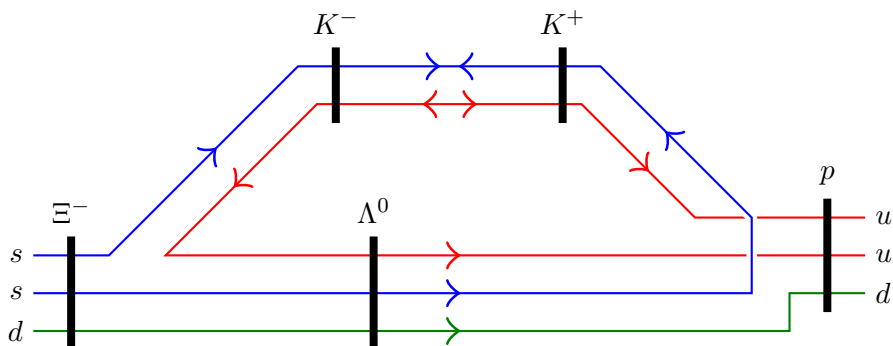


Figure 3. Schematic representation of a possible process responsible for the Ξ^-/p mixing. The process goes through a $u\bar{u}$ pair creation. The colourless $K^- = s\bar{u}$ travels around the torus and turns into a $K^+ = \bar{s}u$. Finally an $s\bar{s}$ pair annihilates.

order to extract the Ω^- mass one has to take the infinite-volume limit of the two-point function (or effective mass) first, and then extract the long-distance behaviour. Similarly the $\Xi^- = ssd$ mixes with the $p = uud$ via a $K^- = s\bar{u}$ traveling around the torus (see figure 3). This process has again $\Delta F_s = -2$ and $\Delta F_u = +2$.

In QCD_C alone, flavour violation is an exponentially-suppressed effect in the size of the box, like any other finite volume correction. Adding electromagnetic interactions make finite volume corrections generically inverse powers of L , due to the massless photon. The detailed analysis of flavour violating process in $\text{QCD}+\text{QED}_C$ requires to keep track of the flavour numbers in the process. This analysis, in the framework of an effective field theory of hadrons, is carried out in detail in the appendix A, but the main results that we prove in this appendix can be easily explained. Flavour violating process in $\text{QCD}+\text{QED}_C$ cannot be mediated by the photon. A particle with the same flavour numbers that are violated must travel around the torus, and since only massive particles carry flavour in $\text{QCD}+\text{QED}_C$, these effects are exponentially suppressed.

For example, in the case of the already-mentioned mixing between the Ξ^- and the proton, the one-loop diagram of figure 3 is of order $\exp(-m_K L)$. But the general case is much more complicated, since the Ξ^- can also mix with the proton and an arbitrary number of photons, or with a neutron- π^+ state. As it is proved in appendix A, flavour violating process in this case are suppressed by a factor $\exp(-\mu L)$ with

$$\mu = \left[M_{K^\pm}^2 - \left(\frac{M_{\Xi^-}^2 - M_{\Lambda^0}^2 + M_{K^\pm}^2}{2M_{\Xi^-}} \right)^2 \right]^{1/2}. \quad (4.7)$$

Note that this effects are generically very suppressed, since the corresponding coefficient in the Ξ^- two-point function is proportional to the square of the transition amplitude, i.e. to $\exp(-2\mu L) \sim \mathcal{O}(10^{-10})$. A similar analysis for the case of the mixing of the Ω^- results in an amplitude suppressed by a factor $\mathcal{O}(10^{-8})$.

We close this section by remarking that the renormalization of $\text{QCD}+\text{QED}_C$ is not affected by electric charge and flavour breaking effects discussed in this section. Indeed these are induced by the boundary conditions and locality guarantees that the ultraviolet

	1C*	2C*	3C*
$\xi(1)$	-0.77438614142	-1.4803898065	-1.7475645946
$\xi(2)$	-0.30138022444	-1.8300453641	-2.5193561521
$\xi(4)$	0.68922257439	-2.1568872986	-3.8631638072

Table 1. Values of the first three coefficients $\xi(s)$ in the case of C* boundary conditions in 1, 2 or 3 spatial directions and periodic boundary conditions in the others (columns 2,3 and 4 respectively).

structure of the theory is independent of them. This applies both to the couplings of the Lagrangian and to the renormalization constants and mixing coefficients of any composite operator.

5 Finite-volume effects on hadron masses

The finite-volume corrections to the mass of a stable hadron of non-vanishing charge q , which is valid only at first order in e^2 and up to corrections in the size of the box that fall off faster than any power, can be written as

$$\frac{\Delta m(L)}{m} = \frac{e^2}{4\pi} \left\{ \frac{q^2 \xi(1)}{2mL} + \frac{q^2 \xi(2)}{\pi(mL)^2} - \frac{1}{4\pi mL^4} \sum_{\ell=1}^{\infty} \frac{(-1)^\ell (2\ell)!}{\ell! L^{2(\ell-1)}} \mathcal{T}_\ell \xi(2+2\ell) \right\} + \dots, \quad (5.1)$$

where m is the particle mass in infinite volume, and $m(L) = m + \Delta m(L)$ is the particle mass in finite volume. Typical examples of stable hadrons to which this formula applies are the proton, the neutron, the pions, the kaons, D and B mesons.

The derivation of eq. (5.1) is given in appendix B. Here we discuss the structure of eq. (5.1) that is in fact very simple. \mathcal{T}_ℓ is the ℓ -th derivative with respect to \mathbf{k}^2 of the (infinite-volume) forward Compton amplitude for the scattering of a photon with energy $|\mathbf{k}|$ on the charged hadron at rest, in the limit $\mathbf{k} \rightarrow \mathbf{0}$. The boundary conditions enter only in the definition of the generalised zeta function

$$\xi(s) = \sum_{\mathbf{n} \neq \mathbf{0}} \frac{(-1)^{(\mathbf{n})}}{|\mathbf{n}|^s}. \quad (5.2)$$

This formula is valid for real $s > 3$, while the values $s = 1$ and 2 are obtained by analytic continuation. An explicit representation of the $\xi(s)$ coefficients, which is valid for all values of s we are interested in, is given in eq. (B.34). The values of the first three coefficients $\xi(s)$ are given in table 1 in the case of C* boundary conditions in 1, 2 or 3 spatial directions.

The $1/L$ and $1/L^2$ terms are universal, i.e. they depend only on the mass and charge of the hadron, and not on its spin and internal structure. These terms vanish in the case of a neutral particle. The dependence upon spin and internal structure is encoded in the coefficients \mathcal{T}_ℓ and is suppressed with respect to the universal part, as it contributes at $\mathcal{O}(1/L^4)$. No inverse odd power of L appears in the expansion, other than the leading $1/L$ point-like contribution.

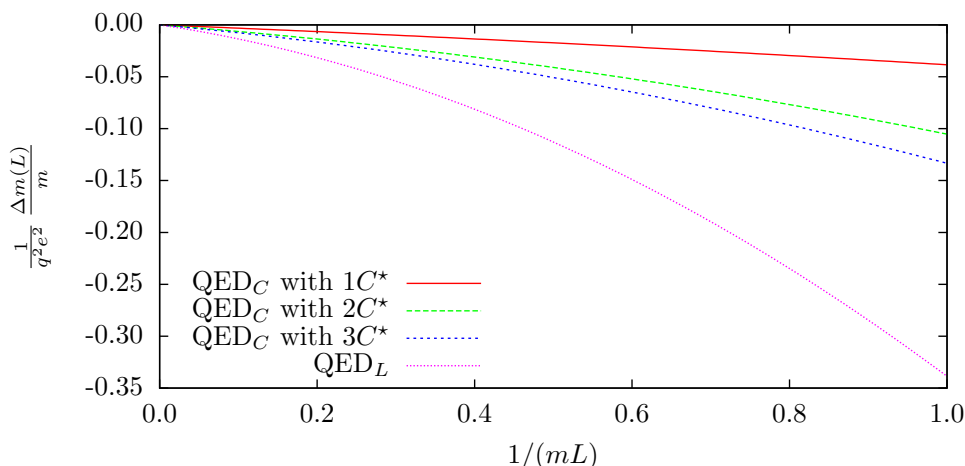


Figure 4. Leading finite-volume corrections to the mass of a stable particle of charge qe in QED_C and QED_L . The plot shows the universal $1/L$ and $1/L^2$ contributions. Spin and structure-dependent contributions are $\mathcal{O}(1/L^3)$ in QED_L , and $\mathcal{O}(1/L^4)$ in QED_C .

A formula very similar to eq. (5.1) has been derived in refs. [2, 18, 19] in the case of QED_L , i.e. the theory with the quenched spatial zero-modes of the electromagnetic field. According to refs. [2, 18, 19] the $1/L$ and $1/L^2$ terms are universal also in QED_L , while spin and structure-dependent terms contribute at $\mathcal{O}(1/L^3)$.

It is remarkable that, because of the locality of QED_C , spin and structure-dependent contributions are much more suppressed with respect to QED_L . Moreover, also the universal $1/L$ and $1/L^2$ contributions are considerably smaller in QED_C with respect to QED_L . This is shown in figure 4 where the results of refs. [2, 18] are compared with the $1/L$ and $1/L^2$ terms of eq. (5.1).⁵

6 Lattice formulation

In the context of lattice non-compact QED, the implementation of C^* boundary conditions and of the proposed interpolating operators is straightforward. One can extract the leading order $\mathcal{O}(e^2)$ electromagnetic contributions either with the techniques described in [3], or by doing a QED dynamical simulation as suggested in refs. [2–7]. In the non-compact formulation a way to damp the longitudinal modes of the gauge field is needed, gauge-fixing being the most common choice. Here we will focus on the compact formulation of the theory in a manifest gauge-invariant way.

In the compact formulation on the lattice, the gauge field is replaced by the link variable $U(x, \mu)$ which lives in the gauge group $U(1)$ and satisfies the boundary conditions

$$U(x + \hat{L}_k, \rho) = U(x, \rho)^*, \tag{6.1}$$

⁵Notice that the universal finite volume effects are considerably smaller when C^* boundary conditions are enforced along a single spatial direction. In this case, however, cubic symmetry is broken and this might represent a limitation in applications such as spectroscopy of higher-spin states.

along the spatial directions, and generic boundary conditions (i.e. periodic, SF, open, open-SF) along the temporal direction. For the moment we focus on the simpler case of QED_C coupled to a single fermion field with unitary charge. The generalization to QCD+QED_C will be discussed at the end of this section.

We want to argue now that, in order to be able to discretize the interpolating operators proposed in section 3 in a completely gauge-invariant fashion, we need a rather unconventional action for compact QED_C. Notice that in the standard formulation of compact QED, the perturbative series is generated by identifying $U(x, \mu) = e^{iA_\mu(x)}$ and by expanding in powers of the gauge field. The discretization of the interpolating operator (3.9) would need to take the square root of the link variable. This operation is not gauge covariant, and should be avoided while aiming at a completely gauge-invariant formulation. The root of this complication lies in the fact that, because of the boundary conditions, the electric flux generated by a single charge must escape the box in a symmetric way through the $x_k = 0$ and $x_k = L$ planes. The dynamical unit charge generated by the interpolating operator of eq. (3.9) is located in x and sees effectively two image half charges located in $x + \hat{L}_k$ and $x - \hat{L}_k$.

As it will be clear by the end of this section, this issue is completely removed by choosing the following action for compact QED_C with a single matter field,

$$\begin{aligned}
 S &= S_\gamma + S_m, \\
 S_\gamma &= \frac{2}{e^2} \sum_x \sum_{\mu\nu} [1 - P(x, \mu, \nu)], \\
 S_m &= \sum_x \bar{\psi}(x) D[U^2] \psi(x).
 \end{aligned}
 \tag{6.2}$$

The plaquette is defined as usual,

$$P(x, \mu, \nu) = U(x, \mu) U(x + \hat{\mu}, \nu) U(x + \hat{\nu}, \mu)^{-1} U(x, \nu)^{-1},
 \tag{6.3}$$

while the Wilson-Dirac operator has an unconventional coupling to the gauge field,

$$\begin{aligned}
 D[U^2] &= m + \frac{1}{2} \sum_{\mu=0}^3 \{ \gamma_\mu (\nabla_\mu^* [U^2] + \nabla_\mu [U^2]) - \nabla_\mu^* [U^2] \nabla_\mu [U^2] \}, \\
 \nabla_\mu [U^2] \psi(x) &= U(x, \mu)^2 \psi(x + \hat{\mu}) - \psi(x), \\
 \nabla_\mu^* [U^2] \psi(x) &= \psi(x) - U(x - \hat{\mu}, \mu)^{-2} \psi(x - \hat{\mu}).
 \end{aligned}
 \tag{6.4}$$

Any other discretization of the Dirac operator (preserving charge conjugation) can be employed as well.

The proposed action is invariant under local gauge transformations of the form

$$\begin{aligned}
 U(x, \mu) &\rightarrow \Lambda(x) U(x, \mu) \Lambda(x + \hat{\mu})^{-1}, \\
 \psi(x) &\rightarrow \Lambda(x)^2 \psi(x), \\
 \bar{\psi}(x) &\rightarrow \bar{\psi}(x) \Lambda(x)^{-2},
 \end{aligned}
 \tag{6.5}$$

where $\Lambda(x) \in U(1)$ satisfies boundary conditions

$$\Lambda(x + \hat{L}_k) = \Lambda(x)^* . \quad (6.6)$$

The action possesses also a \mathbb{Z}_2^4 center symmetry. For each direction μ one can flip the sign of all link variables in the direction μ on the three-dimensional slice defined by $x_\mu = 0$ without changing the value of the action. Before discussing the interpolating operators, we want to show that the action (6.2) is perturbatively equivalent to the usual QED action in the continuum limit.

In order to set up a perturbative expansion, we need to identify the minima of the action at $\mathcal{O}(e^0)$. These are given by all configurations with $P(x, \mu, \nu) = 1$. In appendix C we show that there is a discrete set of gauge-inequivalent minima labeled by the elements of the set

$$\Omega = \{(z_0, z_1, z_2, 1) \mid z_0^2 = z_1^2 = z_2^2 = 1\} . \quad (6.7)$$

Given a minimum of the action at $\mathcal{O}(e^0)$, it is always possible to find a vector $z \in \Omega$ such that the chosen minimum is gauge-equivalent to the following gauge field

$$\bar{U}_z(x, \mu) = \begin{cases} z_\mu & \text{if } x_\mu = L_\mu - 1 , \\ 1 & \text{otherwise .} \end{cases} \quad (6.8)$$

Because of center symmetry one might expect also minima with $z_3 = -1$. However each minimum with $z_3 = -1$ is gauge-equivalent to some minimum with $z_3 = 1$ (this is a byproduct of the construction given in appendix C).

The perturbative expansion around the minimum $\bar{U}_z(x, \mu)$ is set up by defining

$$U(x, \mu) = \bar{U}_z(x, \mu) e^{\frac{i}{2} A_\mu(x)} , \quad (6.9)$$

and by adding a gauge-fixing term S_{gf} to the action, which we will not do explicitly. We only observe that S_{gf} is a function of the fluctuation $A_\mu(x)$ only, and not of the classical vacuum $\bar{U}_z(x, \mu)$. Given a generic functional $\mathcal{F}[U, \psi, \bar{\psi}]$ of the fields, the perturbative expansion to some order $\mathcal{O}(e^n)$ of its expectation value is given by

$$\langle \mathcal{F}[U, \psi, \bar{\psi}] \rangle = \frac{1}{Z} \sum_{z \in \Omega} \int \mathcal{D}A \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{F}[\bar{U}_z e^{\frac{i}{2} A}, \psi, \bar{\psi}] e^{-S[e^{\frac{i}{2} A}, \psi, \bar{\psi}] - S_{\text{gf}}[A]} + \mathcal{O}(e^n) , \quad (6.10)$$

where we have used that the action is center-invariant and therefore it does not depend on $\bar{U}_z(x, \mu)$ once the substitution (6.9) is used. The normalization Z is given by

$$Z = 8 \int \mathcal{D}A \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-S[e^{\frac{i}{2} A}, \psi, \bar{\psi}] - S_{\text{gf}}[A]} \{1 + \mathcal{O}(e^n)\} . \quad (6.11)$$

If the observable \mathcal{F} is charged under center symmetry, its expectation value vanishes. On the other hand, center-invariant observables get mapped naturally into corresponding observables in the non-compact setup. In fact, if \mathcal{F} is invariant under center symmetry, then the z dependence drops out of the path integral and the standard perturbation expansion about $\bar{U} = 1$ is recovered,

$$\langle \mathcal{F}[U, \psi, \bar{\psi}] \rangle = \frac{8}{Z} \int \mathcal{D}A \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{F}[e^{\frac{i}{2} A}, \psi, \bar{\psi}] e^{-S[e^{\frac{i}{2} A}, \psi, \bar{\psi}] - S_{\text{gf}}[A]} + \mathcal{O}(e^n) , \quad (6.12)$$

provided that $S[e^{\frac{i}{2}A}, \psi, \bar{\psi}]$ is the standard QED action up to irrelevant operators.

This can be verified by replacing the definition (6.9) into the action and by expanding in powers of the fields. The 1/2 factor in the exponent of (6.9) combines with the unconventional normalization of the gauge action in eqs. (6.2) in such a way that the canonical normalization of the gauge field is restored,

$$P(x, \mu, \nu) = 1 + \frac{i}{2}F_{\mu\nu}(x) - \frac{1}{8}F_{\mu\nu}^2(x) + \dots, \tag{6.13}$$

$$S_\gamma = \frac{2}{e^2} \sum_x \sum_{\mu\nu} [1 - P(x, \mu, \nu)] = \frac{1}{4e^2} \sum_x \sum_{\mu\nu} F_{\mu\nu}^2(x) + \text{irrelevant operators}.$$

Also the same 1/2 factor in the exponent of (6.9) combines with the second power of the link variable in the Dirac operator (6.4) in such a way that the correct coupling of the electron to the gauge field is restored,

$$U(x, \mu)^2 = 1 + iA_\mu(x) + \dots, \tag{6.14}$$

$$S_m = \sum_x \bar{\psi}(x) \left\{ \gamma_\mu \left[\frac{\partial_\mu + \partial_\mu^*}{2} + iA_\mu(x) \right] + m \right\} \psi(x) + \text{irrelevant operators}.$$

The elementary charge (charge is quantized in compact QED) interacts with the gauge field with strength 1/2. However the dynamical fermion has an electric charge that is twice the elementary charge, which generates a coupling of strength 1 to the gauge field. This structure is also reflected by the gauge transformations (6.5).

In the proposed setup, thanks to the identification (6.9), the interpolating operator (3.9) can be discretized in a straightforward fashion,

$$\Psi_{\mathbf{s}}(x) = \prod_{s=-x_k}^{-1} U(x + s\hat{k}, k)^{-1} \psi(x) \prod_{s=0}^{L-x_k-1} U(x + s\hat{k}, k). \tag{6.15}$$

Notice that the the above operator is charged under center symmetry. However in practice only the product $\Psi_{\mathbf{s}}(x)\bar{\Psi}_{\mathbf{s}}(y)$ is relevant, which is center invariant.

For completeness we present also a possible discretization of the operator (3.7). We introduce the field

$$A_\mu^{\mathbf{c}}(x) = \Delta^{-1} \partial_k^* \hat{F}_{k\mu}(x), \tag{6.16}$$

where $\Delta = \partial_k \partial_k^*$ is the three-dimensional discrete Laplace operator defined with anti-periodic boundary conditions, and $\hat{F}_{\rho\sigma}(x)$ is some discretization of the field tensor (e.g. the clover plaquette). It is straightforward to verify that $A_\mu^{\mathbf{c}}(x)$ satisfies the discrete Coulomb constraint $\partial_k^* A_k^{\mathbf{c}}(x) = 0$. In the continuum limit $A_\mu^{\mathbf{c}}(x)$ is nothing but the gauge field in Coulomb gauge.⁶ The operator (3.7) can be discretized by using the relation

$$\Psi_{\mathbf{c}}(x) = \Psi_{\mathbf{s}}(x) e^{-\frac{i}{2} \sum_{s=0}^L A_k^{\mathbf{c}}(x+s\hat{k})}, \tag{6.17}$$

⁶In the continuum limit:

$$\partial_k A_k^{\mathbf{c}}(x) = \Delta^{-1} \partial_k \partial_j \hat{F}_{kj}(x) = 0,$$

$$A_\mu^{\mathbf{c}}(x) = \Delta^{-1} \partial_k \{ \partial_k A_\mu(x) - \partial_\mu A_k(x) \} = A_\mu(x) - \partial_\mu \{ \Delta^{-1} \partial_k A_k(x) \},$$

i.e. $A_\mu^{\mathbf{c}}(x)$ is gauge-equivalent to $A_\mu(x)$ and satisfies the Coulomb-gauge constraint.

which is exact in the continuum limit, and easily verified in Coulomb gauge. In fact in Coulomb gauge and in the continuum eq. (6.17) is completely equivalent to eq. (3.9), given the relations $A_\mu(x) = A_\mu^c(x)$ and $\Psi_c(x) = \psi(x)$.

The generalization of the proposed strategy to the case of compact QCD+QED_C is straightforward. We need to introduce the link variables $V(x, \mu) \in \text{SU}(3)$ for the colour field with the boundary conditions

$$V(x + \hat{L}_k, \rho) = V(x, \rho)^*, \tag{6.18}$$

and the corresponding plaquette:

$$Q(x, \mu, \nu) = V(x, \mu)V(x + \hat{\mu}, \nu)V(x + \hat{\nu}, \mu)^{-1}V(x, \nu)^{-1}. \tag{6.19}$$

For sake of simplicity we choose the standard Wilson action for the colour field. The photon action requires a further rescaling, since quarks have fractional charge,

$$\begin{aligned} S &= S_g + S_\gamma + S_m, \\ S_g &= \frac{1}{g^2} \sum_x \sum_{\mu\nu} \text{tr}[1 - Q(x, \mu, \nu)], \\ S_\gamma &= \frac{18}{e^2} \sum_x \sum_{\mu\nu} [1 - P(x, \mu, \nu)], \\ S_m &= \sum_f \sum_x \bar{\psi}_f(x) D_f[U, V] \psi_f(x). \end{aligned} \tag{6.20}$$

Moreover the Dirac operator has to implement the correct coupling of up-type ($q_f = 2/3$) and down-type ($q_f = -1/3$) quarks to the electromagnetic field,

$$D_f[U, V] = m_f + \frac{1}{2} \sum_{\mu=0}^3 \{ \gamma_\mu (\nabla_\mu^* [U^{6q_f} V] + \nabla_\mu [U^{6q_f} V]) - \nabla_\mu^* [U^{6q_f} V] \nabla_\mu [U^{6q_f} V] \}. \tag{6.21}$$

We remind that QCD with non-degenerate Wilson-Dirac quarks (with or without QED) has a mild sign problem, i.e. the fermionic determinant is positive in the continuum limit but can be negative because of lattice artefacts. In appendix D we show that C* boundary conditions do not make this sign problem worse.

7 Conclusions

A local solution to the problem of electrically charged particles in a finite volume was proposed in [21–23, 29], and it is based on C* boundary conditions for all fields along one or more spatial directions. Because of the boundary conditions Gauss’s law does not prevent the propagation of charged particles on a finite volume (as opposed to the case of periodic boundary conditions). We have analyzed in detail the properties of QED in isolation and of QED coupled to QCD with C* boundary conditions (QED_C and QCD+QED_C respectively), and we have discussed how this setup can be used in spectroscopy calculations.

We have devoted part of the paper to construct interpolating operators that have the quantum numbers of charged particles and that are also invariant under local gauge transformations. These can be used to probe the physical sector of the Hilbert space of the theory with non-perturbative accuracy without having to rely on gauge-fixing at intermediate stages of calculation. To this end we have discussed the details of the implementation of the proposed interpolating operators in the compact lattice formulation of the theory.

We have discussed the symmetries of QED_C and $\text{QCD}+\text{QED}_C$ in depth. In particular we signal that C^* boundary conditions violate flavour and electric-charge conservation partially, in such a way that this does not represent a limitation to the use of C^* boundary conditions in most of the relevant applications. Even though finite-volume effects vanish generally like some inverse power of the box size because of the photon, we have shown that flavour and electric-charge violations are exponentially suppressed in the box size.

We have calculated the finite-volume corrections to the masses of charged particles with C^* boundary conditions at $\mathcal{O}(\alpha_{em})$. We have shown that the leading $1/L$ and $1/L^2$ finite-volume corrections are universal, i.e. they depend on neither spin nor internal structure. Similar results have been previously obtained in the non-local formulation QED_L . When compared with these previous result, the finite-volume corrections of QED_C are found to be significantly smaller. In particular, the non-universal spin and structure-dependent corrections are $\mathcal{O}(1/L^3)$ in QED_L and $\mathcal{O}(1/L^4)$ in QED_C . We have also shown that these non-universal terms are related with physical quantities, namely the derivatives of the forward Compton scattering amplitudes.

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A Exponential suppression of flavour mixing

Let $\Xi(x)$ be some interpolating operator for some fixed spin-component of the negatively charged $\Xi^- = ssd$ and $\Xi_+(x)$ its C-even component. We consider the finite-volume Minkowskian retarded two-point function at zero momentum, its spectral decomposition and the dispersion relation:

$$C(E; L) = i \int_{\mathbb{R} \times L^3} d^4x \theta(x_0) e^{iEx_0} \langle \Xi_+(x)^\dagger \Xi_+(0) \rangle = \int_0^\infty d\mu \frac{\rho(\mu; L)}{\mu - E - i\epsilon}, \quad (\text{A.1})$$

$$\rho(E; L) = \frac{1}{\pi} \text{Im} C(E; L). \quad (\text{A.2})$$

In infinite volume the spectral density vanishes for $E < M_{\Xi^-}$. In a finite box, because of C^* boundary conditions, the lowest state contributing to the two-point function is a

proton state (via a strangeness-violating process) and the spectral density vanishes only for $E < M_p(L)$. We want to show that the spectral density vanishes exponentially with the volume for energies lower than M_{Ξ^-} .

More precisely we choose some energy $E < M_{\Xi^-}$ and a smooth test function $\phi_E(\mu)$ which vanishes for $\mu > E$. Then we want to show that, in the $L \rightarrow \infty$ limit

$$\ln \int_0^\infty d\mu \rho(\mu; L) \phi_E(\mu) \leq -2LM(E) + \mathcal{O}(\ln L), \tag{A.3}$$

where the mass that controls the exponential decay is a decreasing function of $E < M_{\Xi^-}$ and

$$\mathcal{M}(E) \geq \mathcal{M}(M_{\Xi^-}) = \left[M_{K^\pm}^2 - \left(\frac{M_{\Xi^-}^2 - M_{\Lambda^0}^2 + M_{K^\pm}^2}{2M_{\Xi^-}} \right)^2 \right]^{1/2}. \tag{A.4}$$

Notice that the spectral density at finite volume is a sum of delta functions localised on the eigenvalues of the Hamiltonian in the given channel,⁷ which is the reason why we need to consider a test function in order to write a precise statement. Before proceeding we comment on the fact that the analysis presented in this appendix can be easily extended to other channels (e.g. to the mixing of the Ω^- with lightest states).

We assume that the leading finite-volume corrections in the two-point function $C(E; L)$ are described by some arbitrarily-complicated Lagrangian field theory with small couplings, which effectively describe the dynamics of hadrons and photons at large distance in the framework of a perturbative expansion (after gauge-fixing for the photon). In order to avoid IR divergences at any stage of our calculation, we assume that the photon is massive. We will find that the mass $\mathcal{M}(E)$ does not depend on the mass of the photon. Each infinite-volume stable particle is described by an elementary field in the effective Lagrangian. Because of locality the finite-volume theory is described by the infinite-volume Lagrangian density. In particular vertices conserve flavour. Fields are assumed to have definite flavour numbers, and fields with all flavour numbers equal to zero are assumed to have definite C-parity.

We think of the two-point function $C(E; L)$ order by order in perturbation theory as a sum of Feynman diagrams. According to Cutkosky's rules, a Feynman diagram contributes to the spectral density $\rho(E; L)$ via the dispersion relation (A.2) only if a cut between its external vertices exists such that the sum of the masses of the cut propagators is smaller than E . Notice that all states propagating between the two external vertices must have $(-1)^B = -1$ and $(-1)^S = 1$ where B is the baryon number and S is the strangeness number. It is easy to check that (at the physical masses) states with such quantum numbers and with energy lower than M_{Ξ^-} can contain no strange particle. Therefore a Feynman diagram for the two-point function contributes to the spectral density for $E < M_{\Xi^-}$ only if a cut exists between the external vertices such that no strange particle propagates through the cut. The set of these diagrams is denoted by \mathcal{D}_s (see figure 5 for an example). The spectral

⁷At fixed order in perturbation theory, the spectral density is a sum of delta functions and their derivatives, localized on the eigenvalues of the free Hamiltonian.

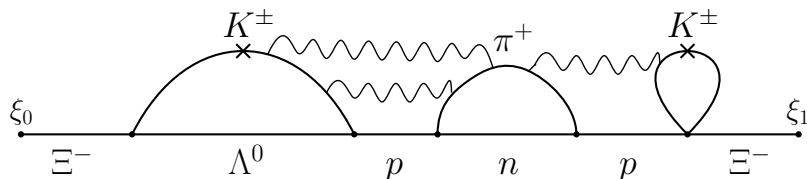


Figure 5. Example of a Feynman diagram in \mathcal{D}_s . This is a contribution to the $\langle \Xi_+(x)^\dagger \Xi_+(0) \rangle$ two-point function. Propagators with a cross are of the flavour-violating type, and they exist only because of the C^* -boundary conditions. Either the proton or the pair $n + \pi^+$ (in both cases with an arbitrary number of photons) can go on-shell with an energy lower than M_{Ξ^-} .

density for $E < M_{\Xi^-}$ can be represented as

$$\rho(E; L) = \frac{1}{\pi} \text{Im} \sum_{\mathcal{G} \in \mathcal{D}_s} \imath \left\{ \prod_{a \in V(\mathcal{G}) - \xi_0} \int_{\mathbb{R} \times L^3} d^4 x(a) \right\} \theta(x_0(\xi_1)) e^{\imath E x_0(\xi_1)} F_{\mathcal{G}}^M(x) |_{x(\xi_0)=0}, \quad (\text{A.5})$$

where ξ_1 and ξ_0 are the two external vertices of the diagram \mathcal{G} , and $V(\mathcal{G})$ is the set of all vertices. $F_{\mathcal{G}}^M(x)$ is a function of the coordinates of all vertices of the graph, and it is given by a product of propagators in coordinate space, various derivatives of propagators and numerical coefficients. We will refer to the function $F_{\mathcal{G}}^M(x)$ as *Feynman integrand*.

Structure of the Feynman integrand. We denote by $L(\mathcal{G})$ the set of lines of the diagram \mathcal{G} . Each line ℓ originates from the vertex $i(\ell)$ and terminates in the vertex $f(\ell)$ (line orientation is chosen arbitrarily). Each line ℓ corresponds to the Wick contraction of two fields located in $i(\ell)$ and $f(\ell)$. Let $F(\ell, i(\ell))$ and $F(\ell, f(\ell))$ be the vectors that contain all flavour numbers of these two fields, $F = (U, D, S, \dots)$. It is convenient to define $F(\ell, a) = 0$ if the line ℓ is not attached to the vertex a . Since a field can be Wick-contracted either with itself or with its charge conjugate, each line is uniquely associated to a mass m_ℓ . The line ℓ corresponds to a propagator

$$\Delta_{C_\ell}^M(\delta_\ell x; m_\ell, L) = \sum_{\mathbf{n}_\ell \in \mathbb{Z}^3} C_\ell^{\mathcal{G}}(\mathbf{n}_\ell) \Delta_M(\delta_\ell x_0, \delta_\ell \mathbf{x} + L \mathbf{n}_\ell; m_\ell), \quad (\text{A.6})$$

where $\Delta_M(x, m)$ is the infinite-volume Minkowkian propagator, $\delta_\ell x = x(f(\ell)) - x(i(\ell))$, $\mathbf{n}_\ell = (0, \mathbf{n}_\ell)$, and $C_\ell^{\mathcal{G}}(\mathbf{n}_\ell)$ is a function defined by one of the following possibilities:

Type 1. Line ℓ arises from the Wick contraction of two flavourless C-even fields,

$$F(\ell, i(\ell)) = F(\ell, f(\ell)) = 0, \quad C_\ell^{\mathcal{G}}(\mathbf{n}_\ell) = 1. \quad (\text{A.7})$$

Type 2. Line ℓ arises from the Wick contraction of two flavourless C-odd fields,

$$F(\ell, i(\ell)) = F(\ell, f(\ell)) = 0, \quad C_\ell^{\mathcal{G}}(\mathbf{n}_\ell) = (-1)^{\langle \mathbf{n}_\ell \rangle}. \quad (\text{A.8})$$

Type 3. Line ℓ arises from the Wick contraction of two flavourful fields with opposite flavour,

$$F(\ell, i(\ell)) = -F(\ell, f(\ell)) \neq 0, \quad C_\ell^{\mathcal{G}}(\mathbf{n}_\ell) = \delta_{\langle \mathbf{n}_\ell \rangle, 0}. \quad (\text{A.9})$$

Type 4. Line ℓ arises from the Wick contraction of two flavourful fields with same flavour,

$$F(\ell, i(\ell)) = F(\ell, f(\ell)) \neq 0, \quad C_\ell^{\mathcal{G}}(\mathbf{n}_\ell) = \delta_{\langle \mathbf{n}_\ell, 1 \rangle}. \quad (\text{A.10})$$

Notice that conservation of flavour at the internal vertices is expressed by the equation

$$\sum_{\ell} F(\ell, a) = 0, \quad \text{for } a \in V(\mathcal{G}) - \{\xi_0, \xi_1\}. \quad (\text{A.11})$$

The function $F_{\mathcal{G}}^M(x)$ has the following structure

$$F_{\mathcal{G}}^M(x) = \sum_{\mathbf{n}} F_{\mathcal{G}}^M(x, \mathbf{n}), \quad F_{\mathcal{G}}^M(x, \mathbf{n}) = \mathbb{V}_{\mathcal{G}}^M \prod_{\ell \in L(\mathcal{G})} C_\ell^{\mathcal{G}}(\mathbf{n}_\ell) \Delta_M(\delta_\ell x + Ln_\ell; m_\ell), \quad (\text{A.12})$$

where $\mathbb{V}_{\mathcal{G}}^M$ is a differential operator acting on all the coordinates $x(a)$ (in fact derivatives might be inserted in between propagators), and includes also couplings and combinatorial factors. The detailed structure of $\mathbb{V}_{\mathcal{G}}^M$ is of no interest for the current discussion.

Boundary conditions for the Feynman integrand. C^* -boundary conditions for the fields imply some peculiar boundary conditions for the Feynman integrand. Shifting the coordinate of a single vertex by

$$x(a) \rightarrow x(a) + \hat{L}_i \quad (\text{A.13})$$

is equivalent to replacing the operator inserted at the vertex a with its charge-conjugate (the propagators have to be modified accordingly). The diagram obtained by this procedure is denoted by $c_a(\mathcal{G})$. Since the interaction Lagrangian and the considered interpolating operators are invariant under charge-conjugation, \mathcal{G} is a diagram contributing to the two-point function if and only if $c_a(\mathcal{G})$ is a diagram contributing to the two-point function. It is also easy to check that the class \mathcal{D}_s is closed under the action of c_a . By iterating the action of c_a , and by noticing that c_a^2 is the identity we get

$$F_{\mathcal{G}}^M(x_0, \mathbf{x} + L\boldsymbol{\lambda}) = F_{c_a^\lambda(\mathcal{G})}^M(x_0, \mathbf{x}), \quad \boldsymbol{\lambda}(a) \in \mathbb{Z}^3, \quad (\text{A.14})$$

$$c^\lambda(\mathcal{G}) = \prod_{a \in V(\mathcal{G})} c_a^{\langle \boldsymbol{\lambda}(a) \rangle}(\mathcal{G}). \quad (\text{A.15})$$

Under the action of c_a , the vertex operator does not change. Propagators of type 1 attached to the vertex a (at only one of the endpoints) are invariant, propagators of type 2 flip sign, propagators of type 3 are replaced with propagators of type 4 and *vice versa*. In formulae this is equivalent to:

$$\mathbb{V}_{c_a^\lambda(\mathcal{G})}^M = \mathbb{V}_{\mathcal{G}}^M, \quad (\text{A.16})$$

$$C_\ell^{c^\lambda(\mathcal{G})}(\mathbf{n}_\ell) = C_\ell^{\mathcal{G}}(\mathbf{n}_\ell - \delta_\ell \boldsymbol{\lambda}). \quad (\text{A.17})$$

The boundary conditions for the function $F_{\mathcal{G}}^M(x, \mathbf{n})$ follow

$$F_{\mathcal{G}}^M(x_0, \mathbf{x} + L\boldsymbol{\lambda}, \mathbf{n}) = F_{c_a^\lambda(\mathcal{G})}^M(x_0, \mathbf{x}, \mathbf{n} + \delta \boldsymbol{\lambda}). \quad (\text{A.18})$$

We can use the above boundary conditions to restrict the sum over the pairs $(\mathcal{G}, \mathbf{n})$ and simultaneously extend the coordinate integration range to the whole \mathbb{R}^4 , by means of a

construction that has been discussed already in [25]. We will say that the two pairs $(\mathcal{G}, \mathbf{n})$ and $(\mathcal{G}', \mathbf{n}')$ are *gauge-equivalent* if and only if $\boldsymbol{\lambda}(a) \in \mathbb{Z}^3$ with $a \in V(\mathcal{G})$ exists such that:

$$\mathcal{G}' = c^\lambda(\mathcal{G}), \tag{A.19}$$

$$\mathbf{n}'_\ell = \mathbf{n}_\ell + \delta_\ell \boldsymbol{\lambda} = \mathbf{n}_\ell + \boldsymbol{\lambda}(f(\ell)) - \boldsymbol{\lambda}(i(\ell)). \tag{A.20}$$

The field \mathbf{n} defined on lines is referred to as *gauge field*, and the field $\boldsymbol{\lambda}$ defined on vertices is referred to as *gauge transformation*. The set of all possible pairs $(\mathcal{G}, \mathbf{n})$ splits into equivalence classes denoted by $[(\mathcal{G}, \mathbf{n})]$. As shown in [25], given two equivalent gauge fields the gauge transformation that relates the two of them is unique up to a global gauge transformation. The sum over the pairs $(\mathcal{G}, \mathbf{n})$ can be written as a sum over the equivalence classes and a sum over the gauge transformations with $\boldsymbol{\lambda}(\xi_0) = 0$. The spectral density for $E < M_{\Xi^-}$ becomes

$$\rho(E; L) = \frac{1}{\pi} \text{Im} \sum_{\substack{[(\mathcal{G}, \mathbf{n})] \\ \text{s.t. } \mathcal{G} \in \mathcal{D}_s}} \sum_{\substack{\boldsymbol{\lambda} \text{ s.t.} \\ \boldsymbol{\lambda}(\xi_0) = 0}} \imath \left\{ \prod_{a \in V(\mathcal{G}) - \xi_0} \int_{\mathbb{R} \times L^3} d^4 x(a) \right\} \times \\ \times \theta(x_0(\xi_1)) e^{\imath E x_0(\xi_1)} F_{c^\lambda(\mathcal{G})}^M(x, \mathbf{n} + \delta \boldsymbol{\lambda})|_{x(\xi_0) = 0}. \tag{A.21}$$

By using the boundary conditions (A.18), one can use the sum over the gauge transformations to reconstruct the integrals over \mathbb{R}^4 :

$$\rho(E; L) = \frac{1}{\pi} \text{Im} \sum_{\substack{[(\mathcal{G}, \mathbf{n})] \\ \text{s.t. } \mathcal{G} \in \mathcal{D}_s}} \imath \left\{ \prod_{a \in V(\mathcal{G}) - \xi_0} \int_{\mathbb{R}^4} d^4 x(a) \right\} \times \\ \times \theta(x_0(\xi_1)) e^{\imath E x_0(\xi_1)} F_{\mathcal{G}}^M(x, \mathbf{n})|_{x(\xi_0) = 0}. \tag{A.22}$$

Strangeness flow in Feynman diagrams. We introduce some general definitions.

Paths. A path P connecting the vertices $a \neq b$ is a set of lines, with the property that a sequence $a = v_1, v_2, \dots, v_N = b$ of pairwise different vertices exists, together with a labelling $\ell_1, \ell_2, \dots, \ell_{N-1}$ of all lines in P , such that v_k, v_{k+1} are the endpoints of ℓ_k .

Loops and Wilson loops. A loop C is a set of lines, with the property that a sequence v_1, v_2, \dots, v_N of pairwise different vertices exists, together with a labelling $\ell_1, \ell_2, \dots, \ell_N$ of all lines in C , such that v_k, v_{k+1} are the endpoints of ℓ_k for $k = 1, \dots, N - 1$, and v_N, v_1 are endpoints of ℓ_N . The Wilson loop associated to C is defined by

$$W(C, \mathbf{n}) = \sum_{\ell \in C} \mathbf{n}_\ell. \tag{A.23}$$

Notice that a Wilson loop is gauge invariant.

Trees and axial gauge. A tree \mathcal{T} in a connected graph is a maximal set of lines that contains no loops. If \mathcal{T} is a tree of \mathcal{G} , for any pair of vertices $a \neq b$ of \mathcal{G} , there is a unique path $P \subseteq \mathcal{T}$ connecting a and b . Any connected graph with more than one vertex has at least one non-empty tree. Given a tree \mathcal{T} , a gauge field \mathbf{n} is said to be in axial gauge

with respect to \mathcal{T} if $\mathbf{n}_\ell = \mathbf{0}$ for any $\ell \in \mathcal{T}$. It is easy to show that any gauge field is gauge-equivalent to some gauge field in axial gauge with respect to \mathcal{T} .

We give a closer look at the flavour structure of diagrams in \mathcal{D}_s , focusing in particular on strangeness. A line ℓ is said to be *strange* if $S(\ell, i(\ell)) \neq 0$, and *strangeless* otherwise. For any diagram $\mathcal{G} \in \mathcal{D}_s$, we define the subdiagram \mathcal{G}_s by taking only the strange lines in \mathcal{G} and vertices that are attached to these lines. Clearly the vertices ξ_0 and ξ_1 corresponding to the interpolating operators belong to \mathcal{G}_s . Because of the defining property of \mathcal{D}_s , there is no path in \mathcal{G}_s connecting ξ_0 and ξ_1 . We define $\mathcal{G}_{s,0}$ as the connected component of \mathcal{G}_s containing ξ_0 . By specializing eq. (A.11) to strangeness, and by observing that strangeness cannot flow outside of $\mathcal{G}_{s,0}$, one obtains the following:

Proposition A.1. *Strangeness is conserved within $\mathcal{G}_{s,0}$ at all vertices of $\mathcal{G}_{s,0}$ except ξ_0 , i.e.*

$$\sum_{\ell \in L(\mathcal{G}_{s,0})} S(\ell, a) = 0, \quad \text{for } a \in V(\mathcal{G}_{s,0}) - \xi_0. \quad (\text{A.24})$$

Lemma A.2. *For any pair $(\mathcal{G}, \mathbf{n})$ such that $\mathcal{G} \in \mathcal{D}_s$ and $F_{\mathcal{G}}^M(x, \mathbf{n})$ is not identically zero, then a loop C exists in $\mathcal{G}_{s,0}$ such that $|W(C, \mathbf{n})| \geq 1$.*

Proof. We consider a tree \mathcal{T} in $\mathcal{G}_{s,0}$, and we assume without loss of generality that $(\mathcal{G}, \mathbf{n})$ is in axial gauge with respect to the tree \mathcal{T} . Notice that all lines in $\mathcal{G}_{s,0}$ are flavourful, therefore they can be either of type 3 (*flavour-preserving*) or of type 4 (*flavour-violating*). If $\ell \in \mathcal{T}$ then $\mathbf{n}_\ell = \mathbf{0}$ by definition of axial gauge. In this case ℓ must be flavour-preserving, otherwise the propagator would contribute with a $\delta_{\langle \mathbf{n}_\ell \rangle, 1} = 0$ factor to $F_{\mathcal{G}}^M(x, \mathbf{n})$.

If all lines in $\mathcal{G}_{s,0}$ were flavour-preserving, by conservation of strangeness at the internal vertices, eq. (A.24), we would have

$$\begin{aligned} 0 &= \sum_{a \in V(\mathcal{G}_{s,0}) - \xi_0} \sum_{\ell \in L(\mathcal{G}_{s,0})} S(\ell, a) = \sum_{a \in V(\mathcal{G}_{s,0})} \sum_{\ell \in L(\mathcal{G}_{s,0})} S(\ell, a) - \sum_{\ell \in L(\mathcal{G}_{s,0})} S(\ell, \xi_0) = \\ &= \sum_{\ell \in L(\mathcal{G}_{s,0})} [S(\ell, i(\ell)) + S(\ell, f(\ell))] - \sum_{\ell \in L(\mathcal{G}_{s,0})} S(\ell, \xi_0) = - \sum_{\ell \in L(\mathcal{G}_{s,0})} S(\ell, \xi_0), \end{aligned} \quad (\text{A.25})$$

which is in contradiction with the fact that the interpolating operator has strangeness equal to ± 2 . Therefore at least a flavour-violating line $\bar{\ell} \in L(\mathcal{G}_{s,0}) - \mathcal{T}$ exists. Since the propagator of a flavour-violating line comes with a factor $\delta_{\langle \mathbf{n}_{\bar{\ell}} \rangle, 1}$ then necessarily $\mathbf{n}_{\bar{\ell}} \neq \mathbf{0}$.

Consider the path P in \mathcal{T} that connects $i(\bar{\ell})$ to $f(\bar{\ell})$, then it is straightforward to prove that $C = P \cup \{\bar{\ell}\}$ is a loop in $\mathcal{G}_{s,0}$ and

$$|W(C, \mathbf{n})| = |\mathbf{n}_{\bar{\ell}}| \neq 0. \quad (\text{A.26})$$

The thesis follows from the fact that the components of $\mathbf{n}_{\bar{\ell}}$ are integers. □

Time-ordering and Euclidean kernel. It is convenient to separate different time-orderings in integral (A.22). Formally the set $T(\mathcal{G})$ of all time-orderings of \mathcal{G} is defined as the set of permutations of $V(\mathcal{G})$, i.e. the set of all bijective functions between $V(\mathcal{G})$

and $\{1, 2, \dots, |V(\mathcal{G})|\}$ where $|V(\mathcal{G})|$ is the number of vertices of \mathcal{G} . Given a time-ordering $\tau \in T(\mathcal{G})$, and two vertices $a, b \in V(\mathcal{G})$ such that $\tau(a) < \tau(b)$, we will say that a is *before* b and b is *after* a (with respect to τ). We define the time-ordering function associated to τ as

$$\theta_\tau(x) = \prod_{\substack{a, b \in V(\mathcal{G}) \\ \text{s.t. } \tau(a) < \tau(b)}} \theta(x_0(b) - x_0(a)), \quad (\text{A.27})$$

and we insert the identity in the integral (A.22) in the form of

$$1 = \sum_{\tau \in T(\mathcal{G})} \theta_\tau(x). \quad (\text{A.28})$$

Not all time-orderings contribute to the spectral density for $E < M_{\Xi^-}$. States with no strange particles need to be able to propagate at some intermediate time between the two external vertices. Therefore only time-orderings such that ξ_1 is after any vertex in $\mathcal{G}_{s,0}$ contribute. We define $T_s(\mathcal{G})$ the set of such time-orderings. Eq. (A.22) becomes

$$\begin{aligned} \rho(E; L) = \frac{1}{\pi} \text{Im} \sum_{\substack{[(\mathcal{G}, \mathbf{n})] \\ \text{s.t. } \mathcal{G} \in \mathcal{D}_s}} \sum_{\tau \in T_s(\mathcal{G})} \int_{\mathbb{R}^4} d^4x(a) \left\{ \prod_{a \in V(\mathcal{G}) - \xi_0} \int_{\mathbb{R}^4} d^4x(a) \right\} \times \\ \times \theta_\tau(x) e^{iEx_0(\xi_1)} F_{\mathcal{G}}^M(x, \mathbf{n})|_{x(\xi_0)=0}. \end{aligned} \quad (\text{A.29})$$

We choose a diagram and a time-ordering contributing to the previous formula. Without loss of generality we can assume that each line is oriented in such a way that its final point is not before its initial point. Let v_-^τ be the latest vertex in $\mathcal{G}_{s,0}$, i.e. the vertex in $\mathcal{G}_{s,0}$ with the property that any other vertex in $\mathcal{G}_{s,0}$ is before it. Let v_+^τ be the vertex right after v_-^τ , i.e. the vertex defined by $\tau(v_+^\tau) = \tau(v_-^\tau) + 1$.

We construct the subdiagram \mathcal{G}_+^τ (resp. \mathcal{G}_-^τ) by taking all the vertices in \mathcal{G} not before v_+^τ (resp. not after v_-^τ) and all lines in \mathcal{G} connecting any pair of these vertices. Let L_0^τ be the set of lines with one endpoint in \mathcal{G}_-^τ and one in \mathcal{G}_+^τ . This decomposition induces a factorization of the integrand in eq. (A.29). The time-ordering function factorizes as

$$\theta_\tau(x) = \theta(x_0(v_+^\tau) - x_0(v_-^\tau)) \theta_{\tau_+}(x) \theta_{\tau_-}(x), \quad (\text{A.30})$$

$$\theta_{\tau_\pm}(x) = \prod_{\substack{a, b \in V(\mathcal{G}_\pm^\tau) \\ \text{s.t. } \tau(a) < \tau(b)}} \theta(x_0(b) - x_0(a)), \quad (\text{A.31})$$

where τ_+ (resp. τ_-) is the time-ordering restricted to \mathcal{G}_+^τ (resp. \mathcal{G}_-^τ). The Feynman integrand factorizes as

$$F_{\mathcal{G}}^M(x, \mathbf{n}) = \sum_{\mu} F_{\mu, \mathcal{G}_+^\tau}^M(x, \mathbf{n}) F_{\mu, \mathcal{G}_-^\tau}^M(x, \mathbf{n}) \prod_{\ell \in L_0^\tau} C_\ell^{\mathcal{G}}(\mathbf{n}_\ell) \Delta_M^+(\delta_\ell x + Ln_\ell; m_\ell), \quad (\text{A.32})$$

where μ is some collective Lorentz index (in the following we will omit the sum over μ). Notice that $F_{\mu, \mathcal{G}_+^\tau}^M(x, \mathbf{n})$ (resp. $F_{\mu, \mathcal{G}_-^\tau}^M(x, \mathbf{n})$) contain differential operators acting on coordinates

of the final (resp. initial) points of the lines in L_0^τ . $\Delta_M^+(x, m)$ is the retarded Minkowskian propagator which we can conveniently write in time-momentum representation

$$\Delta_M^+(x; m) = \theta(x_0) \int \frac{d^3 p}{(2\pi)^3 2E} e^{-i(Ex_0 - \mathbf{p}\mathbf{x})}, \quad \text{with } E = \sqrt{m^2 + \mathbf{p}^2}. \quad (\text{A.33})$$

We plug the factorizations (A.31) and (A.32) and the explicit representation of the retarded propagator into eq. (A.29), we substitute $x_0(a) \rightarrow x_0(a) + x_0(v_-)$ for any $a \in V(\mathcal{G}_+)$, and we use invariance under translations of $F_{\mu, \mathcal{G}_+}^M(x, \mathbf{n})$. The integrals over the coordinates factorizes over the two subgraphs:

$$\begin{aligned} \rho(E; L) = & \frac{1}{\pi} \text{Im} \sum_{\substack{[\mathcal{G}, \mathbf{n}] \\ \text{s.t. } \mathcal{G} \in \mathcal{D}_s}} \sum_{\tau \in T_s(\mathcal{G})} \left\{ \prod_{\ell \in L_0^\tau} \int \frac{d^3 p_\ell}{(2\pi)^3 2E_\ell} \right\} \times \\ & \times (2\pi)^3 \delta^3(\sum_{\ell \in L_0^\tau} \mathbf{p}_\ell) K_{\mu, \mathcal{G}, \tau}^-(E, \mathbf{p}, \mathbf{n}) R_{\mu, \mathcal{G}, \tau}^+(E, \mathbf{p}, \mathbf{n}). \end{aligned} \quad (\text{A.34})$$

The explicit expression for $R_{\mu, \mathcal{G}, \tau}^+(E, \mathbf{p}, \mathbf{n})$ is given for sake of completeness, but we will not need it in the current discussion

$$\begin{aligned} R_{\mu, \mathcal{G}, \tau}^+(E, \mathbf{p}, \mathbf{n}) = & \frac{\prod_{\ell \in L_0^\tau} C_\ell^\mathcal{G}(\mathbf{n}_\ell)}{\sum_{\ell \in L_0^\tau} E_\ell - E - i\epsilon} \left\{ \prod_{a \in V(\mathcal{G}_+^\tau)} \int_{\mathbb{R}^4} d^4 x(a) \right\} \theta_{\tau_+}(x) \times \\ & \times F_{\mu, \mathcal{G}_+^\tau}^M(x, \mathbf{n}) \delta^4(x(v_+^\tau)) e^{iE x_0(\xi_1)} \prod_{\ell \in L_0^\tau} e^{-iE_\ell x_0(f(\ell))} e^{i\mathbf{p}_\ell \mathbf{x}(f(\ell))}. \end{aligned} \quad (\text{A.35})$$

The explicit expression for $K_{\mu, \mathcal{G}, \tau}^-(E, \mathbf{p}, \mathbf{n})$ is given after Wick rotation of the coordinate integrals $x_0(a) \rightarrow -ix_0(a)$:

$$\begin{aligned} K_{\mathcal{G}, \tau}^-(E, \mathbf{p}, \mathbf{n}) = & w_{\mu, \mathcal{G}, \tau} \left\{ \prod_{a \in V(\mathcal{G}_-^\tau)} \int_{\mathbb{R}^4} d^4 x(a) \right\} \delta^4(x(\xi_0)) \theta_{\tau_-}(x) F_{\mu, \mathcal{G}_-^\tau}^E(x, \mathbf{n}) \times \\ & \times e^{Ex_0(v_-^\tau)} e^{-\sum_{\ell \in L_0^\tau} E_\ell [x_0(v_-^\tau) - x_0(i(\ell))]} e^{-i\sum_{\ell \in L_0^\tau} \mathbf{p}_\ell [\mathbf{x}(i(\ell)) + L\mathbf{n}_\ell]}, \end{aligned} \quad (\text{A.36})$$

where $E_\ell = \sqrt{m_\ell^2 + \mathbf{p}_\ell^2}$, $F_{\mathcal{G}_-^\tau}^E(x, \mathbf{n})$ is constructed as $F_{\mathcal{G}_-^\tau}^M(x, \mathbf{n})$ except that the Minkowskian propagators and vertices are replaced by the Euclidean ones, and $w_{\mu, \mathcal{G}, \tau}$ is some constant phase factor. The Wick rotation is allowed for $K_{\mathcal{G}, \tau}^-(E, \mathbf{p}, \mathbf{n})$ because all states propagating in between the interpolating operator ξ_0 and the latest vertex v_-^τ have energy that is higher than E by construction. We will refer to the function $K_{\mathcal{G}, \tau}^-(E, \mathbf{p}, \mathbf{n})$ as *Euclidean kernel* associated to the diagram $\mathcal{G} \in \mathcal{D}_s$ and the time-ordering $\tau \in T_s(\mathcal{G})$.

We highlight the following observation, which follows from the construction of the Euclidean kernel.

Observation A.3. *The latest vertex v_-^τ of $\mathcal{G}_{s,0}$ is also the latest vertex of \mathcal{G}_-^τ . Since \mathcal{G}_-^τ contains all vertices of \mathcal{G} not after v_-^τ , and all lines of \mathcal{G} with both endpoints not after v_-^τ , then $\mathcal{G}_{s,0}$ is a subdiagram of \mathcal{G}_-^τ .*

Large-volume behaviour of the Euclidean kernel. We will see that the Euclidean kernel provides the exponential suppression in the infinite-volume limit. We will establish this result in a few steps.

Theorem A.4. *For large L , we have*

$$\ln |K_{\mu, \mathcal{G}, \tau}^{-}(E, \mathbf{p}, \mathbf{n})| = -L\mathcal{E}_{\mathcal{G}, \tau}(E, \mathbf{p}, \mathbf{n}) + \mathcal{O}(\ln L), \quad (\text{A.37})$$

where the function $\mathcal{E}_{\mathcal{G}, \tau}(E, \mathbf{p}, \mathbf{n})$ is given by

$$\begin{aligned} \mathcal{E}_{\mathcal{G}, \tau}(E, \mathbf{p}, \mathbf{n}) &= \\ &= \min_{x \in D_{\mathcal{G}, \tau}} \left\{ -Ex_0(v_{-}^{\tau}) + \sum_{\ell \in L_0^{\tau}} E_{\ell}[x_0(v_{-}^{\tau}) - x_0(i(\ell))] + \sum_{\ell \in L(\mathcal{G}_{-}^{\tau})} m_{\ell} |\delta_{\ell} x + n_{\ell}| \right\}, \end{aligned} \quad (\text{A.38})$$

$$D_{\mathcal{G}, \tau} = \{(x(a))_{a \in V(\mathcal{G}_{-}^{\tau})} \mid x(a) \in \mathcal{R}^4, \theta_{\tau_{-}}(x) = 1, x(\xi_0) = 0\}. \quad (\text{A.39})$$

Proof. We use the heat-kernel representation for the Euclidean propagator

$$\Delta_E(x; m) = \int_0^{\infty} ds \frac{e^{-\frac{x^2}{4s} - m^2 s}}{(4\pi s)^2}. \quad (\text{A.40})$$

When plugging this in eq. (A.36), we need to introduce a Schwinger parameter s_{ℓ} for each line $\ell \in L(\mathcal{G}_{-}^{\tau})$. By substituting $s_{\ell} \rightarrow s_{\ell} L/2m_{\ell}$ and $x(a) \rightarrow Lx(a)$ we get the general form for the Euclidean kernel

$$\begin{aligned} K_{\mu, \mathcal{G}, \tau}^{-}(E, \mathbf{p}, \mathbf{n}) &= \prod_{\ell \in L(\mathcal{G}_{-}^{\tau})} \int_0^{\infty} ds_{\ell} \prod_{a \in V(\mathcal{G}_{-}^{\tau}) - \xi_0} \int_{\mathbb{R}^4} d^4 x(a) \delta(x_0(\xi_0)) \theta_{\tau_{-}}(x) \times \\ &\times L^{\alpha} \frac{P_{\mu}(s, x, \mathbf{n})}{Q(s)} e^{-L\{X(s, x, E, \mathbf{p}, \mathbf{n}) - i \sum_{\ell \in L_0^{\tau}} \mathbf{p}_{\ell} [\mathbf{x}(i(\ell)) + \mathbf{n}_{\ell}]\}}, \end{aligned} \quad (\text{A.41})$$

where $P(s, x, \mathbf{n})$ and $Q(s)$ are polynomials that come from the derivatives in the vertex operator and explicit powers of s in the heat-kernel representation, and

$$\begin{aligned} X(s, x, E, \mathbf{p}, \mathbf{n}) &= \\ &= -Ex_0(v_{-}^{\tau}) + \sum_{\ell \in L_0^{\tau}} E_{\ell}[x_0(v_{-}^{\tau}) - x_0(i(\ell))] + \sum_{\ell \in L(\mathcal{G}_{-}^{\tau})} \frac{m_{\ell}}{2} \left\{ s_{\ell} + \frac{1}{s_{\ell}} |\delta_{\ell} x + n_{\ell}|^2 \right\}. \end{aligned} \quad (\text{A.42})$$

The large- L expansion of the integral in eq. (A.41) is given by a saddle-point approximation, i.e. by expanding about the minima of X . This yields the asymptotic behaviour (A.37) with

$$\mathcal{E}_{\mathcal{G}, \tau}(E, \mathbf{p}, \mathbf{n}) = \min_{x \in D_{\mathcal{G}, \tau}} \min_{s_{\ell} \in [0, \infty)} X(s, x, E, \mathbf{p}, \mathbf{n}). \quad (\text{A.43})$$

Eq. (A.38) is obtained by performing the trivial minimization over each s_{ℓ} . □

The statement of theorem A.4 makes sense because $\mathcal{E}_{\mathcal{G}, \tau}(E, \mathbf{p}, \mathbf{n})$ is strictly positive. We will show this fact in two steps, and we will provide also a lower bound for this function.

Theorem A.5. *The function $\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n})$ defined in eq. (A.38) satisfies*

$$\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n}) \geq 0, \quad \text{for } E < M_{\Xi^-}. \quad (\text{A.44})$$

Proof. Let N be the number of vertices of the diagram \mathcal{G}_-^τ . We assume that the orientation of lines in \mathcal{G}_-^τ is chosen in such a way that

$$\tau(f(\ell)) \geq \tau(i(\ell)). \quad (\text{A.45})$$

We construct an auxiliary graph \mathcal{H} by starting from an empty graph, and by adding elements to it accordingly to a set of rules.

1. We grow \mathcal{H} by adding all the vertices of \mathcal{G}_-^τ . At this stage:

$$V(\mathcal{H}) = V(\mathcal{G}_-^\tau), \quad L(\mathcal{H}) = \emptyset. \quad (\text{A.46})$$

We equip the graph \mathcal{H} with the time-ordering function τ inherited from \mathcal{G}_-^τ .

2. For each *mother* line ℓ of \mathcal{G}_-^τ such that $\tau(f(\ell)) - \tau(i(\ell)) \leq 1$, we add the *daughter* line ℓ to \mathcal{H} with the same incidence relations (notice that the endpoints of ℓ are already in \mathcal{H}).
3. For each *mother* line ℓ of \mathcal{G}_-^τ such that $\tau(f(\ell)) - \tau(i(\ell)) > 1$, we imagine to cut the line ℓ at each intermediate timeslice. More precisely we add the $n = \tau(f(\ell)) - \tau(i(\ell)) - 1$ intermediate vertices v_1, \dots, v_n and the $n + 1$ *daughter* lines ℓ_0, \dots, ℓ_n to \mathcal{H} with the following incidence relations:

$$i(\ell_0) = i(\ell), \quad f(\ell_0) = v_1, \quad (\text{A.47})$$

$$i(\ell_k) = v_k, \quad f(\ell_k) = v_{k+1}, \quad \text{for } k = 1, \dots, n-1, \quad (\text{A.48})$$

$$i(\ell_n) = v_n, \quad f(\ell_n) = f(\ell). \quad (\text{A.49})$$

We also time-order the extra vertices and we declare that

$$\tau(v_k) = \tau(i(\ell)) + k. \quad (\text{A.50})$$

We associate a mass and a \mathbb{Z}^3 gauge field to each line of \mathcal{H} . The masses of the daughter lines are all equal to the mass of the mother line, while the gauge field of the original line is transferred completely only to the first daughter line, i.e.

$$M_{\ell_k} = m_\ell, \quad (\text{A.51})$$

$$\mathbf{n}_{\ell_k} = \mathbf{n}_\ell \delta_{k,0}. \quad (\text{A.52})$$

All quantum numbers are also naturally transferred from the mother line to the daughter lines.

4. For each *mother* line ℓ of L_0^τ such that $\tau(v_-^\tau) - \tau(i(\ell)) > 0$, we add a final point at the latest timeslice and we imagine to cut the line ℓ at each intermediate timeslice. More precisely we add the $n = \tau(v_-^\tau) - \tau(i(\ell))$ vertices v_1, \dots, v_n and the n *daughter* lines $\ell_0, \dots, \ell_{n-1}$ to \mathcal{H} with the following incidence relations:

$$i(\ell_0) = i(\ell), \quad f(\ell_0) = v_1, \quad (\text{A.53})$$

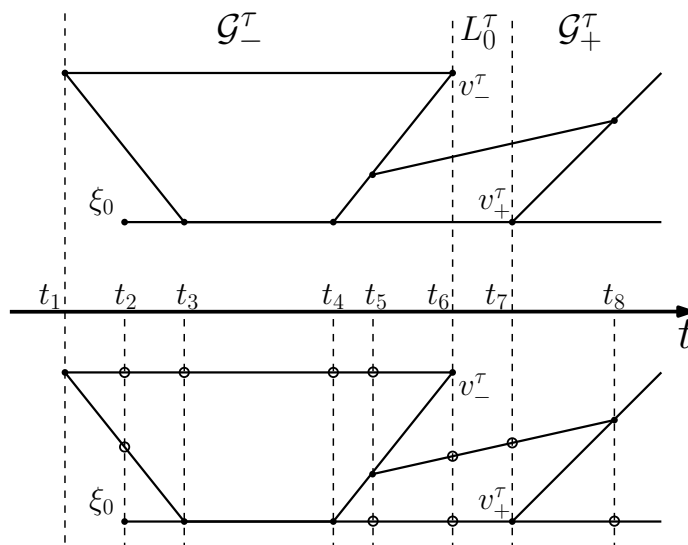


Figure 6. Exemplification of the construction given in the proof of theorem A.5. We start with a diagram whose vertices have been time-ordered (top diagram). Each vertex defines a timeslice. The diagram in the bottom is obtained from the top one by inserting a new vertex every time a line intersects a timeslice. Vertices in the same timeslice are forced to have the same time coordinate.

$$i(\ell_k) = v_k, \quad f(\ell_k) = v_{k+1}, \quad \text{for } k = 1, \dots, n-1. \quad (\text{A.54})$$

Analogously to the previous case, we declare:

$$\tau(v_k) = \tau(i(\ell)) + k, \quad (\text{A.55})$$

$$M_{\ell_k} = E_\ell, \quad (\text{A.56})$$

$$\mathbf{n}_{\ell_k} = \mathbf{n}_\ell \delta_{k,0}, \quad (\text{A.57})$$

and we transfer the quantum numbers of the mother line to the daughter lines.

The above construction is schematically represented in figure 6. The auxiliary diagram \mathcal{H} is useful to rewrite the function $\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n})$ defined in eq. (A.38) in a way that its timeslice structure be manifest.

We define $V_k(\mathcal{H})$ for $k = 1, \dots, N$ as the set that contains all vertices a with $\tau(a) = k$, i.e.

$$V_k(\mathcal{H}) = \tau^{-1}(k). \quad (\text{A.58})$$

The sets $V_k(\mathcal{H})$ for $k = 1, \dots, N$ constitute a partition of $V(\mathcal{H})$,

$$V(\mathcal{H}) = \bigsqcup_{k=1}^N V_k(\mathcal{H}). \quad (\text{A.59})$$

We will refer to $V_k(\mathcal{H})$ as the k -th *timeslice* of \mathcal{H} . We define $L_k(\mathcal{H})$ for $k = 1, \dots, N-1$ as the set that contains all lines ℓ such that $i(\ell)$ is in the k -th timeslice and $f(\ell)$ is in the $(k+1)$ -th timeslice. The only lines of \mathcal{H} that are left out are the looplevels ℓ with $i(\ell) = f(\ell)$

which we collect in the set $L_{\text{loop}}(\mathcal{H})$,

$$L(\mathcal{H}) = \bigsqcup_{k=1}^{N-1} L_k(\mathcal{H}) \sqcup L_{\text{loop}}(\mathcal{H}). \quad (\text{A.60})$$

We change the way in which we associate coordinates to vertices. We associate the time-coordinate t_k to the timeslice $V_k(\mathcal{H})$, and independent spatial coordinates $\mathbf{x}(a)$ to each vertex $a \in V(\mathcal{H})$. We force all vertices in the same timeslice to have the same time coordinate. Therefore the four-dimensional coordinate vector is mapped into

$$x(a) = (t_{\tau(a)}, \mathbf{x}(a)). \quad (\text{A.61})$$

Notice that in each timeslice $V_k(\mathcal{H})$ there is only one vertex of the original diagram \mathcal{G}_-^τ , therefore t_k does coincide with the temporal coordinate of this vertex.

By using iteratively the property that the shortest path between two points is the straight line, in the form of

$$\begin{aligned} & \min_{\mathbf{x}_1} \left\{ \sqrt{(t_{k+2} - t_{k+1})^2 + |\mathbf{x}_2 - \mathbf{x}_1|^2} + \sqrt{(t_{k+1} - t_k)^2 + |\mathbf{x}_1 - \mathbf{x}_0|^2} \right\} = \\ & = \sqrt{(t_{k+2} - t_k)^2 + |\mathbf{x}_2 - \mathbf{x}_0|^2}, \quad \text{for } t_{k+2} > t_{k+1} > t_k, \end{aligned} \quad (\text{A.62})$$

and the property that the shortest path between a point and a plane is the the straight line that is orthogonal to the plane, in the form of

$$\min_{\mathbf{x}_1} \sqrt{(t_{k+1} - t_k)^2 + |\mathbf{x}_1 - \mathbf{x}_0|^2} = t_{k+1} - t_k, \quad \text{for } t_{k+1} > t_k, \quad (\text{A.63})$$

and by recalling that $\tau(v_-^\tau) = N$ as v_-^τ is the latest vertex in \mathcal{G}_-^τ , one can easily prove that

$$\begin{aligned} & \mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n}) = \\ & = \min_{\mathbf{x}} \min_{t_1 < t_2 < \dots < t_N} \left\{ -E[t_N - t_{\tau(\xi_0)}] + \sum_{\ell \in L(\mathcal{H})} M_\ell |x(f(\ell)) - x(i(\ell)) + n_\ell| \right\}. \end{aligned} \quad (\text{A.64})$$

We choose quantities Δ_ℓ associated to the lines of \mathcal{H} satisfying the following constraints

$$\begin{aligned} \Delta_\ell &= 0, & \text{for looplines } \ell \in L_{\text{loop}}(\mathcal{H}), \\ \Delta_\ell &= 0, & \text{for } \ell \in L_k(\mathcal{H}) \text{ with } k < \tau(\xi_0), \\ 0 &\leq \Delta_\ell \leq M_\ell, & \text{for any } \ell, \\ E &= \sum_{\ell \in L_k(\mathcal{H})} \Delta_\ell, & \text{for any } k \geq \tau(\xi_0). \end{aligned} \quad (\text{A.65})$$

Notice that the last two constraints are in tension with each other. Quantities Δ_ℓ satisfying such constraints exist for $E < M_{\Xi^-}$ thanks to the following observation.

Observation A.6. *By construction of \mathcal{G}_-^τ , only states with energy not lower than M_{Ξ^-} propagate at any time between the vertices ξ_0 and v_-^τ , i.e.*

$$\sum_{\ell \in L_k(\mathcal{H})} M_\ell \geq M_{\Xi^-}, \quad \text{for any } k \geq \tau(\xi_0). \quad (\text{A.66})$$

Besides the above constraints, the quantities Δ_ℓ are largely arbitrary (and we will use this arbitrariness later on). The contribution $E[t_N - t_\tau(\xi_0)]$ in eq. (A.64) can be distributed over the lines of \mathcal{H} yielding

$$\begin{aligned} \mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n}) &= \tag{A.67} \\ &= \min_{\mathbf{x}} \min_{t_1 < t_2 < \dots < t_N} \sum_{\ell \in L(\mathcal{H})} \{-\Delta_\ell[x_0(f(\ell)) - x_0(i(\ell))] + M_\ell|x(f(\ell)) - x(i(\ell)) + n_\ell|\} , \end{aligned}$$

We can provide a lower bound for each term of the above sum by using the following inequality

$$-\Delta|\delta t| + M\sqrt{(\delta t)^2 + z^2} \geq |z|\sqrt{M^2 - \Delta^2}, \tag{A.68}$$

valid for any z and δt , as long as $M \geq \Delta$. Therefore we get an estimate for $\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n})$ in which the time minimization has disappeared

$$\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n}) \geq \min_{\mathbf{x}} \sum_{\ell \in L(\mathcal{H})} |\mathbf{x}(f(\ell)) - \mathbf{x}(i(\ell)) + \mathbf{n}_\ell| \sqrt{M_\ell^2 - \Delta_\ell^2}, \tag{A.69}$$

and which shows explicitly that

$$\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n}) \geq 0, \quad \text{for } E < M_{\Xi^-}. \tag{A.70}$$

□

Theorem A.7. *The function $\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n})$ defined in eq. (A.38) satisfies*

$$\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n}) \geq \mathcal{M}(E), \quad \text{for } E < M_{\Xi^-}, \tag{A.71}$$

where the function $\mathcal{M}(E)$ is given by

$$\mathcal{M}(E) = \begin{cases} M_{K^\pm} & \text{if } 0 < E \leq M_p \\ \left[M_{K^\pm}^2 - \left(\frac{E - M_p}{2} \right)^2 \right]^{1/2} & \text{if } M_p \leq E \leq \frac{M_{\Lambda^0}^2 - M_{K^\pm}^2}{M_p} \\ \left[M_{K^\pm}^2 - \left(\frac{E^2 - M_{\Lambda^0}^2 + M_{K^\pm}^2}{2E} \right)^2 \right]^{1/2} & \text{if } \frac{M_{\Lambda^0}^2 - M_{K^\pm}^2}{M_p} \leq E < M_{\Xi^-} \end{cases}. \tag{A.72}$$

Proof. We use the construction in the proof of theorem A.5. Since each term in the sum in the r.h.s. of eq. (A.69) is positive, a looser lower bound on the function $\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n})$ can be provided by restricting the sum to a subset of $L(\mathcal{H})$.

We choose a strange loop C in $\mathcal{G}_{s,0}$ with $|W(C, \mathbf{n})| \geq 1$. Such a loop exists thanks to lemma A.2. Since $\mathcal{G}_{s,0}$ is a subgraph of \mathcal{G}_-^τ , C is also a loop in \mathcal{G}_-^τ . We construct the loop \tilde{C} of \mathcal{H} by replacing each mother line in C with the corresponding daughter lines. Since the gauge field of each mother line is equal to the sum of the gauge fields of the corresponding daughter lines, it is clear that

$$|W(\tilde{C}, \mathbf{n})| = |W(C, \mathbf{n})| \geq 1. \tag{A.73}$$

By using this particular loop in eq. (A.69), we get the following bound for $\mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n})$:

$$\begin{aligned} \mathcal{E}_{\mathcal{G},\tau}(E, \mathbf{p}, \mathbf{n}) &\geq \min_{\mathbf{x}} \sum_{\ell \in \tilde{C}} |\mathbf{x}(f(\ell)) - \mathbf{x}(i(\ell)) + \mathbf{n}_\ell| \sqrt{M_\ell^2 - \Delta_\ell^2} \geq \\ &\geq \mathcal{M}(E, \Delta) \min_{\mathbf{x}} \sum_{\ell \in \tilde{C}} |\mathbf{x}(f(\ell)) - \mathbf{x}(i(\ell)) + \mathbf{n}_\ell| \geq \\ &\geq \mathcal{M}(E, \Delta) |W(\tilde{C}, \mathbf{n})| \geq \mathcal{M}(E, \Delta), \end{aligned} \tag{A.74}$$

where we have used the triangular inequality iteratively along the loop, and we have defined

$$\mathcal{M}(E, \Delta) = \min_{\ell \in \tilde{C}} \sqrt{M_\ell^2 - \Delta_\ell^2}. \tag{A.75}$$

The Δ_ℓ 's are arbitrary quantities satisfying the constraints in eq. (A.65). We can use this arbitrariness in order to optimize the above lower bound.

We separate two cases: either \tilde{C} is a single loopline or \tilde{C} has more than one line, none of which being a loopline. In the first case, $\Delta_\ell = 0$ for $\ell \in \tilde{C}$ and

$$\mathcal{M}(E, \Delta) = M_\ell \geq M_{K^\pm}, \tag{A.76}$$

where the last inequality comes from the fact that the K^\pm is the lightest strange particle.

We consider now the second possibility, i.e. \tilde{C} has more than one line none of which being a loopline,

$$\tilde{C} \subseteq \bigsqcup_{k=1}^{N-1} L_k(\mathcal{H}). \tag{A.77}$$

We define

$$\tilde{C}_k = \tilde{C} \cap L_k(\mathcal{H}). \tag{A.78}$$

The minimization in eq. (A.75) can be performed in two steps, according to

$$\mathcal{M}(E, \Delta) = \min_{\substack{k \text{ s.t.} \\ \tilde{C}_k \neq \emptyset}} \min_{\ell \in \tilde{C}_k} \sqrt{M_\ell^2 - \Delta_\ell^2}. \tag{A.79}$$

We choose a k such that \tilde{C}_k is not empty. If $k < \tau(\xi_0)$ then all Δ_ℓ are equal to zero therefore:

$$\min_{\ell \in \tilde{C}_k} \sqrt{M_\ell^2 - \Delta_\ell^2} = \min_{\ell \in \tilde{C}_k} M_\ell \geq M_{K^\pm}. \tag{A.80}$$

Let us consider $k \geq \tau(\xi_0)$. Since the loop has to close, \tilde{C}_k contains an even number of lines. We separate two possibilities again: the number of lines in \tilde{C}_k with $(-1)^B = 1$ is either even or odd.

If the number of lines in \tilde{C}_k with $(-1)^B = 1$ is even, since all states propagating between ξ_0 and ξ_1 must have $(-1)^B = -1$, there must be a line ℓ_0 in $L_k(\mathcal{H}) - \tilde{C}$ with $(-1)^B = -1$. Since the proton is the lightest particle with $(-1)^B = -1$ then surely $M_{\ell_0} \geq M_p$. We also pick two lines ℓ_1 and ℓ_2 in \tilde{C}_k and we observe that $M_{\ell_1}, M_{\ell_2} \geq M_{K^\pm}$. We assign

$$\Delta_{\ell_0} = \min \{E, M_p\},$$

$$\begin{aligned} \Delta_{\ell_1} &= \Delta_{\ell_2} = \max \left\{ 0, \frac{E - M_p}{2} \right\}, \\ \Delta_\ell &= 0, \quad \text{for } \ell \in L_k(\mathcal{H}) - \{\ell_0, \ell_1, \ell_2\}. \end{aligned} \tag{A.81}$$

By using the fact that $E < M_{\Xi^-}$ one can easily check that the constraints in eq. (A.65) are satisfied. By replacing all masses in the strange loop with M_{K^\pm} we get

$$\min_{\ell \in \tilde{C}_k} \sqrt{M_\ell^2 - \Delta_\ell^2} \geq \begin{cases} M_{K^\pm} & \text{if } E \leq M_p \\ \left[M_{K^\pm}^2 - \left(\frac{E - M_p}{2} \right)^2 \right]^{1/2} & \text{if } E \geq M_p \end{cases}. \tag{A.82}$$

If the number of lines in \tilde{C}_k with $(-1)^B = 1$ is odd, then there is at least a line ℓ_1 in \tilde{C}_k with $(-1)^B = -1$. Since the Λ^0 is the lightest strange particle with $(-1)^B = -1$ then surely $M_{\ell_1} \geq M_{\Lambda^0}$. We also pick another line ℓ_2 in \tilde{C}_k . We assign

$$\begin{aligned} \Delta_{\ell_1} &= \min \left\{ E, \frac{E^2 + M_{\Lambda^0}^2 - M_{K^\pm}^2}{2E} \right\}, \\ \Delta_{\ell_2} &= \max \left\{ 0, \frac{E^2 - M_{\Lambda^0}^2 + M_{K^\pm}^2}{2E} \right\}, \\ \Delta_\ell &= 0, \quad \text{for } \ell \in L_k(\mathcal{H}) - \{\ell_1, \ell_2\}. \end{aligned} \tag{A.83}$$

By using the fact that $E < M_{\Xi^-}$ one can easily check that the constraints in eq. (A.65) are satisfied. By replacing the mass M_{ℓ_1} with M_{Λ^0} and all other masses in the strange loop with M_{K^\pm} we get

$$\min_{\ell \in \tilde{C}_k} \sqrt{M_\ell^2 - \Delta_\ell^2} \geq \begin{cases} M_{K^\pm} & \text{if } E \leq \sqrt{M_{\Lambda^0}^2 - M_{K^\pm}^2} \\ \left[M_{K^\pm}^2 - \left(\frac{E^2 - M_{\Lambda^0}^2 + M_{K^\pm}^2}{2E} \right)^2 \right]^{1/2} & \text{if } E \geq \sqrt{M_{\Lambda^0}^2 - M_{K^\pm}^2} \end{cases}. \tag{A.84}$$

By combining all discussed cases, we get that it is always possible to choose the quantities Δ_ℓ in such a way that the constraints in eq. (A.65) are satisfied and

$$\mathcal{M}(E, \Delta) \geq \mathcal{M}(E), \tag{A.85}$$

where $\mathcal{M}(E)$ is defined in eq.(A.72). This concludes the proof of the theorem. □

Large-volume behaviour of the spectral density. One can easily reproduce the whole construction presented in this appendix around the external vertex ξ_1 instead of ξ_0 . The general structure of the spectral density is:

$$\begin{aligned} \rho(E; L) &= \frac{1}{\pi} \sum_{[(\mathcal{G}, \mathbf{n})]} \sum_{\tau} \left\{ \prod_{\ell \in L_\tau^-} \int \frac{d^3 p_\ell}{(2\pi)^3 2E_\ell} \right\} (2\pi)^3 \delta^3(\sum_{\ell \in L_\tau^-} \mathbf{p}_\ell) \times \\ &\times \left\{ \prod_{\ell \in L_\tau^+} \int \frac{d^3 p_\ell}{(2\pi)^3 2E_\ell} \right\} (2\pi)^3 \delta^3(\sum_{\ell \in L_\tau^+} \mathbf{p}_\ell) \times \end{aligned}$$

$$\times K_{\mu,\mathcal{G},\tau}^-(E, \mathbf{p}, \mathbf{n}) R_{\mu\nu,\mathcal{G},\tau}^0(E, \mathbf{p}, \mathbf{n}) K_{\nu,\mathcal{G},\tau}^+(E, \mathbf{p}, \mathbf{n}), \quad (\text{A.86})$$

where $K_{\mu,\mathcal{G},\tau}^-(E, \mathbf{p}, \mathbf{n})$ and $K_{\nu,\mathcal{G},\tau}^+(E, \mathbf{p}, \mathbf{n})$ are Euclidean kernels that include a flavour-violating strange loop connected to ξ_0 and ξ_1 respectively. The Euclidean kernels satisfy

$$\ln |K_{\mu,\mathcal{G},\tau}^\pm(E, \mathbf{p}, \mathbf{n})| \leq -L\mathcal{M}(E) + \mathcal{O}(\ln L), \quad (\text{A.87})$$

thanks to theorems A.4 and A.7. The desired eq. (A.3) follows by observing that $R_{\mathcal{G},\tau}^0(E, \mathbf{p}, \mathbf{n})$ has a finite large- L limit and the phase-space integral generates at most powers in the volume.

B Corrections to hadron masses in finite volume

In this appendix we want to calculate the power-like finite-volume corrections to the masses of stable hadrons due to electromagnetic interactions at order e^2 .

Stable hadrons are identified by their (finite-volume) flavour numbers. For instance the charged pion has baryon number $B = 0 \pmod 2$, strangeness $F_s = 0 \pmod 2$ and electric charge $Q = 1 \pmod 2$. Given some flavour sector defining the target stable hadron h and some momentum \mathbf{p} , we denote by $|h(\mathbf{p}), \sigma\rangle$ the lightest eigenstates of the QCD Hamiltonian H_0 in the given flavour sector, with momentum \mathbf{p} and with energy $E_{h,0}(\mathbf{p}, L)$. We assume that states with zero momentum are lighter than the others, and we refer to their energy as the $\mathcal{O}(e^0)$ finite-volume mass

$$E_{h,0}(\mathbf{p}, L) > E_{h,0}(\mathbf{0}, L) \equiv m_0(L), \quad \text{if } \mathbf{p} \neq \mathbf{0}. \quad (\text{B.1})$$

The states $|h(\mathbf{0}), \sigma\rangle$ with $\sigma = 1, \dots, d_s$ transform under some (possibly spinorial) representation of the cubic group. Normalization is chosen such that one recovers the relativistic normalization in infinite volume

$$\langle h(\mathbf{p}), \sigma | h(\mathbf{p}'), \sigma' \rangle = 2E_{h,0}(\mathbf{p}, L) L^3 \delta_{\mathbf{p},\mathbf{p}'} \delta_{\sigma,\sigma'}. \quad (\text{B.2})$$

The mass shift due to electromagnetic interactions is given by the Cottingham formula [30], which can be generalized easily to the case of finite volume by replacing the momentum integrals with the appropriate sums, yielding for the mass of the hadron h in finite volume

$$m(L) = m_0(L) - \frac{e^2}{4m_0(L)} \frac{1}{L^3} \sum_{\mathbf{k} \in \Pi_-} \int \frac{dk_0}{2\pi} \frac{T_{\mu\mu}(k; L)}{k^2}, \quad (\text{B.3})$$

$$T_{\mu\nu}(k; L) = \int d^4x e^{-ikx} \langle h(\mathbf{0}) | T \{ j_\mu(x) j_\nu(0) \} | h(\mathbf{0}) \rangle_c, \quad (\text{B.4})$$

where the subscript c stands for

$$\langle \psi | A | \psi' \rangle_c = \langle \psi | A | \psi' \rangle - \langle \psi | \psi' \rangle \langle 0 | A | 0 \rangle, \quad (\text{B.5})$$

and $j_\mu(x)$ is the Heisenberg electric-current operator in Euclidean spacetime

$$j_\mu(x) = e^{x_0 H_0} e^{-i\mathbf{x}\mathbf{P}} j_\mu(0) e^{-x_0 H_0} e^{i\mathbf{x}\mathbf{P}}, \quad (\text{B.6})$$

evolved with the QCD Hamiltonian H_0 , and normalized in such a way that the electric charge is

$$Q(x_0) = -i \int d^3x j_0(x_0, \mathbf{x}). \quad (\text{B.7})$$

Notice that the electric current $j_\mu(x)$ is C-odd and therefore it is also anti-periodic in space. It follows that the spatial momentum \mathbf{k} in eq. (B.4) must belong to the set Π_- . In eq. (B.4) we have also used the shorthand notation

$$\langle h(\mathbf{0})|A|h(\mathbf{0})\rangle = \frac{1}{d_s} \sum_{\sigma} \langle h(\mathbf{0}), \sigma|A|h(\mathbf{0}), \sigma\rangle \quad (\text{B.8})$$

which is particularly useful as the spin will play no special role in the calculation of this appendix.

Because of the exponentially-raising operator $e^{x_0 H}$ in eq. (B.6), it is not obvious that the x_0 -integral in eq. (B.4) converges. However the states that propagate in between the two currents have the same flavour numbers as the external state and they are odd under charge conjugation. In particular it follows that they cannot have zero momentum and they are therefore strictly heavier than the external state. In this situation the integral is shown to converge and an explicit calculation yields

$$T_{\mu\nu}(k; L) = M_{\mu\nu}(k; L) + M_{\nu\mu}(-k; L), \quad (\text{B.9})$$

$$\begin{aligned} M_{\mu\nu}(k; L) &= \int d^4x \theta(x_0) e^{-ikx} \langle h(\mathbf{0})|j_\mu(x)j_\nu(0)|h(\mathbf{0})\rangle_c \\ &= \langle h(\mathbf{0})|j_\mu(0) \frac{L^3 \delta_{\mathbf{P}, \mathbf{k}}}{H_0 - m_0(L) + ik_0} j_\nu(0)|h(\mathbf{0})\rangle \\ &\quad - 2m_0(L) L^3 \langle 0|j_\mu(0) \frac{L^3 \delta_{\mathbf{P}, \mathbf{k}}}{H_0 + ik_0} j_\nu(0)|0\rangle. \end{aligned} \quad (\text{B.10})$$

The retarded function $M_{\mu\nu}(k; L)$ is analytical for any complex k_0 except for the simple poles along the positive imaginary axis. In order to make contact with the original Minkowskian Cottingham formula [30], the reader can easily check that $T_{\mu\nu}(ik_0 - \epsilon, \mathbf{k}; \infty)$ is the forward Compton amplitude for the scattering of a virtual photon with quadrimomentum k from the hadron h at rest.

Formula (B.3) contains UV divergences which need to be subtracted. Notice that the electric current $j_\mu(x)$ does not require renormalization. Therefore the purely-QCD expectation value $\langle h(\mathbf{0})|\text{T}\{j_\mu(x)j_\nu(0)\}|h(\mathbf{0})\rangle_c$ appearing in eq. (B.4) is UV-finite for $x \neq 0$. The operator product expansion of $j_\mu(x)j_\nu(0)$ implies that $T_{\mu\nu}(k, L)$ vanishes like k^{-2} (up to logarithms) at large k , which makes the integral in eq. (B.3) logarithmically divergent. Following [31] we renormalize the Euclidean Cottingham formula by introducing a Pauli-Villard regulator for the photon propagator and by adding appropriate counterterms:

$$\begin{aligned} m(L) &= m_0(L) + \\ &+ \lim_{\Lambda \rightarrow \infty} \left\{ -\frac{e^2}{4m_0(L)} \frac{1}{L^3} \sum_{\mathbf{k} \in \Pi_-} \int \frac{dk_0}{2\pi} \frac{T_{\mu\mu}(k; L) \Lambda^2}{k^2(k^2 + \Lambda^2)} + \langle h(\mathbf{0})|C(\Lambda)|h(\mathbf{0})\rangle_c \right\}. \end{aligned} \quad (\text{B.11})$$

In this formula we assume that the regulator needed to define $T_{\mu\nu}(k, L)$ has been already removed. The counterterms have the form:

$$C(\Lambda) = c_\theta(\Lambda)\theta_{\mu\mu}(0) + \sum_f c_f(\Lambda)m_f\bar{\psi}_f\psi_f(0), \quad (\text{B.12})$$

where $\theta_{\mu\nu}$ is the (Euclidean) energy-momentum tensor. Since QCD+QED_C is a local theory, the coefficients $c(\Lambda)$ can be chosen to be L -independent by choosing renormalization conditions in infinite volume.

We are ready now to manipulate eq. (B.11) in order to extract the power-like finite-volume corrections to the mass.

Lemma B.1. *The QCD quantities appearing in eq. (B.11) have only exponentially-suppressed finite-volume corrections,*

$$\begin{aligned} m_0(L) - m_0(\infty) &= \mathcal{O}(e^{-m_\pi L}), \\ T_{\mu\mu}(k; L) - T_{\mu\mu}(k; \infty) &= \mathcal{O}(e^{-\frac{\sqrt{3}}{2}m_\pi L}), \quad \text{for any real } k \neq 0, \\ \langle h(\mathbf{0})|C(\Lambda)|h(\mathbf{0})\rangle_c - \lim_{L \rightarrow \infty} \langle h(\mathbf{0})|C(\Lambda)|h(\mathbf{0})\rangle_c &= \mathcal{O}(e^{-\frac{\sqrt{3}}{2}m_\pi L}). \end{aligned} \quad (\text{B.13})$$

Proof. A possible proof of this lemma, which we will not give here, can be obtained by using intermediate results and theorems in [25], under the assumption that the leading finite-volume corrections are described by some arbitrarily-complicated Lagrangian massive field theory with small couplings, which effectively describe the dynamics of hadrons at large distance. All above quantities can be decomposed in terms of dressed propagators and (1PI) proper vertices with possible insertions and with two on-shell external legs. For all these quantities, the general conclusions of theorems 2.4, 2.5 and 2.6 hold, leading to a proof of the lemma. Notice that for a general theory, the finite-volume effects on the masses are $\mathcal{O}(e^{-\frac{\sqrt{3}}{2}m_{gap}L})$ however this is not the case in QCD [32]. Some of the technology of [25] is adapted to the case of C^* -boundary conditions in appendix A. \square

Thanks to lemma B.1, we can write for the finite-volume correction to the mass

$$\begin{aligned} \Delta m(L) &\equiv m(L) - m(\infty) \\ &= -\frac{e^2}{4m_0} \lim_{\Lambda \rightarrow \infty} \left\{ \frac{1}{L^3} \sum_{\mathbf{k} \in \Pi_-} - \int \frac{d^3k}{(2\pi)^3} \right\} \int \frac{dk_0}{2\pi} \frac{T_{\mu\mu}(k)\Lambda^2}{k^2(k^2 + \Lambda^2)} + \\ &\quad + \mathcal{O}(e^{-m_\pi L}) + e^2 \mathcal{O}(e^{-\frac{\sqrt{3}}{2}m_\pi L}), \end{aligned} \quad (\text{B.14})$$

where it is understood that we mean $L = \infty$ whenever we drop the L dependence.

We introduce an arbitrary function $\eta(z)$ of a real variable z with the properties: (a) $\eta(z)$ is infinitely differentiable for any value of z , (b) $\eta(z) = \eta(-z)$, (c) $\eta(z) = 1$ for $|z| \leq M^2/2$ for some arbitrary $M > 0$, (d) $\eta(z) = 0$ for $|z| \geq M^2$. We rewrite the finite-volume correction to the mass as

$$\Delta m(L) = -\frac{e^2}{4m_0} \left\{ \frac{1}{L^3} \sum_{\mathbf{k} \in \Pi_-} - \int \frac{d^3k}{(2\pi)^3} \right\} \eta(\mathbf{k}^2) \int \frac{dk_0}{2\pi} \frac{T_{\mu\mu}(k)}{k^2} + R(L), \quad (\text{B.15})$$

where the reminder $R(L)$ is

$$R(L) = \lim_{\Lambda \rightarrow \infty} \left\{ \frac{1}{L^3} \sum_{\mathbf{k} \in \Pi_-} - \int \frac{d^3 k}{(2\pi)^3} \right\} \mathcal{I}_\Lambda(\mathbf{k}) + \mathcal{O}(e^{-m_\pi L}),$$

$$\mathcal{I}_\Lambda(\mathbf{k}^2) = -\frac{e^2}{4m_0} [1 - \eta(\mathbf{k}^2)] \int \frac{dk_0}{2\pi} \frac{T_{\mu\mu}(k) \Lambda^2}{k^2(k^2 + \Lambda^2)}. \quad (\text{B.16})$$

Lemma B.2. *The infinite-volume Euclidean amplitude $T_{\mu\mu}(k)$ is infinitely differentiable for any $k \in \mathbb{R}^4 \setminus \{0\}$.*

Proof. See appendix B.1. □

Thanks to lemma B.2 and to the fact that the factor $1 - \eta(\mathbf{k}^2)$ regularizes the singularity in $\mathbf{k} = 0$, $\mathcal{I}_\Lambda(\mathbf{k}^2)$ is infinitely differentiable in $\mathbf{k} \in \mathbb{R}^3$. The reminder $R(L)$ is the difference between the integral of a smooth function and its approximation as a Riemann sum, which vanishes in the infinite-volume limit faster than any inverse power of L ,

$$\lim_{L \rightarrow \infty} L^\omega R(L) = 0, \quad \text{for all } \omega > 0. \quad (\text{B.17})$$

By plugging the eq. (B.9) into eq. (B.15), and by folding the k_0 integral we get

$$\Delta m(L) = -\frac{e^2}{2m_0} \left\{ \frac{1}{L^3} \sum_{\mathbf{k} \in \Pi_-} - \int \frac{d^3 k}{(2\pi)^3} \right\} \eta(\mathbf{k}^2) \int \frac{dk_0}{2\pi} \frac{M_{\mu\mu}(k)}{k^2} + R(L). \quad (\text{B.18})$$

The integrand is holomorphic in the half plane $\text{Im } k_0 \leq 0$ except for the single pole in $k_0 = -i|\mathbf{k}|$. Therefore the k_0 integral can be calculated as a Cauchy integral by closing the contour at infinity in the lower half plane yielding

$$\Delta m(L) = -\frac{e^2}{4m_0} \left\{ \frac{1}{L^3} \sum_{\mathbf{k} \in \Pi_-} - \int \frac{d^3 k}{(2\pi)^3} \right\} \eta(\mathbf{k}^2) \frac{M_{\mu\mu}(-i|\mathbf{k}|, \mathbf{k})}{|\mathbf{k}|} + R(L). \quad (\text{B.19})$$

We will see that the power-law finite-volume corrections come from the behaviour of the integrand in eq. (B.19) around $\mathbf{k} = \mathbf{0}$.

Lemma B.3. *Because of rotational symmetry, the on-shell retarded function $M_{\mu\mu}(-i|\mathbf{k}|, \mathbf{k})$ is a function of \mathbf{k} only via $|\mathbf{k}|$. It can be decomposed as*

$$M_{\mu\mu}(-i|\mathbf{k}|, \mathbf{k})|_{|\mathbf{k}|=\kappa} = \frac{\mathcal{M}_{-1}}{\kappa} + \mathcal{M}(\kappa), \quad (\text{B.20})$$

where the function $\mathcal{M}(\kappa)$ is analytical for complex values of κ in a neighbourhood of zero, and

$$\mathcal{M}_{-1} = -2m_0 q^2, \quad (\text{B.21})$$

where q is the electric charge of the hadron h .

Proof. See appendix B.1. □

We can use now Poisson summation formula in order to express the discrete sum in eq. (B.19) over spatial momenta in terms of Fourier integrals. Since the momentum \mathbf{k} belongs to the anti-periodic set $\hat{\Pi}_-$, an extra sign appears in Poisson summation formula

$$\sum_{\mathbf{k} \in \hat{\Pi}_-} f(\mathbf{k}) = \sum_{\mathbf{n} \in \mathbb{Z}_3} (-1)^{\langle \mathbf{n} \rangle} \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{n}\mathbf{k}} f(\mathbf{k}), \quad (\text{B.22})$$

where $\langle \mathbf{n} \rangle$ has been defined in eq. (2.22). The term $\mathbf{n} = \mathbf{0}$ in the previous expression corresponds to the infinite-volume integral. By plugging the definition (B.20) into eq. (B.19), and after calculating the angular integral in \mathbf{k} , we get

$$\begin{aligned} \Delta m(L) = & -\frac{e^2 \mathcal{M}_{-1}}{8m_0 \pi^2 L} \sum_{\mathbf{n} \in \mathbb{Z}_3 / \{0\}} \frac{(-1)^{\langle \mathbf{n} \rangle}}{|\mathbf{n}|} \int_0^\infty d\kappa \eta(\kappa^2) \frac{\sin(\kappa|\mathbf{n}|L)}{\kappa} - \\ & - \frac{e^2}{8\pi^2 m_0 L} \sum_{\mathbf{n} \in \mathbb{Z}_3 / \{0\}} \frac{(-1)^{\langle \mathbf{n} \rangle}}{|\mathbf{n}|} \int_0^\infty d\kappa \eta(\kappa^2) \mathcal{M}(\kappa) \sin(\kappa|\mathbf{n}|L) + R(L). \end{aligned} \quad (\text{B.23})$$

We exploit the arbitrariness we have in choosing the function $\eta(\kappa^2)$ and assume that it has support in the analyticity domain of $\mathcal{M}(\kappa)$. Thanks to lemma B.3 the function $\eta(\kappa^2)\mathcal{M}(\kappa)$ is smooth for any $\kappa > 0$, and has all right derivatives in $\kappa = 0$. The expansion in powers of $1/L$ can be written in terms of the following generalized zeta function

$$\xi(s) = \sum_{\mathbf{n} \in \mathbb{Z}_3 / \{0\}} \frac{(-1)^{\langle \mathbf{n} \rangle}}{|\mathbf{n}|^s}, \quad (\text{B.24})$$

which is analytically extended to a meromorphic function in the whole complex plane, and holomorphic for $\text{Re } s > 0$.

The first integral in (B.23) can be understood by defining the function

$$\tilde{\eta}(x) = \int_{-\infty}^\infty \frac{d\kappa}{2\pi} \eta(\kappa^2) e^{i\kappa x}. \quad (\text{B.25})$$

Since $\eta(k^2)$ is a Schwartz function so is $\tilde{\eta}(x)$, and in particular it decays at infinity faster than any inverse power of x . The sum

$$\frac{2}{\pi} \sum_{\mathbf{n} \in \mathbb{Z}_3 / \{0\}} \frac{(-1)^{\langle \mathbf{n} \rangle}}{|\mathbf{n}|} \int_0^\infty d\kappa \eta(\kappa^2) \frac{\sin(\kappa|\mathbf{n}|L)}{\kappa} = \sum_{\mathbf{n} \in \mathbb{Z}_3 / \{0\}} \frac{(-1)^{\langle \mathbf{n} \rangle}}{|\mathbf{n}|} \int_{-|\mathbf{n}|L}^{|\mathbf{n}|L} dx \tilde{\eta}(x) \quad (\text{B.26})$$

converges to $\xi(1)$, and the corrections decay faster than any power in $1/L$. The second integral in (B.23) has a Taylor expansion in $(|\mathbf{n}|L)^{-1}$ that can be extracted by using iteratively the identity

$$\int_0^\infty d\kappa f(\kappa) \sin(x\kappa) = \frac{1}{x} f(0) - \frac{1}{x^2} \int_0^\infty d\kappa f''(\kappa) \sin(x\kappa). \quad (\text{B.27})$$

Putting everything together we obtain the desired expansion of the finite-volume corrections to the mass

$$\Delta m(L) = -\frac{e^2 \mathcal{M}_{-1}}{16m_0 \pi L} \xi(1) - \frac{e^2}{8\pi^2 m_0} \sum_{\ell=0}^\infty \frac{(-1)^\ell}{L^{2+2\ell}} \mathcal{M}_{2\ell} \xi(2+2\ell) + \dots, \quad (\text{B.28})$$

where the dots stand for contributions that decay faster than any power of $1/L$, and $\mathcal{M}_{2\ell}$ is the (2ℓ) -th derivative of $\mathcal{M}(\kappa)$ in $\kappa = 0$. Notice that the on-shell forward Compton amplitude is given by

$$\mathcal{T}(\mathbf{k}^2) = T_{\mu\mu}(\imath|\mathbf{k}| - \epsilon, \mathbf{k}) = M_{\mu\mu}(\imath|\mathbf{k}|, \mathbf{k}) + M_{\mu\mu}(-\imath|\mathbf{k}|, \mathbf{k}) = \mathcal{M}(|\mathbf{k}|) + \mathcal{M}(-|\mathbf{k}|), \quad (\text{B.29})$$

therefore the coefficients $\mathcal{M}_{2\ell}$ are trivially related to the derivatives

$$\mathcal{M}_{2\ell} = \frac{(2\ell)!}{2(\ell!)} \frac{d^\ell}{d(\kappa^2)^\ell} \mathcal{T}(0) \equiv \frac{(2\ell)!}{2(\ell!)} \mathcal{T}_\ell \quad (\text{B.30})$$

of the on-shell forward Compton amplitude for the scattering of soft photons on the hadron h at rest.

We also notice that the coefficients \mathcal{M}_{-1} and \mathcal{T}_0 depend only on the mass and charge of the hadron, and not on its spin or internal structure. For the scattering amplitude we use the classical result [33, 34] (also reviewed in section 13.5 of [35]):

$$\mathcal{T}_0 = \lim_{\mathbf{k} \rightarrow \mathbf{0}} T_{\mu\mu}(\imath|\mathbf{k}| - \epsilon, \mathbf{k}) = -4q^2. \quad (\text{B.31})$$

We conclude this appendix by providing a representation of the zeta function $\xi(s)$ defined in eq. (B.24) which is useful for numerical calculation. We use the identity

$$\frac{1}{|\mathbf{n}|^{s/2}} = \frac{1}{\Gamma(s/2)} \int_0^{u_*} du u^{\frac{s}{2}-1} e^{-u\mathbf{n}^2} + \frac{1}{\Gamma(s/2)} \int_{u_*}^\infty du u^{\frac{s}{2}-1} e^{-u\mathbf{n}^2}, \quad (\text{B.32})$$

we plug it into eq. (B.24) and we use the Poisson summation formula

$$\sum_{\mathbf{n} \in \mathbb{Z}_3} e^{-u\mathbf{n}^2 + \imath\pi\langle \mathbf{n} \rangle} = \left(\frac{\pi}{u}\right)^{\frac{3}{2}} \sum_{\mathbf{k} \in \hat{\Pi}_-} e^{-\frac{\mathbf{k}^2}{4u}}, \quad (\text{B.33})$$

only in the integral over $u \in [0, u_*]$. At this point all integrals can be calculated explicitly in terms of the upper incomplete gamma functions:

$$\xi(s) = \frac{1}{\Gamma(s/2)} \left\{ -\frac{2u_*^{s/2}}{s} + \frac{\pi^{3/2}}{2^{s-3}} \sum_{\mathbf{k} \in \hat{\Pi}_-} (\mathbf{k}^2)^{\frac{s-3}{2}} \Gamma\left(\frac{3-s}{2}, \frac{\mathbf{k}^2}{4u_*}\right) + \sum_{\mathbf{n} \neq \mathbf{0}} \frac{(-1)^{\langle \mathbf{n} \rangle}}{|\mathbf{n}|^{s/2}} \Gamma(s/2, u_* \mathbf{n}^2) \right\}. \quad (\text{B.34})$$

The upper incomplete gamma function $\Gamma(\tau, z)$ is defined for all complex values of τ except non-positive integers, and it decays exponentially as $|z| \rightarrow \infty$. Therefore the infinite sums in the previous formula are rapidly convergent. Also this representation is valid for all values of s needed in the mass formula. The splitting variable $u_* > 0$ is completely arbitrary and can be used to check the result of numerical calculation.

B.1 Analyticity properties

In this subsection we work in Minkowski spacetime with metric $g = \text{diag}(1, -1, -1, -1)$. We also set $L = \infty$. We introduce the Minkowskian electric current:

$$J_\mu(x) = e^{\imath(x_0 H_0 - \mathbf{xP})} J_\mu(0) e^{-\imath(x_0 H_0 - \mathbf{xP})}, \quad (\text{B.35})$$

which is related to the Euclidean one introduced in eq. (B.4) via

$$J^0(0) = -\imath j_0(0), \quad J^k(0) = j_k(0). \quad (\text{B.36})$$

While in finite volume, because of C^* -boundary conditions, eigenstates of the momentum are also eigenstates of the charge-conjugation operator, this is not necessarily true in infinite volume. We perform a change of basis which does not affect the quantities we are interested in, and we choose to work with simultaneous eigenstates of energy, momentum and electric charge.

We consider the retarded two-point function in the forward limit

$$W_+(k) = \imath \lim_{\mathbf{p} \rightarrow \mathbf{0}} \int d^4x e^{\imath kx} \theta(x_0) \langle h(\mathbf{p}) | J_\mu(x) J^\mu(0) | h(\mathbf{0}) \rangle_c, \quad (\text{B.37})$$

which is related to the function $M_{\mu\mu}(k)$ introduced in eq. (B.10) in infinite volume through a Wick rotation

$$M_{\mu\mu}(k_0, \mathbf{k}) = -W_+(-\imath k_0, \mathbf{k}). \quad (\text{B.38})$$

The subtraction of the disconnected part in eq. (B.37) can be expanded:

$$\begin{aligned} & \int d^4x e^{\imath kx} \theta(x_0) \langle h(\mathbf{p}) | J_\mu(x) J^\mu(0) | h(\mathbf{0}) \rangle_c \\ &= \int d^4x e^{\imath kx} \theta(x_0) \left\{ \langle h(\mathbf{p}) | J_\mu(x) J^\mu(0) | h(\mathbf{0}) \rangle - 2E(\mathbf{p}) (2\pi)^3 \delta^3(\mathbf{p}) \langle 0 | J_\mu(x) J^\mu(0) | 0 \rangle \right\}. \end{aligned} \quad (\text{B.39})$$

Notice that in this formula we cannot just take $\mathbf{p} = \mathbf{0}$ because the disconnected contribution gives a geometrical divergence proportional to $\delta^3(\mathbf{0})$. Therefore the limit in eq. (B.37) is essential in order to define properly the subtraction. However notice that for any $\mathbf{p} \neq \mathbf{0}$ the delta function vanishes exactly and it does not contribute to the limit ($\lim_{\mathbf{p} \rightarrow \mathbf{0}} \delta^3(\mathbf{p}) = 0$), allowing us to write equivalently

$$W_+(k) = \imath \lim_{\mathbf{p} \rightarrow \mathbf{0}} \int d^4x e^{\imath kx} \theta(x_0) \langle h(\mathbf{p}) | J_\mu(x) J^\mu(0) | h(\mathbf{0}) \rangle, \quad (\text{B.40})$$

It is possible to prove that this limit is finite, which we will assume in the remaining of this appendix.⁸

⁸By means of the LSZ reduction formula, the function $C_+(k)$ defined in (B.50) can be expressed as linear combinations of the *reduced Green's functions* defined in eq. (16.52), chapter 16 of [36]. On the other hand, as we will notice later on, $W_+(k)$ is uniquely determined by $C_+(k)$. The finiteness of the limit $\mathbf{p} \rightarrow \mathbf{0}$ in eq. (B.50) and consequently in eq. (B.40) derives from the analyticity properties of the *reduced Green's functions* stated in Theorem 16.8, chapter 16 of [36]. The reader should notice that the connected part and the limit are systematically dropped in the classical literature, e.g. [30].

By calculating the coordinate integral in eq. (B.40) one gets

$$W_+(k) = \lim_{\mathbf{p} \rightarrow \mathbf{0}} \langle h(\mathbf{p}) | J_\mu(0) \frac{(2\pi)^3 \delta^3(\mathbf{P} - \mathbf{p} - \mathbf{k})}{H_0 - E(\mathbf{p}) - k_0 - i\epsilon} J^\mu(0) | h(\mathbf{0}) \rangle, \quad (\text{B.41})$$

where we have introduced the energy of the external states

$$E(\mathbf{p}) = \sqrt{m_0^2 + \mathbf{p}^2}. \quad (\text{B.42})$$

Notice that, since the external state corresponds to a stable hadron, the states propagating in between the two currents in eq. (B.41) have energy not smaller than m_0 . Therefore the retarded function $W_+(k)$ has poles only for non-negative values of k_0 .

It is useful to separate the single particle component from the continuous part of the spectrum:

$$W_+(k) = \frac{Z_{1P}(\mathbf{k}^2)}{E(\mathbf{k}) - m_0 - k_0 + i\epsilon} + Z_{MP}(k_0, \mathbf{k}^2), \quad (\text{B.43})$$

$$Z_{1P}(\mathbf{k}^2) = \frac{1}{d_s} \sum_{\mu, \sigma, \sigma'} \frac{g^{\mu\mu}}{2E(\mathbf{k})} |\langle h(\mathbf{0}), \sigma | J_\mu(0) | h(\mathbf{k}), \sigma' \rangle|^2. \quad (\text{B.44})$$

We want to study the analyticity properties of $Z_{1P}(\mathbf{k}^2)$ and $Z_{MP}(k_0, \mathbf{k}^2)$ in the spatial momentum \mathbf{k} (the analyticity properties in k_0 are obvious from the spectral decomposition (B.41)), which we summarize here:

1. $Z_{1P}(\mathbf{k}^2)$ is analytical for any real value of \mathbf{k} , and can be analytically continued to a complex neighbourhood of $\mathbf{k}^2 = 0$;
2. The Euclidean function $Z_{MP}(-ik_0, \mathbf{k}^2)$ is analytical for any real value of \mathbf{k} ;
3. The on-shell function $Z_{MP}(-|\mathbf{k}|, \mathbf{k}^2)$ is analytical for any real value of \mathbf{k} ;
4. The on-shell function $Z_{MP}(|\mathbf{k}|, \mathbf{k}^2)$ is analytical for real values of \mathbf{k} in a neighbourhood of $\mathbf{k} = \mathbf{0}$, and can be analytically continued to a complex neighbourhood of $|\mathbf{k}| = 0$.

From these properties it follows that:

1. The off-shell Euclidean Compton amplitude

$$\begin{aligned} T(k_0, \mathbf{k}) &= M_{\mu\mu}(k_0, \mathbf{k}) + M_{\mu\mu}(-k_0, -\mathbf{k}) \\ &= -\frac{2[E(\mathbf{k}) - m_0]Z_{1P}(\mathbf{k}^2)}{[E(\mathbf{k}) - m_0]^2 + k_0^2} - Z_{MP}(ik_0, \mathbf{k}^2) - Z_{MP}(-ik_0, \mathbf{k}^2) \end{aligned} \quad (\text{B.45})$$

is analytical for any real value of $\mathbf{k} \neq \mathbf{0}$ (lemma B.2).

2. The on-shell quantity

$$M_{\mu\mu}(-i|\mathbf{k}|, \mathbf{k}) = -\frac{Z_{1P}(\mathbf{k}^2)}{E(\mathbf{k}) - m_0 + |\mathbf{k}|} - Z_{MP}(-|\mathbf{k}|, \mathbf{k}^2), \quad (\text{B.46})$$

as a function of $|\mathbf{k}|$, admits a meromorphic extension to a complex neighbourhood of $|\mathbf{k}| = 0$. In particular it admits a Laurent series in $|\mathbf{k}| = 0$, the first term being:

$$M_{\mu\mu}(-i|\mathbf{k}|, \mathbf{k}) = -\frac{Z_{1P}(0)}{|\mathbf{k}|} + \mathcal{O}(|\mathbf{k}|^0). \quad (\text{B.47})$$

We will show that, eq. (B.65), $Z_{1P}(0) = 2m_0q^2$ (lemma B.3).

3. The on-shell Compton amplitude

$$T(i|\mathbf{k}| - \epsilon, \mathbf{k}) = -\frac{2[E(\mathbf{k}) - m_0]Z_{1P}(\mathbf{k}^2)}{[E(\mathbf{k}) - m_0]^2 - \mathbf{k}^2 - i\epsilon} - Z_{MP}(|\mathbf{k}|, \mathbf{k}^2) - Z_{MP}(-|\mathbf{k}|, \mathbf{k}^2) \quad (\text{B.48})$$

is an analytic function of \mathbf{k}^2 in a complex neighbourhood of $\mathbf{k}^2 = 0$. This follows from the analyticity properties discussed above, from the fact that the odd powers in $|\mathbf{k}|$ generated by the expansion of $Z_{MP}(\pm|\mathbf{k}|, \mathbf{k}^2)$ cancel out, and from the fact that

$$\lim_{\mathbf{k} \rightarrow \mathbf{0}} \frac{2[E(\mathbf{k}) - m_0]}{[E(\mathbf{k}) - m_0]^2 - \mathbf{k}^2 - i\epsilon} = -\frac{1}{m_0}. \quad (\text{B.49})$$

The full analyticity properties of $W_+(k)$, and consequently of $Z_{1P}(\mathbf{k}^2)$ and $Z_{MP}(k_0, \mathbf{k}^2)$, can be derived by the analyticity properties of four-point reduced Green's functions discussed in chapter 16 of [36]. However we provide here a hopefully more digestible proof of the particular properties we are interested in, based on the Jost-Lehmann-Dyson representation of the expectation values of certain retarded commutators. We also point out that the same analyticity properties we are interested in can also be obtained by assuming an effective theory describing hadrons and by using results and methods discussed in section 2.4 of ref. [25] and in appendix A.

Analysis of $Z_{1P}(\mathbf{k}^2)$. We notice first that $Z_{1P}(\mathbf{k}^2)$ can be extracted also from the retarded commutator

$$\begin{aligned} C_+(k) &= i \lim_{\mathbf{p} \rightarrow \mathbf{0}} \int d^4x e^{ikx} \theta(x_0) \langle h(\mathbf{p}) | [J_\mu(x), J^\mu(0)] | h(\mathbf{0}) \rangle \\ &= W_+(k) + W_-(k), \end{aligned} \quad (\text{B.50})$$

where $W_-(k)$ is a functions with poles only for negative value of k_0 . Therefore the following reduction formula holds

$$\begin{aligned} \lim_{k_0 \rightarrow E(\mathbf{k}) - m_0} [E(\mathbf{k}) - m_0 - k_0] C_+(k) \\ = \lim_{k_0 \rightarrow E(\mathbf{k}) - m_0} [E(\mathbf{k}) - m_0 - k_0] W_+(k) = Z_{1P}(\mathbf{k}^2). \end{aligned} \quad (\text{B.51})$$

Then we extract the single-hadron pole from both orderings of the retarded commutator by means of the following trick. We introduce the auxiliary retarded commutator

$$\tilde{C}_+(k) = i \lim_{\mathbf{p} \rightarrow \mathbf{0}} \int d^4x e^{ikx} \theta(x_0) \langle h(\mathbf{p}) | [\bar{J}_\mu(x), \bar{J}^\mu(0)] | h(\mathbf{0}) \rangle, \quad (\text{B.52})$$

$$\bar{J}_\mu(x) = (-\square + 2im_0\partial_0)J^\mu(x). \quad (\text{B.53})$$

The relation between this retarded commutator and the original one is obtained through integration by parts of the differential operator $(-\square + 2im_0\partial_0)$

$$(k^2 + 2m_0k_0)(k^2 - 2m_0k_0)C_+(k) = \tilde{C}_+(k) + \tilde{P}(k). \quad (\text{B.54})$$

The boundary term has the form

$$\tilde{P}(k) = i \lim_{\mathbf{p} \rightarrow \mathbf{0}} \int d^4x \delta(x_0) e^{ikx} \langle h(\mathbf{p}) | [\mathcal{D}J_\mu(x), J^\mu(0)] | h(\mathbf{0}) \rangle \quad (\text{B.55})$$

where \mathcal{D} is some local differential operator. The integrand of $\tilde{P}(k)$ involves only commutators of local operators at equal time, which are linear combinations of delta functions and their derivatives. Therefore $\tilde{P}(k)$ is a polynomial in the quadrimomentum k . In terms of the auxiliary retarded commutator, the reduction formula reads

$$Z_{1P}(\mathbf{k}^2) = \frac{1}{8m_0 E(\mathbf{k}) [E(\mathbf{k}) - m_0]} \lim_{k_0 \rightarrow E(\mathbf{k}) - m_0} [\tilde{C}_+(k) + \tilde{P}(k)]. \quad (\text{B.56})$$

The analyticity properties of the modified retarded commutator can be exposed by means of the Jost-Lehmann-Dyson (JLD) representation [37, 38],

$$\tilde{C}_+(k) = \int_{\tilde{\mathcal{S}}} \frac{d^4 u d\lambda^2 \tilde{\rho}(u, \lambda^2)}{(k-u)^2 - \lambda^2 + i(k_0 - u_0)\epsilon}, \quad (\text{B.57})$$

where the JLD spectral function $\tilde{\rho}(u, \lambda^2)$ is uniquely determined by the retarded commutator. The integration domain $\tilde{\mathcal{S}}$ encodes all known information about the spectrum, and can be represented as the set of 5-tuples (u, λ^2) such that

$$\begin{cases} \sqrt{(\mathbf{u} - \mathbf{k})^2 + \lambda^2} + u_0 \geq \sqrt{M_1^2 + \mathbf{k}^2} - m \\ \sqrt{(\mathbf{u} - \mathbf{k})^2 + \lambda^2} - u_0 \geq \sqrt{M_2^2 + \mathbf{k}^2} - m \end{cases}, \quad (\text{B.58})$$

for any value of the momentum \mathbf{k} . The masses M_1 and M_2 are determined in the following way. Consider the commutator

$$\begin{aligned} & \lim_{\mathbf{p} \rightarrow \mathbf{0}} \int d^4 x e^{ikx} \langle h(\mathbf{p}) | [\bar{J}_\mu(x), \bar{J}^\mu(0)] | h(\mathbf{0}) \rangle \\ &= \lim_{\mathbf{p} \rightarrow \mathbf{0}} \langle h(\mathbf{p}) | \bar{J}_\mu(0) (2\pi)^4 [\delta(P - p - k) - \delta(P - p + k)]_{p=(E(\mathbf{p}), \mathbf{p})} \bar{J}^\mu(0) | h(\mathbf{0}) \rangle, \end{aligned} \quad (\text{B.59})$$

with $P = (H_0, \mathbf{P})$. The two delta functions come from the two different orderings of the currents in the commutator. M_1 and M_2 are the masses of the lightest states propagating in between the two currents in the first and second ordering respectively. Had we considered the original current $J_\mu(x)$, the lightest state would have been the hadron h itself. However it is easy to check that the insertion of the operators $(-\square + 2im_0\partial_0)$ kills the contribution of the single-hadron states in the above commutator, therefore

$$M_1 = M_2 = m + \Delta \quad (\text{B.60})$$

where $\Delta > 0$ is some mass gap (if no bound states exist $\Delta = 2m_\pi$).

The relevant limit for the reduction formula (B.56) is

$$\begin{aligned} f(\mathbf{k}^2) &= \lim_{k_0 \rightarrow E(\mathbf{k}) - m_0} [\tilde{C}_+(k) + \tilde{P}(k)] \\ &= P(E(\mathbf{k}), \mathbf{k}) + \int_{\tilde{\mathcal{S}}} \frac{d^4 u d\lambda^2 \tilde{\rho}(u, \lambda^2)}{[E(\mathbf{k}) - m_0 - u_0]^2 - (\mathbf{k} - \mathbf{u})^2 - \lambda^2}. \end{aligned} \quad (\text{B.61})$$

The denominator vanishes only if

$$u_0 \pm \sqrt{(\mathbf{k} - \mathbf{u})^2 + \lambda^2} = E(\mathbf{k}) - m_0, \quad (\text{B.62})$$

which is satisfied for no real value of \mathbf{k} if (u, λ^2) is in the domain $\tilde{\mathcal{S}}$.

As pointed out in [38], if (u, λ^2) is in the domain $\tilde{\mathcal{S}}$ then necessarily

$$|u_0| + |\mathbf{u}| \leq m_0. \quad (\text{B.63})$$

Thanks to this, it is easy to show that two positive constants κ and α exist such that the denominator in eq. (B.61) is limited from below by

$$|[E(\mathbf{k}) - m_0 - u_0]^2 - (\mathbf{k} - \mathbf{u})^2 - \lambda^2| \geq |u_0^2 - \mathbf{u}^2 - \lambda^2| - \alpha|\mathbf{k}| \geq \Delta^2 - \alpha|\mathbf{k}| \quad (\text{B.64})$$

for any $(u, \lambda^2) \in \tilde{\mathcal{S}}$ and for any complex \mathbf{k} such that $|\mathbf{k}| < \kappa$. In the last step we have used eqs. (B.58) for $\mathbf{k} = \mathbf{0}$. From the above bound it is clear that if κ is small enough, then the denominator never vanishes. Therefore $f(\mathbf{k}^2)$ can be continued by analyticity to a complex neighbourhood of $\mathbf{k}^2 = 0$.

From eq. (B.56) it might seem that $Z_{1\text{P}}(\mathbf{k}^2)$ has a singularity in $\mathbf{k} \rightarrow \mathbf{0}$. However this limit is fixed by symmetries:

$$\lim_{\mathbf{k} \rightarrow \mathbf{0}} Z_{1\text{P}}(\mathbf{k}^2) = \lim_{\mathbf{k} \rightarrow \mathbf{0}} \frac{1}{d_s} \sum_{\mu, \sigma, \sigma'} \frac{g^{\mu\mu}}{2E(\mathbf{k})} |\langle h(\mathbf{0}), \sigma | J_\mu(0) | h(\mathbf{k}), \sigma' \rangle|^2 = 2m_0 q^2, \quad (\text{B.65})$$

where q is the electric charge of the hadron h . This relation implies that $f(0) = 0$ and $Z_{1\text{P}}(\mathbf{k}^2)$ is an analytic function for any real value of \mathbf{k}^2 , and for complex values of \mathbf{k}^2 in a neighbourhood of zero.

Analysis of $Z_{\text{MP}}(k_0, \mathbf{k}^2)$. $Z_{\text{MP}}(k_0, \mathbf{k}^2)$ is obtained by selecting all poles in $W_+(k)$, or equivalently in $C_+(k)$, with $\text{Re } k_0 > E(\mathbf{k}) - m_0$. In this case we find more convenient to write $C_+(k)$ in terms of the auxiliary retarded commutator

$$\hat{C}_+(k) = i \lim_{\mathbf{p} \rightarrow \mathbf{0}} \sum_{\sigma} \int d^4x e^{ikx} \theta(x_0) \langle h(\mathbf{p}) | [\bar{J}_\mu(x), J^\mu(0)] | h(\mathbf{0}) \rangle. \quad (\text{B.66})$$

In complete analogy to eq. (B.54), the original retarded commutator can be written in terms of the auxiliary one as

$$(k^2 + 2m_0 k_0) C_+(k) = \hat{C}_+(k) + \hat{P}(k), \quad (\text{B.67})$$

where $\hat{P}(k)$ is a polynomial in the quadrimomentum k . The above equation can be inverted by noticing that all poles of $C_+(x)$ have negative imaginary part. We introduce a JLD representation for the retarded commutator $\hat{C}_+(k)$ and we get

$$C_+(k) = \frac{1}{k^2 + 2m_0 k_0 + i(k_0 + m_0)\epsilon} \left\{ \hat{P}(k) + \int_{\hat{\mathcal{S}}} \frac{d^4u d\lambda^2 \hat{\rho}(u, \lambda^2)}{(k-u)^2 - \lambda^2 + i(k_0 - u_0)\epsilon} \right\}. \quad (\text{B.68})$$

The integration domain $\hat{\mathcal{S}}$ is the set of 5-tuples (u, λ^2) such that

$$\left\{ \begin{array}{l} \sqrt{(\mathbf{u} - \mathbf{k})^2 + \lambda^2} + u_0 \geq \sqrt{(m + \Delta)^2 + \mathbf{k}^2} - m \\ \sqrt{(\mathbf{u} - \mathbf{k})^2 + \lambda^2} - u_0 \geq \sqrt{m^2 + \mathbf{k}^2} - m \end{array} \right\}, \quad (\text{B.69})$$

for any value of the momentum \mathbf{k} . The denominator outside of the integral in eq. (B.68) has poles for $\text{Re } k_0 \leq E(\mathbf{k}) - m_0$ which do not contribute to $Z_{\text{MP}}(k_0, \mathbf{k}^2)$. The integrand can be decomposed in partial fractions

$$\frac{1}{(k-u)^2 - \lambda^2 + i(k_0 - u_0)\epsilon} = \frac{1}{2X} \left(\frac{1}{k_0 - u_0 - X + i\epsilon} - \frac{1}{k_0 - u_0 + X + i\epsilon} \right), \quad (\text{B.70})$$

$$X = \sqrt{(\mathbf{k} - \mathbf{u})^2 + \lambda^2}, \quad (\text{B.71})$$

and only the first one contributes with a pole to $Z_{\text{MP}}(k_0, \mathbf{k}^2)$. By calculating the residue at this pole we get

$$Z_{\text{MP}}(k_0, \mathbf{k}^2) = \int_{\hat{\mathcal{S}}} d^4 u d\lambda^2 \frac{\hat{\rho}(u, \lambda^2)}{2X[(u_0 + X + m_0)^2 - E(\mathbf{k})^2]} \frac{1}{k_0 - u_0 - X + i\epsilon}. \quad (\text{B.72})$$

Using the definition of the domain $\hat{\mathcal{S}}$ it is straightforward to check that the denominator $2X[(u_0 + X + m_0)^2 - E(\mathbf{k})^2]$ never vanishes for any real value of \mathbf{k} and for any value of $(u, \lambda^2) \in \hat{\mathcal{S}}$. We derive some particular properties.

The Wick-rotated function

$$Z_{\text{MP}}(-ik_0, \mathbf{k}^2) = \int_{\hat{\mathcal{S}}} d^4 u d\lambda^2 \frac{\hat{\rho}(u, \lambda^2)}{2X[(u_0 + X + m_0)^2 - E(\mathbf{k})^2]} \frac{1}{-ik_0 - u_0 - X}. \quad (\text{B.73})$$

is analytical for any real value of k , since the two denominators never vanish (as $u_0 + X > 0$).

The on-shell function

$$Z_{\text{MP}}(-|\mathbf{k}|, \mathbf{k}^2) = \int_{\hat{\mathcal{S}}} d^4 u d\lambda^2 \frac{\hat{\rho}(u, \lambda^2)}{2X[(u_0 + X + m_0)^2 - E(\mathbf{k})^2]} \frac{1}{-|\mathbf{k}| - u_0 - X}. \quad (\text{B.74})$$

is analytical for any real value of \mathbf{k} , since the two denominators never vanish (as $|\mathbf{k}| + u_0 + X \geq u_0 + X > 0$). Moreover, as a function of $|\mathbf{k}|$, $Z_{\text{MP}}(-|\mathbf{k}|, \mathbf{k}^2)$ can be analytically continued to a complex neighbourhood of $|\mathbf{k}| = 0$.

The on-shell function

$$Z_{\text{MP}}(|\mathbf{k}|, \mathbf{k}^2) = \int_{\hat{\mathcal{S}}} d^4 u d\lambda^2 \frac{\hat{\rho}(u, \lambda^2)}{2X[(u_0 + X + m_0)^2 - E(\mathbf{k})^2]} \frac{1}{|\mathbf{k}| - u_0 - X + i\epsilon}. \quad (\text{B.75})$$

is analytical for real values of \mathbf{k} such that

$$|\mathbf{k}| < \Delta, \quad (\text{B.76})$$

as in this range the denominator $|\mathbf{k}| - u_0 - X$ can be shown not to vanish for any value of $(u, \lambda^2) \in \hat{\mathcal{S}}$. As a function of $|\mathbf{k}|$, $Z_{\text{MP}}(|\mathbf{k}|, \mathbf{k}^2)$ can be analytically continued to a complex neighbourhood of $|\mathbf{k}| = 0$.

C Classical vacua of compact QED_C

We consider an abelian gauge field on a lattice with C^* boundary conditions along the directions included in the set \mathcal{C}

$$U(x + \hat{L}_\mu, \rho) = \begin{cases} U(x, \rho) & \text{if } \mu \notin \mathcal{C} \\ U(x, \rho)^* & \text{if } \mu \in \mathcal{C} \end{cases}, \quad (\text{C.1})$$

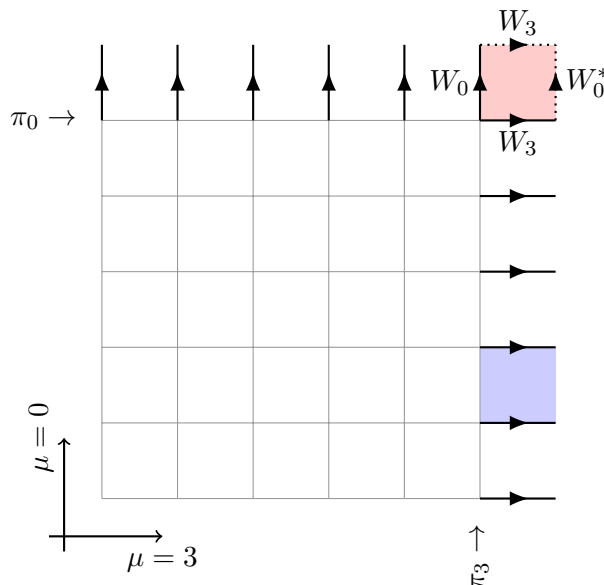


Figure 7. A two-dimensional representation of the problem discussed in this appendix. Direction $\mu = 0$ is periodic, while direction $\mu = 3$ is C^* -periodic. In simultaneous axial gauge, the only links that are different from unity are the ones represented with a thick line and an arrow (*active link variables*). The condition that the blue plaquette be equal to one implies that the two active link variables in the plaquette are equal. Nontrivial constraints come from minimum condition for the red plaquette at the intersection of the π_0 and π_3 hyperplanes.

where the coordinates are integer numbers in the range

$$0 \leq x_\mu \leq L_\mu - 1. \quad (\text{C.2})$$

We assume direction $\mu = 3$ C^* -periodic, and direction $\mu = 0$ periodic.

We want to characterise all gauge-field configurations corresponding to absolute minima of the Wilson action. In terms of the plaquette $P(x, \mu, \nu)$ the minimum condition reads

$$P(x, \mu, \nu) = 1. \quad (\text{C.3})$$

We can always gauge-transform to axial gauge along a given direction μ , i.e. to a gauge in which all the link variables $U(x, \mu)$ are equal to one except the ones on the hyperplane π_μ defined by the equation

$$\pi_\mu : x_\mu = L_\mu - 1. \quad (\text{C.4})$$

Because of condition (C.3) it is easy to show that we can gauge-transform to simultaneous axial gauge for all directions. We will refer to those link variables that are different from unity as *active link variables* (see figure 7).

Plaquettes at the intersection of two distinct π -planes involve four active link variables, all other plaquettes on the π -planes involve two parallel link variables. Constraint (C.3) on the latter ones, together with the fact that unity is left unchanged by the boundary

conditions, implies

$$U(x, \mu) = U(x + \hat{\nu}, \mu), \text{ for any } x \in \pi_\mu, \nu \neq \mu. \quad (\text{C.5})$$

Using this equation recursively we get that, given some direction μ , all active link variables along μ are equal to each other. We will define

$$W_\mu = U(x, \mu), \text{ for any } x \in \pi_\mu. \quad (\text{C.6})$$

We use now the minimum condition (C.3) for plaquettes at the intersection of two distinct π -planes. Let us consider first the plaquette in some point $x \in \pi_\mu \cap \pi_3$ where μ is a periodic direction (see figure 7):

$$1 = P(x, \mu, 3) = W_\mu W_3 W_\mu W_3^{-1}, \quad (\text{C.7})$$

which implies

$$W_\mu = \pm 1, \text{ if } \mu \notin \mathcal{C}. \quad (\text{C.8})$$

If $\mu \neq 3$ is a C^* direction we get instead

$$1 = P(x, \mu, 3) = W_\mu W_3^{-1} W_\mu W_3^{-1}, \quad (\text{C.9})$$

which implies

$$W_\mu = \pm W_3, \text{ if } \mu \in \mathcal{C}. \quad (\text{C.10})$$

Finally we show that W_3 can be set to 1 with a gauge transformation. Let w be a complex number such that $W_3 = w^{-2}$ and we define the gauge transformation

$$\Lambda(x) = w, \text{ for } 0 \leq x_\mu \leq L_\mu - 1, \quad (\text{C.11})$$

and extended outside the above domain by means of the boundary conditions

$$\Lambda(x + \hat{L}_\mu) = \begin{cases} \Lambda(x) & \text{if } \mu \notin \mathcal{C} \\ \Lambda(x)^* & \text{if } \mu \in \mathcal{C} \end{cases}. \quad (\text{C.12})$$

First notice that this gauge transformation preserves the gauge-field boundary conditions and the axial gauge. All active link variables along periodic directions are left unchanged under this gauge transformation. If μ is a C^* -direction, the active link variable along μ transforms like

$$W_\mu \rightarrow w W_\mu w = W_3^{-1} W_\mu = \pm 1, \quad (\text{C.13})$$

with the particular case of

$$W_3 \rightarrow w W_3 w = W_3^{-1} W_3 = 1. \quad (\text{C.14})$$

This concludes the proof of part 1 of the following proposition.

Proposition C.1. *Let $U(x, \mu)$ be a gauge configuration that minimizes the Wilson action.*

1. A vector z satisfying the conditions

$$z_3 = 1, \quad z_\mu^2 = 1. \tag{C.15}$$

exists such that $U(x, \mu)$ is gauge-equivalent to the gauge configuration

$$\bar{U}_z(x, \mu) = \begin{cases} z_\mu & \text{if } x_\mu = L_\mu - 1 \\ 1 & \text{otherwise} \end{cases}. \tag{C.16}$$

2. The vector z is unique.

Uniqueness is proven by noticing that the vector z is therefore uniquely determined by the original gauge configuration $U(x, \mu)$

$$z_\mu = \begin{cases} W(\mu) & \text{if } \mu \notin \mathcal{C} \\ W(\mu)W(3)^{-1} & \text{if } \mu \in \mathcal{C} \end{cases}, \tag{C.17}$$

where we have introduced the Wilson lines

$$W(\mu) = \prod_{s=0}^{L_\mu-1} U(s\hat{\mu}, \mu). \tag{C.18}$$

It is easy to show that $W(\mu)$ is gauge invariant if and only if μ is a periodic direction, while the L-shaped parallel transport $W(\mu)W(3)^{-1}$ is gauge invariant if and only if μ is a \mathcal{C}^* -direction.

D Anatomy of the sign problem

Integration of the fermion fields in a periodic setup yields the determinant of the Dirac operator. This result relies on the fact that the Grassman variables $\psi(x)$ and $\bar{\psi}(x)$ are independent, which is not true in the case of \mathcal{C}^* boundary conditions. A possible way to get an explicit expression for the fermionic path integral is to use the change of variable

$$\psi_\pm(x) = \frac{\psi(x) \pm C^{-1}\bar{\psi}^T(x)}{\sqrt{2}}, \tag{D.1}$$

and to define the new two-component field

$$\eta(x) = \begin{pmatrix} \psi_+(x) \\ -\psi_-(x) \end{pmatrix}. \tag{D.2}$$

It is straightforward to verify that \mathcal{C}^* boundary conditions for the field $\psi(x)$ are equivalent to

$$\eta(x + \hat{L}_k) = K\eta(x), \quad K = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{D.3}$$

where the matrix K acts on the two components of η . We will refer to these boundary conditions as K boundary conditions.

By using the identity for the Wilson-Dirac operator (valid for a general non-abelian gauge theory)

$$C^{-1}D[V]^T C = D[V^*], \tag{D.4}$$

and a few lines of algebra, one can write the fermionic action in terms of the new fields

$$S_F = \bar{\psi}D[V]\psi = -\frac{1}{2}\eta^T CD[\mathcal{J}(V)]\eta, \tag{D.5}$$

where $D_{\mathcal{J}} \equiv D[\mathcal{J}(V)]$ is the Wilson-Dirac operator calculated with the gauge field $\mathcal{J}(V)$ defined as

$$\mathcal{J}(V) = 1_2 \otimes \text{Re } V + J \otimes \text{Im } V, \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{D.6}$$

The matrices 1_2 and J act on the two components of η . Notice that $\mathcal{J}(V)$ defines a representation of the gauge group, unitarily equivalent to the representation defined by V . Integration of the fermionic action in the form obtained in eq. (D.5) yields

$$\int_{C^* \text{ b.c.s}} \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\bar{\psi}D[V]\psi} = \int_{K \text{ b.c.s}} \mathcal{D}\eta e^{\frac{1}{2}\eta^T CD_{\mathcal{J}}\eta} = \text{Pf}_K CD_{\mathcal{J}}, \tag{D.7}$$

where the subscript K reminds that the derivative appearing in the Dirac operator are defined on the space of fields satisfying K boundary conditions, and $CD_{\mathcal{J}}$ is an antisymmetric complex matrix. In eq. (D.7) $\text{Pf}_K CD_{\mathcal{J}}$ is the Pfaffian of $CD_{\mathcal{J}}$ that, by using the algebraic identities

$$(\text{Pf}_K CD_{\mathcal{J}})^2 = \text{Det}_K CD_{\mathcal{J}} = \text{Det}_K D_{\mathcal{J}}, \tag{D.8}$$

can be related to the determinant of $D_{\mathcal{J}}$. Algorithms for the lattice simulation of theories involving Pfaffians have been discussed in the context of C^* boundary conditions or the closely-related G-parity boundary conditions and also in the context of lattice supersymmetric models (see [39–42] for a list of references on this subject).

We shall now discuss if a sign problem is associated to $\text{Pf}_K CD_{\mathcal{J}}$. By using eq. (D.8) and the γ_5 -hermiticity of the Dirac operator, one concludes easily that the squared Pfaffian is real. We want to show now that a stronger result holds: the Pfaffian itself is real. Let us consider the Pfaffian of the auxiliary operator $C(D_{\mathcal{J}} - s)$ for a generic complex number s . This Pfaffian is a polynomial in the matrix elements and in particular in s ,

$$\text{Pf}_K C(D_{\mathcal{J}} - s) = \prod_{\alpha} (s - \lambda_{\alpha})^{m_{\alpha}}, \tag{D.9}$$

where the λ_{α} 's are distinct roots. The overall normalization is determined by the value of the Pfaffian in the $s \rightarrow \infty$ limit. By using the relation between the Pfaffian and the determinant we calculate the characteristic polynomial of $D_{\mathcal{J}}$

$$\text{Det}_K (D_{\mathcal{J}} - s) = [\text{Pf}_K C(D_{\mathcal{J}} - s)]^2 = \prod_{\alpha} (s - \lambda_{\alpha})^{2m_{\alpha}}. \tag{D.10}$$

The λ_{α} 's are the roots of the characteristic polynomial of $D_{\mathcal{J}}$, i.e. they are the eigenvalues of $D_{\mathcal{J}}$. Notice that the algebraic multiplicity of λ_{α} is $2m_{\alpha}$. Because of γ_5 -hermiticity either

the eigenvalues of $D_{\mathcal{J}}$ are real or they appear in pairs of complex conjugates. Since all multiplicities are even, the determinant is positive if s is real, and consequently the Pfaffian is real. For $s = 0$ one gets

$$\text{Pf}_K CD_{\mathcal{J}} = \prod_{\alpha | \text{Im } \lambda_{\alpha} = 0} \lambda_{\alpha}^{m_{\alpha}} \prod_{\alpha | \text{Im } \lambda_{\alpha} > 0} |\lambda_{\alpha}^{m_{\alpha}}|^2. \quad (\text{D.11})$$

Once established that the fermionic Pfaffian (D.7) is real, we need to wonder about its sign. From eq. (D.11), clearly the Pfaffian is negative only if the Dirac operator $D_{\mathcal{J}}$ has some negative eigenvalues, which can happen with Wilson fermions. However, in the continuum limit, the real part of the eigenvalues of the Dirac operator is always positive (and equal to m) therefore the Pfaffian is positive. At finite lattice spacing the fermionic Pfaffian (D.7) has a mild sign problem that is completely analogous to the single-flavour case with periodic boundary conditions.

A detailed study of the simulations cost of QCD and QCD+QCD with C^* boundary conditions is well beyond the scope of this paper and will be the subject of future investigation. At the same time, before closing this appendix we want to add two side remarks on the numerical implementation of C^* boundary conditions.

The Dirac operator $D_{\mathcal{J}}$ acts on *extended* pseudofermions that have twice as many component as the case with periodic boundary conditions (*regular* pseudofermions). One might wonder whether this implies a factor of two in the simulation cost. This is not expected to be the case, as one can easily argue for QCD in isolation. If the boundary conditions (D.3) are replaced with periodic ones for all components, with a little algebra one can show that the use of the extended pseudofermion is equivalent to Clark and Kennedy's n -th root acceleration [43] with two regular pseudofermions. Therefore, if the volume is large enough (such that the boundary conditions do not affect the spectrum of the Dirac operator), the simulation of QCD with C^* boundary conditions and a single extended pseudofermion is expected to be more efficient than the simulation of QCD with periodic boundary conditions and a single regular pseudofermion. Of course at intermediate volumes competing effects may be generated.

Moreover in the calculation of baryonic correlators with two or three equal valence quarks one has additional fermionic Wick contractions in QCD+QED_C with respect to the standard periodic setup. However, by using arguments similar to the ones discussed in appendix A, one can show that these contributions are exponentially suppressed with the volume. Due to this suppression, it is reasonable to argue that the numerical accuracy needed for evaluating the extra terms might be much lower than that required for the standard contributions.

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