Correlation functions for massive fermions with background instantons

Wen-Yuan Ai[1], Juan S. Cruz[2], Björn Garbrecht[2*], Carlos Tamarit[2]

1 Centre for Cosmology, Particle Physics and Phenomenology,
Université catholique de Louvain, Louvain-la-Neuve B-1348, Belgium
2 Physik-Department T70, James-Franck-Straße,
Technische Universität München, 85748 Garching, Germany
* garbrecht@tum.de

Abstract

We derive correlation functions for fermions with a complex mass in BPST instanton backgrounds in the presence of a general vacuum angle. For this purpose, we first build the Green's functions in the one-instanton background in Euclidean space through a spectral sum in terms of the eigenmodes for the massless case. While this is straightforward for a real mass term, an additional basis transformation among the massless modes of opposite eigenvalues is necessary for a complex mass term. We also construct the Green's functions in real time and relate this approach to recent developments on the theory of vacuum transitions in Minkowski spacetime. These results are then used in order to compute the correlation functions for massive fermions by summing over the background instantons. In these correlation functions, if the infinite-volume limit is taken before the sum over topological sectors, the chiral phases from the mass terms and from the instanton effects are aligned, such that, in absence of additional phases, these do not give rise to observable effects that would violate charge-parity symmetry.

Contents

1 Introduction

The anomalous violation of chiral fermion number through instanton and sphaleron transitions is a characteristic feature of the strong interactions, and for the weak interactions, it is likely to be of key importance for the generation of the baryon asymmetry of the Universe [1–7]. Upon the discovery of the Belavin-Polyakov-Schwartz-Tyupkin (BPST) instanton [3], it was soon realized by 't Hooft that these instanton solutions can also solve the axial U(1) problem [8], which queries why there is no pseudo-Goldstone boson associated with flavour-diagonal chiral rephasings—the η' is much heavier than the mesons in the octet. Although the Adler-Bell-Jackiw anomaly [1, 2] implies that the axial U(1) current is not conserved, it was believed for a while that the anomalous term vanishes when integrated over the whole spacetime because it is a total derivative. However, for the BPST instanton, the anomaly turns out to be nonvanishing globally, thus providing extra breaking for the axial U(1) symmetry and giving rise to the splitting of η' from the meson octet. The violation of chiral fermion number induced by instantons is typically suppressed by the tunneling exponent. At finite temperature, it is however possible to have thermal transitions instead of tunneling. These are described by the sphaleron, i.e. an unstable saddle point of the energy functional for the gauge fields [6].

In the context of thermal field theory and since the instanton corresponds to a Euclidean saddle point solution, calculations are typically carried out using imaginary time. Nonetheless, the main phenomenological applications are within scattering theory or kinetic theory such that it is necessary to transfer the results to the real time of Minkowski space. This is generally possible through the analytic continuation of Green's functions. Nonetheless, it remains of interest to achieve a formulation directly in Minkowski spacetime because it would allow for a first-principle derivation of kinetic theory involving instantons, e.g. in the Schwinger-Keldysh formalism [9, 10], or a more systematic treatment of fermions that are not of the Dirac type, e.g. in chiral gauge theories. A real-time approach would also serve as a check for the correct interpretation of the analytically continued quantities. In view of this, we also discuss in this paper some details on the correlation functions in Minkowski spacetime.

Real-time calculations are typically only feasible when expanding about a saddle point of the action. However, there is no saddle for the action in Minkowski spacetime that would correspond to an instanton configuration. The saddle is recovered when extending the path integral over the degrees of freedom of the bosonic fields into the complex plane and deforming the integration contour. Convergent integration contours that go through the saddle of interest can be found using Picard–Lefschetz theory [11] which has found a number of applications and further developments, for instance, in Refs. [12–17]. Effects from the chiral anomaly for real background fields in Minkowksi space are calculated e.g. in Refs. [18–20].

It is advantageous to derive the Green's function for fermions from a spectral sum, this way the contribution of modes that account for the chiral anomaly, i.e. the zero modes in the massless limit, is readily isolated [4, 5, 21, 22]. Given the spectrum of the massless Dirac operator in the instanton background, this construction is straightforward for the case of a real mass term in Euclidean space. Assuming the mass acts as a perturbation to the eigenspectrum, it is also obvious how to insert a complex mass into the zero-mode contribution to the Green's function. In Section 2.1, we therefore note this result along with some well-known generalities about analytic continuation of the problem. We focus for simplicity on setups with Dirac fermions in the fundamental representation of the gauge group, as in quantum chromodynamics. It is less clear how to construct the spectral sum in Euclidean space in the presence of a complex mass that cannot be treated as a small perturbation. This is because of the occurrence of γ^5, the complex mass term is not proportional to an identity matrix. In Section 2.2, we show that the spectral sum can be built in terms of the eigenfunctions of the massless Dirac operator after an additional orthogonal transformation among the pairs of modes with opposite eigenvalues. As for the eigenmodes, there is a complication in the analytic continuation because the improperly normalizable Euclidean continuum modes will in general not be normalizable when evaluated in real time [15]. In Section 2.3, we therefore discuss in detail how the spectral decomposition of the Green's function can be continued from Euclidean to Minkowski space by rotating the temporal coordinate axis by an angle ϑ. This requires a particular procedure for the continuation of the dual eigenvectors that we refer to as ϑ-conjugation, and in Appendix A, we exemplify this on the Green's function for a Dirac fermion in the homogeneous and isotropic background spacetime. As a result, in Section 2.4, we then show how the spectral sum can be understood in terms of the eigenmodes of the Dirac operator directly in Minkowski spacetime, which requires discussion because this operator is non-Hermitian since the analytically continued gauge field configuration of the instanton is complex. Having reported the results for fermion Green's functions with complex masses, i.e. nonzero chiral phase, we proceed in Section 3 to derive correlation functions, starting with two-point functions in a theory with a single fermion. The correlation functions do not trivially coincide with the Green's functions because in the path integral, the sum over the number of individual instantons as well as the integral over their locations are yet to be carried out. We observe that for a given number of instantons with positive and negative winding numbers, chiral phases from the fermion determinant as well as from the θ-vacuum of the gauge theory multiply all structures—left and right chiral contributions as well as pieces corresponding to the homogeneous background between instantons—by the same factor. Because of the boundary conditions on the gauge field, the integration over the infinite spacetime volume must then be carried out for configurations with fixed total winding number. Thus, after the summations and integrations, the chiral phase of the mass term is aligned with the phase associated with the chirality-violating effects of the instantons. Analogously, when considering higher-point correlation functions in theories with several flavours and complex mass terms, the θ-angle drops out of the final result. In Section 4, we comment on the calculation of correlations beyond the fermionic two-point functions. Concluding remarks are left in Section 5.

2 Green's function for fermions in a one-instanton background in Minkowski space

2.1 Analytic continuation of the instanton solutions and fermion fluctuations between Euclidean and Minkowski space

We discuss here some generalities of the continuation of the instanton solution, the Dirac operator and its Green's function between Euclidean and Minkowski spacetime. For definiteness, we consider Dirac fermions in the fundamental representation in the background of SU(2) BPST (anti-)instantons. We construct the fermion Green's function by regulating the divergence from the fermion zero-mode by a mass term with a nonzero chiral phase. While such a phase can straightforwardly be inserted into the well-known results for the Green's function e.g. from Ref. [21], the explicit discussion of this matter serves us to introduce the general context as well as some notation.

In four-dimensional Euclidean space the BPST instanton with the collective coordinates for the location equal to zero and with winding number $\eta = -1$ is given in terms of the vector potential

$$A_m^{\mathrm{E}}(\vec{x}, x_4) = -\frac{\sigma_{mn}^{\mathrm{E}} x_n^{\mathrm{E}}}{(x^{\mathrm{E}})^2 + \varrho^2}\,, \tag{1}$$

and the expression for the $\eta = +1$, which is the parity conjugate of Eq. (1), is obtained when replacing $\sigma_{mn}^{\mathrm{E}} \to \bar{\sigma}_{mn}^{\mathrm{E}}$. We use the Euclidean tensors

$$\begin{aligned} \sigma_{mn}^{\mathrm{E}} &= \frac{1}{2}\left(\sigma_m^{\mathrm{E}} \bar{\sigma}_n^{\mathrm{E}} - \sigma_n^{\mathrm{E}} \bar{\sigma}_m^{\mathrm{E}}\right)\,, \qquad \sigma_m^{\mathrm{E}} = (\vec{\tau}, \mathrm{i}\mathbb{1})\,, \\ \bar{\sigma}_{mn}^{\mathrm{E}} &= \frac{1}{2}\left(\bar{\sigma}_m^{\mathrm{E}} \sigma_n^{\mathrm{E}} - \bar{\sigma}_n^{\mathrm{E}} \sigma_m^{\mathrm{E}}\right)\,, \qquad \bar{\sigma}_m^{\mathrm{E}} = (\vec{\tau}, -\mathrm{i}\mathbb{1})\,. \end{aligned} \tag{2}$$

Here we follow the notation of Ref. [23] where the generators for SU(2) are chosen as $T^a = \frac{\tau^a}{2\mathrm{i}}$, such that the covariant derivatives take the form $D_m^{\mathrm{E}} = \partial_m + A_m^{\mathrm{E}}$, different from taking $T^a = \frac{\tau^a}{2}$ and $D_m^{\mathrm{E}} = \partial_m - \mathrm{i}A_m^{\mathrm{E}}$, where τ^a are the Pauli matrices. Our Euclidean conventions are such that the coordinates are taken as

$$x_m^{\mathrm{E}} = \{\vec{x}, x_4\}\,, \tag{3}$$

and tensorial quantities are labelled with Latin indices $m, n\ldots$, taking values between 1 and 4. Contractions of indices are carried out through the metric δ_{mn}.

The Euclidean Dirac matrices are given by

$$\gamma_m^{\mathrm{E}} = \begin{pmatrix} 0 & -\mathrm{i}\sigma_m^{\mathrm{E}} \\ \mathrm{i}\bar{\sigma}_m^{\mathrm{E}} & 0 \end{pmatrix}\,. \tag{4}$$

The continuation of Euclidean time to an arbitrarily rotated time contour is parametrized as (cf. Ref. [15])

$$x_4 \to \mathrm{e}^{-\mathrm{i}(\vartheta - \frac{\pi}{2})} t\,, \tag{5}$$

where t is a real parameter. Then, for $\vartheta = \pi/2$, t is just Euclidean time whereas for $\vartheta = 0^+$, it corresponds to Minkowskian time. Here the infinitesimal 0^+ that regulates the continuation of the instanton configuration to Minkowski spacetime can be understood as a prescription to ensure that the path integration captures the transition amplitude from the true vacuum state onto itself [15]. We simply take 0^+ to be zero whenever it does not play a role. For a fixed value of ϑ characterizing a choice of time contour, we label the real coordinates of the (time-rotated) spacetime as

$$x^\mu = (x^0, \vec{x}) = (t, \vec{x})\,, \tag{6}$$

where Greek indices run from 0 to 3. With this parameterization, all equations of motion as well as their solutions do in general depend on ϑ. The ϑ-dependent instanton solutions for the gauge fields can be simply obtained by performing the substitution of Eq. (5) into Eq. (1) or the corresponding Euclidean solution for $\eta = +1$. In particular, the solutions in Minkowski spacetime are obtained when taking $\vartheta = 0^+$. In the following, we clarify when necessary whether we are referring to quantities for general ϑ or for a particular choice. For the remainder of this section we consider the continuation from Euclidean into Minkowski spacetime, maintaining a superscript "E" for Euclidean quantities, and omitting labels for their Minkowskian counterparts.

First, one should note that when recasting expressions in terms of Minkowskian metric tensors (e.g. $-\delta_{mn} \to \eta_{\mu\nu} \equiv \mathrm{diag}(1, -1, -1, -1)$) and Dirac matrices, it is natural to define the components A_μ of the Minkowski gauge field as:

$$A_0(x^0, \vec{x}) = \mathrm{i}A_4^{\mathrm{E}}(\vec{x}, x_4 = ix^0) \text{ and } A_i(x^0, \vec{x}) = A_i^{\mathrm{E}}(\vec{x}, x_4 = ix^0) \text{ for } i = 1, 2, 3\,. \tag{7}$$

When expressing $A_\mu = (-i\tau^a/2)A^a_\mu$, this implies however that the components A^a_μ when evaluated for the $\eta = -1$ instanton solution (Eq. (1)) continued to $\vartheta = 0^+$ are in general complex. Since the physical fields A^a_μ are however real, a deformation of the integration contour of the path integral is required in order to capture the analytically continued solution, which constitutes then a complex saddle point from which appropriate complex integration contours that lead to well-behaved integrands can be obtained by means of steepest-descent flows [11, 12]. In Ref. [15] it is derived how to evaluate the path integration of bosonic fluctuations on the deformed contours using Picard-Lefschetz theory, which would have to be applied here in order to deal with the fluctuations of the gauge field. The saddle point for the fermion field is still given by the vanishing field configuration, and the path integral of the Graßmannian fermion fluctuations can be carried out as usual.

In chiral representation the Dirac matrices for Minkowski spacetime are given by

$$\gamma^0 = \gamma^{\rm E}_4 \text{ and } \gamma^i = {\rm i}\gamma^{\rm E}_i \text{ for } i = 1, 2, 3\,. \tag{8}$$

Note that the form of γ^5 is the same for Euclidean and Minkowski space, and it is defined as $\gamma^5 = {\rm i}\gamma^0\gamma^1\gamma^2\gamma^3 = \gamma^{\rm E}_1\gamma^{\rm E}_2\gamma^{\rm E}_3\gamma^{\rm E}_4$. The Minkowskian Dirac operator is then obtained from the Euclidean one by performing the analytic continuation of Eq. (5) to $\vartheta = 0^+$:

$$\begin{aligned} \not{D}^{\rm E} = (\not{\partial}^{\rm E}_m + \gamma^{\rm E}_m A^{\rm E}_m) \to & \left(-{\rm i}\frac{\partial}{\partial x^0}\gamma^{\rm E}_4 + \vec{\gamma}^{\rm E}\cdot\nabla + \gamma^{\rm E}_4 A^{\rm E}_4(\vec{x}, x_4 = ix^0) + \vec{\gamma}^{\rm E}\cdot\vec{A}^{\rm E}(\vec{x}, x_4 = ix^0)\right) \\ = & -{\rm i}\left(\frac{\partial}{\partial x^0}\gamma^0 + \vec{\gamma}\cdot\nabla + \gamma^0 A_0(x^0, \vec{x}) + \vec{\gamma}\cdot\vec{A}(x^0, \vec{x})\right) = -{\rm i}\not{D}\,, \end{aligned} \tag{9}$$

where $\vec{\gamma}\cdot\nabla \equiv \sum_i \gamma^i\partial_i$ and accordingly for $\vec{\gamma}\cdot\vec{A}$. We can generalize this continuation such as to include a complex mass $m{\rm e}^{{\rm i}\alpha} \equiv m_{\rm R} + {\rm i}m_{\rm I}$, resulting in

$$\not{D}^{\rm E} + m_{\rm R} + {\rm i}\gamma^5 m_{\rm I} \to -\left({\rm i}\not{D} - m_{\rm R} - {\rm i}\gamma^5 m_{\rm I}\right)\,. \tag{10}$$

On the right-hand side, we recover the standard Dirac operator for a massive fermion in Minkowski spacetime. It is a non-Hermitian operator leading to a Lagrangian term that is however Hermitian when sandwiched between $\bar{\psi} = \psi^\dagger\gamma^0$ and ψ and when A^a_μ is real. As noted above, the latter condition is not met for the complex saddle corresponding to the instanton.

When including a complex fermion mass, the Euclidean Green's function $S^{\rm E}(x^{\rm E}, x^{\rm E\prime})$ satisfies

$$(\not{D}^{\rm E} + m_{\rm R} + {\rm i}\gamma^5 m_{\rm I})S^{\rm E}(x^{\rm E}, x^{\rm E\prime}) = \delta^4(x^{\rm E} - x^{\rm E\prime})\,. \tag{11}$$

The most straightforward way of constructing it is from the spectral sum in the massless limit. It is constituted by the solutions to the eigenvalue problem

$$\not{D}^{\rm E}\hat{\psi}^{\rm E}_\lambda = \left(\not{\partial}^{\rm E} + \gamma^{\rm E}_m A^{\rm E}_m\right)\hat{\psi}^{\rm E}_\lambda = \lambda^{\rm E}\hat{\psi}^{\rm E}_\lambda\,, \tag{12}$$

as

$$S^{\rm E}(x^{\rm E}, x^{\rm E\prime}) = \sum\!\!\!\!\!\!\int_{\lambda^{\rm E}} \frac{\hat{\psi}^{\rm E}_\lambda(x^{\rm E})\hat{\psi}^{\rm E\dagger}_\lambda(x^{\rm E\prime})}{\lambda^{\rm E}}\,. \tag{13}$$

Since the Euclidean Dirac operator $\not{D}^{\rm E}$ is anti-Hermitian, its eigenfunctions can readily be assumed to be orthonormal and Eq. (11) be immediately verified. Yet, Eq. (13) is ill-defined because of the fermionic zero mode $\lambda^{\mathrm{E}} = 0$ in the instanton background. The Euclidean index theorem relates the winding number to the difference between the number of right-handed and left-handed zero modes. This gives one left-handed zero-mode for a $\eta = -1$ background, and a right-handed zero mode for $\eta = 1$. The former is given by

$$\psi^{\mathrm{E}}_{0\mathrm{L}}(x^{\mathrm{E}}) = \begin{pmatrix} \chi^{\mathrm{E}}_0(x^{\mathrm{E}}) \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{pmatrix}, \quad \text{where} \quad \chi^{\mathrm{E}}_0(x^{\mathrm{E}}) = \frac{\varrho u}{\pi\left[\varrho^2 + (x^{\mathrm{E}})^2\right]^{\frac{3}{2}}} \tag{14}$$

and u is a 2×2 antisymmetric matrix with a Weyl index α and an index b labelling the fundamental representation of SU(2), i.e. $u^{\alpha b} = \varepsilon^{\alpha b}$, with $\varepsilon^{12} = 1$. As anticipated the mode is left chiral, i.e. $P_{\mathrm{L}}\psi^{\mathrm{E}}_{0\mathrm{L}}(x^{\mathrm{E}}) = \psi^{\mathrm{E}}_{0\mathrm{L}}(x^{\mathrm{E}})$, where $P_{\mathrm{L,R}} = \frac{1\mp\gamma^5}{2}$ are the chiral projectors. The solution $\psi^{\mathrm{E}}_{0\mathrm{R}}$ in the $\eta = +1$ instanton background can be obtained by switching the chiral block in Eq. (14).

A small complex mass term can serve as a regulator of the zero-mode contribution to Eq. (13) because, for fermions in the fundamental representation of the gauge group in the $\eta = -1$ instanton background, one obtains at first order in perturbation theory [21]

$$S^{\mathrm{E}}(x^{\mathrm{E}}, x^{\mathrm{E}\prime}) = \frac{\hat\psi^{\mathrm{E}}_0(x^{\mathrm{E}})\hat\psi^{\mathrm{E}\dagger}_0(x^{\mathrm{E}\prime})}{m\mathrm{e}^{-\mathrm{i}\alpha}} + \sum_{\lambda^{\mathrm{E}}\neq 0}\!\!\!\!\!\!\int \frac{\hat\psi^{\mathrm{E}}_\lambda(x^{\mathrm{E}})\hat\psi^{\mathrm{E}\dagger}_\lambda(x^{\mathrm{E}\prime})}{\lambda^{\mathrm{E}}}\,. \tag{15}$$

From Eq. (10), it then follows that we may analytically continue this solution as

$$\mathrm{i}S(x, x') = S^{\mathrm{E}}(x^{\mathrm{E}}, x^{\mathrm{E}\prime})\big|_{x_4=\mathrm{i}x^0,\, x_4'=\mathrm{i}x'^0}\,, \tag{16}$$

where the dependence on $x^{(\prime)}$ is understood to refer to the components $x^{(\prime)0}$ and $\vec{x}^{(\prime)}$ of the corresponding four-vector $x^{(\prime)\mu}$ as in Eq. (6). This Minkowski-space Green's function approximately solves the equation

$$\left(\mathrm{i}\not{D} - m_{\mathrm{R}} - \mathrm{i}\gamma^5 m_{\mathrm{I}}\right)\mathrm{i}S(x, x') = \mathrm{i}\delta^4(x - x')\,. \tag{17}$$

The above equation can be obtained from an analytic continuation of Eq. (11), with the continuation of the delta function giving $\delta^4(x^{\mathrm{E}} - x^{\mathrm{E}\prime}) \to -\mathrm{i}\delta^4(x - x')$. (For example, one can start with the representation of $\delta(x)$ in terms of its Fourier-transform and analytically continue x away from the real line.) On the other hand, taking Eqs. (11) and (17) as the definitions of the Euclidean and Minkowskian Green's functions, respectively, one can infer from the path integral the following correspondence between the Green's functions and the fermion propagators in the one-instanton background:

$$S^{\mathrm{E}}(x^{\mathrm{E}}, x^{\mathrm{E}\prime}) = -\,\mathrm{i}\langle\psi^{\mathrm{E}}(x^{\mathrm{E}})\psi^{\mathrm{E}\dagger}(x^{\mathrm{E}\prime})\rangle, \qquad \mathrm{i}S(x, x') = \langle\psi(x)\bar\psi(x')\rangle\,. \tag{18}$$

Recalling that the mapping between Euclidean and Minkowskian fermion fields goes as $\psi^{\mathrm{E}}(\vec{x}, x_4 = \mathrm{i}x^0) = \psi(x^0, \vec{x})$, $\psi^{\mathrm{E}\dagger}(\vec{x}, x_4 = \mathrm{i}x^0) = \mathrm{i}\bar\psi(x^0, \vec{x})$ (see e.g. Ref. [24]), one can confirm that the Euclidean and Minkowskian Green's functions are indeed related by the analytic continuation of Eq. (16). Note however that, as it is elaborated upon in Section 2.4, it is not straightforward to show that this analytic continuation has a well-defined spectral representation in terms of (im)properly normalizable eigenfunctions of the Dirac operator in Minkowski spacetime [15].

Equations (15) and (16) show that a mass term with a complex phase can thus be perturbatively included in the leading contribution to the Green's function that corresponds to the Euclidean zero modes in the massless limit. Nonetheless, since the Euclidean Dirac operator for a massive fermion with a general chiral phase is not of definite Hermiticity, it remains of interest whether such a spectral sum in terms of orthonormal eigenfunctions is also possible for a complex mass term without resorting to perturbation theory around the massless configuration, which is what we discuss in the following section.

2.2 Complex fermion mass in Euclidean space

In this section we focus on the Euclidean operator in Eq. (10). The operator $\not{D}^{\rm E}+m e^{{\rm i}\alpha\gamma_5} = \not{D}^{\rm E}+m_{\rm R}+{\rm i}\gamma_5 m_{\rm I}$ has the following properties in certain simplified cases. For $m=0$, it is anti-Hermitian, while for $m_{\rm I}=0$, it is "γ^5-Hermitian", i.e.

$$\left(\not{D}^{\rm E}+m_{\rm R}\right)^\dagger = \gamma^5\left(\not{D}^{\rm E}+m_{\rm R}\right)\gamma^5\,. \tag{19}$$

When using the eigenmodes $\hat{\psi}^{\rm E}_\lambda$ from the massless problem (12) in the presence of a real mass, these still lead to eigenmodes with the eigenvalues

$$\left(\not{D}^{E}+m_{\rm R}\right)\hat{\psi}^{\rm E}_\lambda =(\lambda^{\rm E}+m_{\rm R})\hat{\psi}^{E}_\lambda\,, \tag{20a}$$

$$\left(\not{D}^{\rm E}+m_{\rm R}\right)\gamma^5\hat{\psi}^{\rm E}_\lambda =\gamma^5\left(-\not{D}^{\rm E}+m_{\rm R}\right)\hat{\psi}^{\rm E}_\lambda = (-\lambda^{\rm E}+m_{\rm R})\gamma^5\hat{\psi}^{\rm E}_\lambda\,. \tag{20b}$$

Hence, since the real mass term is proportional to the identity matrix in spinor space, a spectral sum can be computed in terms of the same basis vectors as for the massless case. Moreover, $\hat{\psi}^{\rm E}_\lambda$ and $\gamma^5\hat{\psi}^{\rm E}_\lambda$ are orthogonal for $\lambda^{\rm E}\neq 0$ because they correspond to different eigenvalues of the anti-Hermitian operator $\not{D}^{\rm E}$.

For a complex mass term, where in addition $m_{\rm I}\neq 0$, it it is less obvious that a spectral sum can be constructed in terms of the massless eigenmodes because the mass term is no longer simply proportional to an identity matrix in spinor space. Nonetheless, this can still be accomplished with an additional basis transformation among the pairs $\hat{\psi}^{\rm E}_\lambda$ and $\gamma^5\hat{\psi}^{\rm E}_\lambda$. To see this, we note that for a given pair of massless eigenmodes $\hat{\psi}^{\rm E}_\lambda$ and $\gamma^5\hat{\psi}^{\rm E}_\lambda$ ($\lambda^{\rm E}\neq 0$), the Dirac operator takes the matrix form (in terms of 2×2 blocks)

$$\left(\not{D}^{\rm E}+m_{\rm R}+{\rm i}\gamma^5 m_{\rm I}\right)\begin{pmatrix}\hat{\psi}^{\rm E}_\lambda\\ \gamma^5\hat{\psi}^{\rm E}_\lambda\end{pmatrix} = \begin{pmatrix}\lambda^{\rm E}+m_{\rm R} & {\rm i}m_{\rm I}\\ {\rm i}m_{\rm I} & -\lambda^{\rm E}+m_{\rm R}\end{pmatrix}\begin{pmatrix}\hat{\psi}^{\rm E}_\lambda\\ \gamma^5\hat{\psi}^{\rm E}_\lambda\end{pmatrix}. \tag{21}$$

The eigenvalues of this matrix are

$$\xi^{\rm E}_\pm(\lambda^{\rm E}) = m_{\rm R}\pm\sqrt{(\lambda^{\rm E})^2-m_{\rm I}^2} \tag{22}$$

and the normalized eigenvectors are

$$\psi^{\rm E}_{\xi\pm} = \frac{1}{\sqrt{2\lambda^{\rm E}}}\left(\frac{m_{\rm I}}{\sqrt{\lambda^{\rm E}\mp\sqrt{(\lambda^{\rm E})^2-m_{\rm I}^2}}}\hat{\psi}^{\rm E}_\lambda + {\rm i}\sqrt{\lambda^{\rm E}\mp\sqrt{(\lambda^{\rm E})^2-m_{\rm I}^2}}\gamma^5\hat{\psi}^{\rm E}_\lambda\right). \tag{23}$$

The spinors $\psi^{\rm E}_{\xi\pm}$ are pairwise orthogonal, which can be checked explicitly when making use of the fact that $\not{D}^{\rm E}$ is anti-Hermitian such that $\lambda^{\rm E}$ is purely imaginary. Since the zero mode is chiral, it is still an eigenfunction $\psi^{\rm E}_0\equiv\hat{\psi}^{\rm E}_0$ for the Dirac operator when a complex mass is added. Altogether, we still have an orthonormal system such that the Green's function in the $\eta=-1$ instanton background is given by

$$S^{\rm E}(x^{\rm E},x^{\rm E\prime}) = \frac{\psi^{\rm E}_0(x)\psi^{\rm E\dagger}_0(x^{\rm E\prime})}{m e^{-{\rm i}\alpha}} + \sum\!\!\!\!\!\!\!\int_{\lambda^{\rm E}/{\rm i}>0}\sum_\pm\frac{\psi^{\rm E}_{\xi\pm}(x^{\rm E})\psi^{\rm E\dagger}_{\xi\pm}(x^{\rm E\prime})}{\xi^{\rm E}_\pm}\,. \tag{24}$$

In addition, we note that $(\lambda^{\rm E})^2-m_{\rm I}^2<0$, such that the coefficients of $\hat{\psi}^{\rm E}_\lambda$ and $\gamma^5\hat{\psi}^{\rm E}_\lambda$ in Eq. (23) have the same phase. The basis transformation is thus orthogonal, up to an arbitrary overall phase. Hence, $\psi^{\rm E}_{\xi\pm}$ are also eigenvectors of the Hermitian conjugate operator

$$\left(\not{D}^{\rm E}+m_{\rm R}+{\rm i}\gamma^5 m_{\rm I}\right)^\dagger\left(\begin{array}{c}\hat\psi^{\rm E}_\lambda\\ \gamma^5\hat\psi^{\rm E}_\lambda\end{array}\right)=\left(\begin{array}{cc}-\lambda^{\rm E}+m_{\rm R} & -{\rm i}m_{\rm I}\\ -{\rm i}m_{\rm I} & \lambda^{\rm E}+m_{\rm R}\end{array}\right)\left(\begin{array}{c}\hat\psi^{\rm E}_\lambda\\ \gamma^5\hat\psi^{\rm E}_\lambda\end{array}\right) \tag{25}$$

with eigenvalues $(\xi^{\rm E}_\pm)^*$ because the above operator acts on the pair $\hat\psi^{\rm E}_\lambda$ and $\gamma^5\hat\psi^{\rm E}_\lambda$ as the complex conjugate of the operator in Eq. (21). (If the coefficients of $\hat\psi^{\rm E}_\lambda$ and $\gamma^5\hat\psi^{\rm E}_\lambda$ had not the same phase, the coefficients would have to be complex conjugated in order to obtain the eigenvectors of the complex conjugate matrix.)

The anomalous divergence of the chiral current can now be straightforwardly verified. We first note that

$$\begin{aligned}\partial^{\rm E}_m{\rm tr}\,\gamma^5\gamma^{\rm E}_m\psi^{\rm E}_{\xi\pm}(x^{\rm E})\psi^{\rm E\dagger}_{\xi\pm}(x^{\rm E}) =&{\rm tr}\Big\{\gamma^5\left[\left(\not{D}^{\rm E}+m{\rm e}^{{\rm i}\alpha\gamma^5}-\gamma^{\rm E}_m A^{\rm E}_m-m{\rm e}^{{\rm i}\alpha\gamma^5}\right)\psi^{\rm E}_{\xi\pm}(x^{\rm E})\right]\psi^{\rm E\dagger}_{\xi\pm}(x^{\rm E})\\ &-\gamma^5\psi^{\rm E}_{\xi\pm}(x^{\rm E})\left[\left(\not{D}^{\rm E}-m{\rm e}^{-{\rm i}\alpha\gamma^5}-\gamma^{\rm E}_m A^{\rm E}_m+m{\rm e}^{-{\rm i}\alpha\gamma^5}\right)\psi^{\rm E}_{\xi\pm}(x^{\rm E})\right]^\dagger\Big\}\\ =&{\rm tr}\left\{2\gamma^5\xi^{\rm E}_\pm\psi^{\rm E}_{\xi\pm}(x^{\rm E})\psi^{\rm E\dagger}_{\xi\pm}(x^{\rm E})-2\gamma^5 m{\rm e}^{{\rm i}\alpha\gamma^5}\psi^{\rm E}_{\xi\pm}(x^{\rm E})\psi^{\rm E\dagger}_{\xi\pm}(x^{\rm E})\right\},\end{aligned} \tag{26}$$

and that the according relation also holds for the zero mode $\psi^{\rm E}_0(x^{\rm E})$. The trace is understood to run over the spinor indices, and we have substituted the eigenvalues of the massive Dirac operator and its Hermitian conjugate as discussed above. Substituting this into Eq. (24), we indeed obtain

$$\begin{aligned}&\partial^{\rm E}_m{\rm tr}\,\gamma^5\gamma^{\rm E}_m S^{\rm E}(x^{\rm E},x^{\rm E})\\ =&2\psi^{\rm E\dagger}_0(x^{\rm E})\gamma^5\psi^{\rm E}_0(x^{\rm E})+\sum\!\!\!\!\!\!\!\int_{\lambda^{\rm E}/{\rm i}>0}\sum_\pm 2\psi^{\rm E\dagger}_{\xi\pm}(x^{\rm E})\gamma^5\psi^{\rm E}_{\xi\pm}(x^{\rm E})+2{\rm i}\langle\psi^{\rm E\dagger}(x^{\rm E})\gamma^5 m{\rm e}^{{\rm i}\alpha\gamma^5}\psi^{\rm E}(x^{\rm E})\rangle\,.\end{aligned} \tag{27}$$

We note that the second term on the right-hand side vanishes because the trace of γ^5 over the nonzero modes is not anomalous. The first term on the right gives the usual anomaly upon integration over spacetime and accounting for the unit norm of the zero modes: For a $\eta=\pm1$ background with a right (left)-handed zero mode, one gets a change of chirality by ±2 units. The last term in Eq. (27) reproduces the classical divergence of the current.

From the spectral decomposition we can also observe that the phase of the determinant of the operator $\not{D}^{\rm E}+m_{\rm R}+{\rm i}\gamma^5 m_{\rm I}$ is entirely determined by the zero modes of $\not{D}^{\rm E}$. For a $\eta=\pm1$ instanton background with a right(left)-handed zero mode one has

$$\begin{aligned}\det(-\not{D}^{\rm E}-m_{\rm R}-{\rm i}\gamma^5 m_{\rm I})=&\det(-\not{D}^{\rm E}-m{\rm e}^{{\rm i}\alpha\gamma_5})=-m{\rm e}^{{\rm i}\eta\alpha}\prod_{\lambda^{\rm E}/{\rm i}>0}\xi^{\rm E}_+(\lambda^{\rm E})\xi^{\rm E}_-(\lambda^{\rm E})\\ =&-m{\rm e}^{{\rm i}\eta\alpha}\prod_{\lambda^{\rm E}/{\rm i}>0}(m^2+|\lambda^{\rm E}|^2)\,,\end{aligned} \tag{28}$$

where we have used the fact that $\lambda^{\rm E}$ is purely imaginary. As a consequence, we can write

$$\det(-\not{D}^{\rm E}-m{\rm e}^{{\rm i}\alpha\gamma^5})=-{\rm e}^{{\rm i}\eta\alpha}|\det(-\not{D}^{\rm E}-m{\rm e}^{{\rm i}\alpha\gamma^5})|\,,\quad \eta=\pm1\,. \tag{29}$$

One can use the fact that the instanton and anti-instanton backgrounds are simply related by parity conjugation to prove that the determinants in both backgrounds are related by the substitution $\alpha\to-\alpha$. This is consistent with the phases in Eqs. (28) and (29).

Moreover, according to Eq. (28), $|\det(-\not{D}^{\rm E} - m e^{{\rm i}\alpha\gamma_5})|$ is independent of α, and thus it is identical for both backgrounds. A similar analysis can be done the operator $-\not{\partial}^{\rm E} - m_{\rm R} - {\rm i}\gamma^5 m_{\rm I}$. In this case, since the gauge-field background is trivial with zero winding number, according to the Atiyah–Singer index theorem the number of left zero modes for $\not{\partial}^{\rm E}$ must equal to the number of right zero modes, ending up with a vanishing chiral phase in the determinant:

$$\det(-\not{\partial}^{\rm E} - m e^{{\rm i}\alpha\gamma^5}) = |\det(-\not{\partial}^{\rm E} - m e^{{\rm i}\alpha\gamma^5})|\,. \tag{30}$$

In preparation for the extension of the spectral decomposition of the propagator (24) to arbitrary rotations of the time contour, we consider separately the Euclidean eigenfunctions belonging to the discrete and continuum spectrum and introduce associated notation and properties. The normalizable eigenfunctions belonging to the discrete spectrum are denoted as $\psi_n^{\rm E}$ and their eigenvalues as $\xi_n^{\rm E}$. These modes have a finite norm and are mutually orthogonal under the usual scalar product,

$$(\psi_m^{\rm E}, \psi_n^{\rm E}) = \int {\rm d}^4 x^{\rm E}\, \psi_m^{{\rm E}\dagger}(x^{\rm E})\psi_n^{\rm E}(x^{\rm E}) = \delta_{mn}\,. \tag{31}$$

In regards to the continuum spectrum, involving improperly normalizable eigenfunctions, it can be constructed from solutions which approach plane waves at $x_4 \to -\infty$, characterized by asymptotic momenta $k_m, m = 1, \ldots, 4$. We will thus denote the eigenfunctions as $\psi^{\rm E}_{\{k^{\rm E}\}} = \psi^{\rm E}_{\{\vec{k},k_4\}}$ and their eigenvalues as $\xi^{\rm E}_{\{k^{\rm E}\}} = \xi^{\rm E}_{\{\vec{k}.k_4\}}$. A difference with the work of Ref. [15], which focuses on differential operators in backgrounds invariant under spatial translations like a planar domain-wall, is that the continuum modes will not be given by a single plane wave for all x_4, due to the spatial inhomogeneity of the BPST instanton background. However, one can always choose a basis of modes approaching a single plane wave at $x_4 \to -\infty$ and given by a superposition of plane waves at $x_4 \to \infty$. Indeed, from the results in this section it follows that generic Euclidean modes $\psi_\xi^{\rm E}$ with eigenvalues $\xi^{\rm E}$ satisfy

$$\begin{aligned}(\not{D}^{\rm E} + m e^{{\rm i}\alpha\gamma^5})\psi_\xi^{\rm E}(x^{\rm E}) =& \xi^{\rm E}\psi_\xi^{\rm E}(x^{\rm E})\,,\\ (\not{D}^{\rm E} + m e^{{\rm i}\alpha\gamma^5})^\dagger\psi_\xi^{\rm E}(x^{\rm E}) =& (-\not{D}^{\rm E} + m e^{-{\rm i}\alpha\gamma^5})\psi_\xi^{\rm E}(x^{\rm E}) = (\xi^{\rm E})^*\psi_\xi^{\rm E}(x^{\rm E})\,,\end{aligned} \tag{32}$$

which gives

$$(\not{D}^{\rm E} + m e^{{\rm i}\alpha\gamma^5})(-\not{D}^{\rm E} + m e^{-{\rm i}\alpha\gamma^5})\psi_\xi^{\rm E} = |\xi^E|^2\psi_\xi^{\rm E} = (-(\partial_m + A_m^{\rm E})(\partial_m + A_m^{\rm E}) + m^2)\psi_\xi^{\rm E}\,. \tag{33}$$

Therefore the Euclidean eigenvalue problem implies

$$((\partial_m + A_m^{\rm E})(\partial_m + A_m^{\rm E}) - m^2 + |\xi^E|^2)\psi_\xi^{\rm E} = 0\,. \tag{34}$$

For a solution going asymptotically as a plane wave in the infinite Euclidean past—thus being improperly normalizable and belonging to the continuum spectrum—one has

$$\psi^{\rm E}_{\{k^{\rm E}\}} \sim e^{{\rm i}k_m x_m} \text{ as } x_4 \to -\infty\,, \tag{35}$$

and the Euclidean eigenvalues satisfy (using the fact that the instanton background $A_m^{\rm E}$ goes to zero at infinity)

$$|\xi^{\rm E}_{\{k^{\rm E}\}}|^2 = m^2 + k_m k_m\,. \tag{36}$$

As the background also goes to zero for $x_4 \to +\infty$, the solutions will tend to a superposition of plane waves with the same value of $k^2 = k_m k_m$, fixed in terms of $|\xi^{\rm E}_{\{k_m\}}|^2$ as above. In this sense, the eigenvalue equation is analogous to a wave-mechanical scattering problem. We expect that we can form a basis for the continuum spectrum by considering all possible plane waves at $x_4 \to -\infty$. As the solutions are eigenfunctions of a Hermitian operator, the $\psi^{\rm E}_{\{k_m\}}$ are orthogonal, and they can be normalized so that the norm is a delta function in k-space:

$$(\psi^{\rm E}_{\{k^{\rm E}\}}, \psi^{\rm E}_{\{k^{\rm E\prime}\}}) = \delta^4(k^{\rm E} - k^{\rm E\prime})\,. \tag{37}$$

In the massless limit, as discussed above the continuum eigenvalues must become purely imaginary. Denoting these massless eigenvalues as $\lambda^{\rm E}_{\{k_m\}}$ and using Eq. (36) in the massless limit, if follows that

$$\lambda^{\rm E}_{\{k^{\rm E}\}} = {\rm i}\sqrt{k_m k_m}\,. \tag{38}$$

Then, the results of Eq. (22) imply that the continuum Euclidean eigenvalues for a general complex mass have the form

$$\xi^{\rm E}_{\pm\{k^{\rm E}\}} = m_{\rm R} \pm {\rm i}\sqrt{k_m k_m + m_{\rm I}^2}\,. \tag{39}$$

2.3 Complex fermion mass for an arbitrary rotation of the time contour

In this section we generalize the spectral decomposition of the Euclidean propagator to the case of arbitrary rotations of the time contour, using the methods of Ref. [15] adapted to complex fermion fields in generic, rather than bosonic planar backgrounds. We use superscripts "ϑ" for objects defined for a general time contour. Under the analytic continuation of Eq. (5), the fermionic kinetic term of the Lagrangian involves the operator

$$-\not{D}^{\rm E} - m{\rm e}^{{\rm i}\alpha\gamma^5} \;\to\; {\rm i}\not{D}^{\vartheta} - m{\rm e}^{{\rm i}\alpha\gamma^5}\,, \qquad \not{D}^{\vartheta} \;=\; \gamma^{\vartheta\mu}(\partial_\mu + A^{\vartheta}_\mu(x))\,, \tag{40}$$

with the following γ-matrices and gauge field components:

$$\begin{aligned} \gamma^{\vartheta 0} &= {\rm e}^{{\rm i}\vartheta}\gamma^0\,, & \gamma^{\vartheta i} &= \gamma^i\,, \\ A^{\vartheta 0}(x^0,\vec{x}) &= {\rm i}{\rm e}^{-{\rm i}\vartheta}A^{\rm E}_4(\vec{x}, x_4 = {\rm i}{\rm e}^{-{\rm i}\vartheta}x^0)\,, & A^{\vartheta i}(x^0,\vec{x}) &= A^{\rm E}_i(\vec{x}, x_4 = {\rm i}{\rm e}^{-{\rm i}\vartheta}x^0)\,. \end{aligned} \tag{41}$$

Recall that x^0 is meant to be real, parameterizing the rotated time contour; one also has $\partial_\mu = \partial/\partial x^\mu$ with x^μ the components of the four-vector in Eq. (6). The matrices $\gamma^{\vartheta\mu}$, which have been defined in terms of their Minkowskian counterparts γ^μ, satisfy a Clifford algebra $\{\gamma^{\vartheta\mu}, \gamma^{\vartheta\nu}\} = g^{\vartheta\mu\nu}$, with the metric $g^{\vartheta\mu\nu} = {\rm diag}\{{\rm e}^{2{\rm i}\vartheta}, -1, -1, -1\}$. The latter coincides with the effective metric appearing in the kinetic terms for scalar fields for arbitrary ϑ in Ref. [15]. Note that here we are looking at the analytic continuation between the two operators in Eq. (40). When taking $\vartheta = \pi/2$, the $\gamma^{\vartheta\mu}$ do not render the Euclidean γ-matrices but differ from these by a factor of i. This is due to the signature $(+,-,-,-)$ used in Minkowski spacetime, as opposed to the positive signature in Euclidean spacetime. However ${\rm i}\not{D}^{\vartheta} - m{\rm e}^{{\rm i}\alpha\gamma^5}$ does return to $-\not{D}^{\rm E} - m{\rm e}^{{\rm i}\alpha\gamma^5}$ for $\vartheta = \pi/2$.

As in Ref. [15], one can construct (im)properly normalizable eigenfunctions for the differential operator for arbitrary ϑ by analytic continuation of the corresponding Euclidean eigenfunctions in the time variable and, for the continuum spectrum, additionally in the asymptotic parameter k_4. In order to obtain eigenfunctions ψ^{ϑ}_n in the discrete spectrum it suffices to perform the usual analytic continuation, for which one obtains same eigenvalues as in Euclidean space, safe for the minus sign that follows from Eq. (40) and the fact that the Euclidean eigenvalues were defined as corresponding to the operator $\not{D}^{\rm E}+m e^{{\rm i}\alpha\gamma^5}$:

$$\psi^\vartheta_n(x)=\psi^\vartheta_n(x^0,\vec{x})=\sqrt{{\rm i}e^{-{\rm i}\vartheta}}\,\psi^{\rm E}_n(\vec{x},x_4={\rm i}e^{-{\rm i}\vartheta}x^0)\,,\quad \xi^\vartheta_n=-\xi^{\rm E}_n\,,\quad \text{discrete spectrum.} \tag{42}$$

The factor of $\sqrt{{\rm i}e^{-{\rm i}\vartheta}}$ is taken to lie in the principal branch and is necessary to guarantee a unit norm, defined with an inner product that will be described below. For the continuum spectrum, in order to preserve the plane-wave behaviour at $t\to-\infty$, one needs to rotate the asymptotic parameter k_4, and as a result the continuum eigenvalues in Minkowski spacetime are ϑ-dependent:

$$\begin{aligned}&\psi^\vartheta_{\{k\}}(x)=\psi^\vartheta_{\{k^0,\vec{k}\}}(x^0,\vec{x})=\psi^{\rm E}_{\{\vec{k},-{\rm i}e^{{\rm i}\vartheta}k_0\}}(\vec{x},x_4={\rm i}e^{-{\rm i}\vartheta}x^0)\,,\quad \xi^\vartheta_{\{k^0,\vec{k}\}}=-\xi^{\rm E}_{\{\vec{k},-{\rm i}e^{{\rm i}\vartheta}k_0\}}\,,\\&\text{for the continuum spectrum.}\end{aligned} \tag{43}$$

In the following we denote a generic eigenfunction with eigenvalue ξ^ϑ—either in the discrete or continuum spectrum—as ψ^ϑ_ξ. It turns out that the eigenfunctions constructed as above are orthogonal and complete with respect to the following inner product,

$$(\psi^\vartheta_\xi,\psi^\vartheta_{\xi'})_\vartheta=\int {\rm d}^4x\,\tilde{\psi}^\vartheta_\xi(x)\,\psi^\vartheta_{\xi'}(x)\,, \tag{44}$$

with $\tilde{\psi}^\vartheta$ defined as

$$\begin{aligned}&\tilde{\psi}^\vartheta_n(x^0,\vec{x})=\sqrt{{\rm i}e^{-{\rm i}\vartheta}}\,(\psi^{\rm E}_n(\vec{x},x_4))^\dagger\Big|_{x_4={\rm i}e^{-{\rm i}\vartheta}x^0}={\rm i}e^{-{\rm i}\vartheta}\,(\psi^\vartheta_n(x^0,\vec{x}))^\dagger\Big|_{x^0\to-e^{-2{\rm i}\vartheta}x^0}\,,\\&\text{for the discrete spectrum,}\\&\tilde{\psi}^\vartheta_{\{k^0,\vec{k}\}}(x^0,\vec{x})=\left(\psi^{\rm E}_{\{\vec{k},k_4\}}(\vec{x},x_4)\right)^\dagger\Bigg|_{\substack{x_4={\rm i}e^{-{\rm i}\vartheta}x^0\\ k_4=-{\rm i}e^{{\rm i}\vartheta}k^0}}=\psi^\vartheta_{\{k^0,\vec{k}\}}(x^0,\vec{x})^\dagger\Bigg|_{\substack{x^0\to-e^{-2{\rm i}\vartheta}x^0\\ k^0\to-e^{2{\rm i}\vartheta}k^0}}\,,\\&\text{for the continuum spectrum.}\end{aligned} \tag{45}$$

We refer to this operation indicated by a tilde and to the associated inner product in Eq. (44) as *ϑ-adjoint* and *ϑ-adjoint inner product*, respectively. In Eq. (45), the dagger operation is to be understood assuming that the corresponding coordinates and asymptotic parameters are treated as real, i.e. $\psi^{\rm E}_{\{\vec{k},k_4\}}(\vec{x},x_4)^\dagger$ should be calculated assuming k_m,x_m are real, and the same goes for $k^0,\vec{k},x^0,\vec{x}$ when evaluating $\psi^\vartheta_n(x)^\dagger$. The last equalities in both lines of Eq. (45) follow from the fact that the transformations $x_0\to-e^{-2{\rm i}\vartheta}x^0,\ k_0\to-e^{2{\rm i}\vartheta}k^0$ undo the complex conjugation of the combinations ${\rm i}e^{-{\rm i}\theta}x^0,-{\rm i}e^{{\rm i}\theta}k^0$ corresponding to the Euclidean variables x_4,k_4. A consequence of the above definition is that both ψ^ϑ and $\tilde{\psi}^\vartheta$ are holomorphic functions of x^0 and k^0. Then one can prove orthogonality and completeness of the ϑ eigenfunctions constructed as above by relating all integrals over the parameters x^0,k^0 to their Euclidean counterparts x_4,k_4 using the Cauchy theorem [15]. In particular, the discrete modes have the normalization

$$(\psi^\vartheta_m,\psi^\vartheta_n)_\vartheta=\delta_{mn}\,, \tag{46}$$

where as advertised earlier the prefactors $\sqrt{{\rm i}e^{-{\rm i}\vartheta}}$ in Eqs. (42) and Eq. (45) cancel the Jacobian from the rotation of the contour to the Euclidean time. On the other hand, for the eigenfunctions in the continuum one has

$$(\psi^\vartheta_{\{k\}},\psi^\vartheta_{\{k'\}})_\vartheta=\delta^4(k-k')\,, \tag{47}$$

where in this case the Jacobian from the rotation to Euclidean time is cancelled by the the one arising from the analytic continuation of the Euclidean delta function of the asymptotic momenta.

Proceeding along these lines, and as explained in detail in Ref. [15], the orthogonality and completeness of the basis of eigenfunctions for arbitrary ϑ follow from the analogous properties of the Euclidean spectrum. The former implies that one can resolve the operator $\mathrm{i}\not{D}^\vartheta - m e^{\mathrm{i}\alpha\gamma^5}$ in terms of orthogonal projectors,

$$\mathrm{i}\not{D}^\vartheta - m e^{\mathrm{i}\alpha\gamma^5} = \sum\!\!\!\!\!\!\!\int_{\xi^\vartheta} \xi^\vartheta \psi^\vartheta_\xi(x)\tilde{\psi}^\vartheta_\xi(x') = \sum_n \xi^\vartheta_n\, \psi^\vartheta_n(x)\tilde{\psi}^\vartheta_n(x') + \int \mathrm{d}^4k\, \xi^\vartheta_{\{k\}}\psi^\vartheta_{\{k\}}(x)\tilde{\psi}^\vartheta_{\{k\}}(x')\,, \tag{48}$$

and thus its inverse, i.e. the propagator, is given by

$$\begin{aligned} S^\vartheta(x,x') \equiv (\mathrm{i}\not{D}^\vartheta - m e^{\mathrm{i}\alpha\gamma_5})^{-1}(x,x') &= \sum\!\!\!\!\!\!\!\int_{\xi^\vartheta} \frac{1}{\xi^\vartheta}\, \psi^\vartheta_\xi(x)\tilde{\psi}^\vartheta_\xi(x') \\ &= \sum_n \frac{1}{\xi^\vartheta_n}\, \psi^\vartheta_n(x)\tilde{\psi}^\vartheta_n(x') + \int \mathrm{d}^4k\, \frac{1}{\xi^\vartheta_{\{k\}}}\psi^\vartheta_{\{k\}}(x)\tilde{\psi}^\vartheta_{\{k\}}(x')\,. \end{aligned} \tag{49}$$

The above propagator is nothing but the analytic continuation of its Euclidean counterpart, up to an overall constant:

$$S^\vartheta(x,x') = -\mathrm{i}e^{-\mathrm{i}\vartheta} S^{\mathrm{E}}(x^{\mathrm{E}}, x^{\mathrm{E}\prime})|_{x_4\to \mathrm{i}e^{-\mathrm{i}\vartheta}x^0,\, x_4'\to \mathrm{i}e^{-\mathrm{i}\vartheta}x'^0}\,, \tag{50}$$

The overall minus in Eq. (50) arises as a result of Eq. (40) (or equivalently from the minus signs in the relations between rotated and Euclidean eigenvalues in Eqs. (42) and (43)). The constant $\mathrm{i}e^{-\mathrm{i}\vartheta}$ appears in the contribution from the discrete spectrum due to the different normalization of the modes, see Eqs. (42) and (45), while for the continuum spectrum the same factor arises when relating the integral over the rotated k^0 to its Euclidean counterpart $k_4 = -\mathrm{i}e^{\mathrm{i}\vartheta}k^0$. Note that for $\vartheta = \pi/2$ one recovers the Euclidean result up to a minus sign, arising because the propagator $S^{\vartheta=\pi/2}$ is the inverse of $\not{D}^{\vartheta=\frac{\pi}{2}} - m e^{\mathrm{i}\alpha\gamma^5} = -\not{D}^{\mathrm{E}} - m e^{\mathrm{i}\alpha\gamma^5}$. For $\vartheta = 0^+$, one recovers the relation (16).

As an explicit application of the previous construction for $\vartheta = 0$, in Appendix A we use a spectral sum involving the ϑ-adjoint inner product to derive the free Minkowskian propagator for a fermion with a complex mass term.

2.4 Complex fermion mass in Minkowski spacetime

The results of the previous section can be applied to Minkowski spacetime by taking the limit $\vartheta \to 0^+$. Throughout this section, unless specified otherwise all objects are assumed to be defined in Minkowski spacetime. The relevant differential operator,

$$\mathrm{i}\not{D} - m_{\mathrm{R}} - \mathrm{i}\gamma^5 m_{\mathrm{I}}\,, \tag{51}$$

is Hermitian when evaluated in a background of real A^a_μ and multiplied by γ^0. This may suggest that for such real backgrounds one could define an inner product involving Dirac adjoint spinors rather than the inner product of Eq. (44) defined in terms of the ϑ-adjoint spinors introduced in Eq. (45). For the Dirac adjoint inner product the operator $\mathrm{i}\not{D} - m_{\mathrm{R}} - \mathrm{i}\gamma^5 m_{\mathrm{I}}$ would remain Hermitian, and one would naively expect orthogonal eigenvectors with real eigenvalues, giving a spectral decomposition of the propagator in terms of projectors of the form $\psi_\xi\bar{\psi}_\xi$. However, this is not the case because the Dirac adjoint inner product is not positive definite, and thus the $\psi_\xi\bar{\psi}_\xi$ operators do not behave as projectors. This is best illustrated by considering the case of the free Minkowskian propagator, which is studied in Appendix A; as shown there, when using the Dirac adjoint inner product the eigenfunctions have zero norm and are not orthogonal, while using the ϑ-adjoint inner product one recovers normalizability, orthogonality and completeness, and the usual propagator is recovered from the spectral sum of the tilde projectors. Finally, one could think of defining a propagator from the Hermitian operator $\gamma^0(\mathrm{i}\not{D}-m_\mathrm{R}-\mathrm{i}\gamma^5 m_\mathrm{I})$, but this plays no role for S-matrix elements, which are constructed from Green's functions involving products of spinors ψ, $\bar{\psi}$ and thus defined in terms of the inverse of the operator in Eq. (51). In any case, in the Minkowskian instanton background the background fields A^a_μ are not real, so that Hermiticity cannot be a guiding principle for the choice of operator or inner product.

From the results of the previous sections we therefore infer a spectral decomposition for the Minkowskian Dirac operator and its associated propagator,

$$\left(\mathrm{i}\not{D}-m_\mathrm{R}-\mathrm{i}\gamma^5 m_\mathrm{I}\right)_{x,x'}=\sum\!\!\!\!\!\!\!\int_\xi \xi\psi_\xi(x)\tilde{\psi}_\xi(x')\,,\qquad \mathrm{i}S(x,x')=\mathrm{i}\sum\!\!\!\!\!\!\!\int_\xi \frac{\psi_\xi(x)\tilde{\psi}_\xi(x')}{\xi}\,. \tag{52}$$

An explicit discussion of the analytic continuation of the continuum spectrum of fermionic and bosonic excitations about instantons would be of interest in the future. To this end, we only comment on the fermion zero-mode, that is normalizable in the proper sense and accountable for the effects from the chiral anomaly. By "zero mode" we refer to eigenstates with zero eigenvalue of the *massless* Dirac operator. As these modes have well-defined chirality, they are also eigenstates of the general Dirac operator with a complex mass, with eigenvalue $\xi_{0\mathrm{R}}=-m\mathrm{e}^{\mathrm{i}\alpha}$ for right-handed modes, and $\xi_{0\mathrm{L}}=-m\mathrm{e}^{-\mathrm{i}\alpha}$ for left-handed ones. As follows from the results of the previous section, these discrete zero modes are obtained by analytically continuing the corresponding Euclidean solutions. Then, as in Euclidean spacetime, this gives one right-handed zero-mode for a $\eta=1$ background, and a left-handed zero mode for $\eta=-1$. Applying Eq. (42) to the Euclidean expression of Eq. (14) for the zero mode in the $\eta=-1$ background gives

$$\psi_{0\mathrm{L}}(x^0,\vec{x})\equiv\sqrt{\mathrm{i}}\,\varphi_{0\mathrm{L}}(x^0,\vec{x})=\sqrt{\mathrm{i}}\,\psi^\mathrm{E}_{0\mathrm{L}}(\vec{x},\mathrm{i}x^0)\,, \tag{53}$$

with

$$\varphi_{0\mathrm{L}}(x)=\begin{pmatrix}\chi_0(x)\\ \begin{pmatrix}0\\0\end{pmatrix}\end{pmatrix}\,,\qquad \chi_0(x)=\frac{\varrho u}{\pi(\varrho^2-x^2)^{\frac{3}{2}}}\,, \tag{54}$$

where u is defined below Eq. (14). The zero mode satisfies the property

$$\tilde{\psi}_{0\mathrm{L}}(x)=\sqrt{\mathrm{i}}\,(\varphi_{0\mathrm{L}}(x))^\dagger\,, \tag{55}$$

as follows from the definition of the ϑ-adjoint operation in Eq. (45) and the invariance of $\varphi^\dagger_{0\mathrm{L}}(x)$ under time reflections, as can be readily seen from Eq. (54).

Hence the spectral decomposition of the propagator in Eq. (52) features a contribution involving $\varphi_{0\mathrm{L}}(\varphi_{0\mathrm{L}})^\dagger$. Note that this structure indicates anomalous violation of chirality, as it should, which would not be the case if the spectral decomposition were constructed with the Dirac adjoint inner product. Such construction, which was discarded in the previous section, would involve terms of the form $\varphi_{0\mathrm{L}}\overline{\varphi}_{0\mathrm{L}}$.

Assuming that the zero mode dominates the contributions to the Green's function in the $\eta = -1$ instanton background close to its centre x_0, we thus arrive at the approximation

$$\begin{aligned} \mathrm{i}S(x,x') &= \mathrm{i}S_{\rm cont}(x,x') + \frac{\varphi_{0\rm L}(x-x_0)\,\varphi^\dagger_{0\rm L}(x'-x_0)}{m\mathrm{e}^{-\mathrm{i}\alpha}} \\ &\approx \mathrm{i}S_{0\rm inst}(x,x') + \frac{\varphi_{0\rm L}(x-x_0)\,\varphi^\dagger_{0\rm L}(x'-x_0)}{m\mathrm{e}^{-\mathrm{i}\alpha}}\,, \end{aligned} \tag{56}$$

which captures the dominant contributions from both close to the centre and far away from it. Here, $\mathrm{i}S_{\rm cont}(x,x')$ is the contribution from the continuum spectrum and

$$\mathrm{i}S_{0\rm inst}(x,x') = (-\gamma^\mu\partial_\mu + \mathrm{i}m\mathrm{e}^{-\mathrm{i}\alpha\gamma^5})\int\frac{\mathrm{d}^4p}{(2\pi)^4}\mathrm{e}^{-\mathrm{i}p(x-x')}\frac{1}{p^2-m^2+\mathrm{i}\epsilon} \tag{57}$$

is the propagator in the trivial background with vanishing gauge fields, whose derivation from a spectral decomposition involving the ϑ-adjoint inner product is presented in Appendix A. Furthermore, we have explicitly inserted the dependence on the translational coordinates x_0 of the instanton. Noting that $\mathrm{i}S_{0\rm inst}$ has a spectral decomposition purely in terms of continuum modes and that $\mathrm{i}S_{0\rm inst}(x,x') \approx \mathrm{i}S(x,x')$ for $|x^2|,|x'^2| \gg \rho^2$ is an approximation to the Green's function in the instanton background that is valid at large distances from the centre of the instanton, explains the last equality in Eq. (56). In Eq. (57), we have chosen the ϵ-prescription corresponding to the Feynman propagator, while of course also other boundary conditions are of interest, e.g. in view of applications within the Schwinger-Keldysh formalism. The Fourier integral can be straightforwardly evaluated, while the explicit result is not relevant to this end.

The propagator in the $\eta = +1$ instanton background follows from the $\eta = -1$ case by switching the chiral block of the zero mode in Eq. (54), using the resulting right-handed zero mode $\varphi_{0\rm R}$ in place of $\varphi_{0\rm L}$ in Eq. (56), and replacing $\alpha \to -\alpha$. For a background consisting of a dilute gas of n instantons and $\bar n$ anti-instantons with centres $x_{0,\nu}, x_{0,\bar\nu}$, the propagator can be approximated again by the ordinary contribution plus a sum over the zero-mode contributions of the instantons and anti-instantons:

$$\begin{aligned} \mathrm{i}S_{n,\bar n}(x,x') \approx \mathrm{i}S_{0\rm inst}(x,x') &+ \sum_{\bar\nu=1}^{\bar n}\frac{\varphi_{0\rm L}(x-x_{0,\bar\nu})\varphi^\dagger_{0\rm L}(x'-x_{0,\bar\nu})}{m\mathrm{e}^{-\mathrm{i}\alpha}} \\ &+ \sum_{\nu=1}^{n}\frac{\varphi_{0\rm R}(x-x_{0,\nu})\varphi^\dagger_{0\rm R}(x'-x_{0,\nu})}{m\mathrm{e}^{\mathrm{i}\alpha}}\,. \end{aligned} \tag{58}$$

To end this section, we may note that, using the results of Ref. [15], the determinant of the Minkowski-space operator $\mathrm{i}\not{D} - m_{\rm R} - \mathrm{i}\gamma^5 m_{\rm I}$ can be obtained from the Euclidean result of Eq. (29) by analytic continuation of the time interval $T^{\rm E} \to \mathrm{i}T$ (with $T^{\rm E}$ and T referring to the Euclidean and Minkowskian time intervals of the spacetime volume $VT^{\rm E}$ and VT, respectively),

$$\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5}) = \det(-\not{D}^{\rm E} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\big|_{T^{\rm E}\to\mathrm{i}T}\,. \tag{59}$$

Actually, in physical quantities it is the ratio $\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})/\det(\mathrm{i}\not\partial - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})$ (and the corresponding one in Euclidean space) that enters. And it turns out that for such ratios the T-dependence cancels out. It is shown in Ref. [15] that the T-dependence appears only in the integral over the collective time-coordinate of the instanton which originates from the time-translational zero mode of the gauge-field fluctuations in our case (see Eqs. (68), (69) below). Therefore we simply have

$$\frac{\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}{\det(\mathrm{i}\not\partial - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})} = \frac{\det(-\not{D}^{\rm E} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}{\det(-\not\partial^{\rm E} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}\,. \tag{60}$$

This means, in particular, that the only dependence on the chiral phase α is again coming from the zero modes of $\not{D}^{\mathrm{E}}$ alone. We therefore define

$$\frac{\det(\mathrm{i}\not{D}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}{\det(\mathrm{i}\not{\partial}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}\equiv-\mathrm{e}^{\mathrm{i}\eta\alpha}\Theta\,,\qquad \Theta=\left|\frac{\det(\mathrm{i}\not{D}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}{\det(\mathrm{i}\not{\partial}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}\right|=\left|\frac{\det(-\not{D}^{\mathrm{E}}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}{\det(-\not{\partial}^{\mathrm{E}}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}\right|\,, \tag{61}$$

where Θ is a positive real number. As follows from the discussion in Section 2.2, Θ is the same for both instantons and anti-instantons, hence the omission of a label indicating η.

3 Correlation functions for fermions

In this section we consider correlation functions for massive fermions with chiral phases, working directly in Minkowski spacetime. We first derive the two-point correlator in a theory with a single fermion and after that, we generalize the result to the cases of multiple fermions and higher-order correlators.

For fluctuations about a given classical background—or about a saddle point on a certain complexified contour of path integration, the Green's function can be identified with the leading order approximation to the two-point correlation function. In the case of the vacuum of a non-Abelian gauge theory, the correlation function is to be computed by summing over contributions coming from fluctuations around backgrounds from different topological sectors, i.e. of different winding number. In a dilute instanton gas approximation, such backgrounds are described by configurations with all possible numbers of (anti-)instantons, with arbitrary locations in spacetime. The required summation can be carried out along the lines of Ref. [25], though here we will track explicitly the factors of spacetime volume, rather than using instanton densities (which may be phenomenologically more accurate). In a theory with a single massive Dirac fermion, the two-point correlation function is given by

$$\begin{aligned}\langle\psi(x)\bar\psi(x')\rangle=&\frac{1}{Z}\int\mathcal{D}A\mathcal{D}\bar\psi\mathcal{D}\psi\,\psi(x)\bar\psi(x)\mathrm{e}^{\mathrm{i}S}\,,\\ Z=&\int\mathcal{D}A\mathcal{D}\bar\psi\mathcal{D}\psi\,\mathrm{e}^{\mathrm{i}S}\,,\end{aligned} \tag{62}$$

where S is the Minkowskian action and Z the partition function. In order to relate this to the previously obtained Green's functions in a one-(anti-)instanton background, we denote the numbers of $\eta=-1$ and $\eta=1$ instantons in the spacetime volume VT under consideration by $\bar n$ and n, respectively.

The total winding number of a given background is $\Delta n=n-\bar n$, and consequently configurations with different values of Δn have different boundary conditions for the gauge field configuration. These therefore lead to separate contributions to the path integral. In order to add up these pieces to obtain the partition function or an observable, we need to take into account the fact that the vacuum state is a superposition of configurations with all topological charges or Chern–Simons numbers, i.e. (up to an irrelevant normalization factor)

$$|\mathrm{vac}\rangle=\sum_{n_{\mathrm{CS}}}|n_{\mathrm{CS}}\rangle\,. \tag{63}$$

Here, $|n_{\mathrm{CS}}\rangle$ is a state with a fixed Chern–Simons number. Note that the vacuum angle θ does not explicitly appear here since we choose to absorb it in the topological Lagrangian term $\theta F\tilde{F}/(16\pi^2)$, where F denotes the field strength tensor of the gauge field, $\tilde{F}$ its dual and θ is the vacuum angle of the gauge theory under consideration. It is easy to see that the following arguments do not rely on whether the phase is attributed to the state $|\mathrm{vac}\rangle$ or to the Lagrangian. We choose the latter option such as to simplify notation.

There are then distinct path integrals with different boundary conditions for each winding number $\Delta n = n - \bar{n}$ contained in the spacetime volume. This is because in regular gauge, the integral over the topological term is determined by the configuration of the gauge field at infinity, where the boundary conditions are imposed. It also implies that the individual contributions must be evaluated in the limit $VT \to \infty$, which turns out to be of substantial consequence. We therefore consider these pieces separately. First we have to specify the determinant of the Dirac operator in a general background with winding number $\Delta n = n - \bar{n}$. Naively one may write it as

$$\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})_{n,\bar{n}} = \left(\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\Big|_{\eta=1}\right)^n \left(\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\Big|_{\eta=-1}\right)^{\bar{n}} . \tag{64}$$

However, this would lead to an overcounting of the vacuum fluctuations from the domains of spacetime far away from instantons or anti-instantons, where we recall that e.g. the propagator reduces to its vacuum form in those regions, cf. Eq. (58). In order to count these fluctuations for the trivial background one time and one time only, instead of Eq. (64), the correct contribution is

$$\begin{aligned}
&\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})_{n,\bar{n}}\\
&= \det(\mathrm{i}\not{\partial} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5}) \left(\frac{\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}{\det(\mathrm{i}\not{\partial} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}\Bigg|_{\eta=1}\right)^n \left(\frac{\det(\mathrm{i}\not{D} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}{\det(\mathrm{i}\not{\partial} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})}\Bigg|_{\eta=-1}\right)^{\bar{n}}\\
&= |\det(-\not{\partial}^{\mathrm{E}} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})|\Big|_{T^{\mathrm{E}}\to\mathrm{i}T} \mathrm{e}^{-\mathrm{i}(\bar{n}-n)\alpha}(-\Theta)^{\bar{n}+n} ,
\end{aligned} \tag{65}$$

which can be seen to follow formally from Eq. (58) and where we have used Eqs. (30), (59), (61) and the fact that Θ is independent of the winding number η. Similarly for the functional determinant of the gauge and ghost fields, we have

$$\det{}'_{A_{n,\bar{n}}} = \det{}_{A=0}\left(\frac{\det'_A}{\det_{A=0}}\right)^{n+\bar{n}} , \tag{66}$$

where a prime on the determinant indicates that factors from zero eigenvalues have been deleted. Here $\det_A$ represents the functional determinant of the gauge and ghost fields in the one-instanton backgrounds. We have used that the determinants for $\eta = 1$ and $\eta = -1$ are identical, as can be seen to follow from the fact that the instanton and anti-instanton backgrounds are related by parity conjugation. For notational convenience, we define

$$\varpi \equiv \frac{1}{\sqrt{\det'_A/\det_{A=0}}} . \tag{67}$$

Then for a two-point fermionic correlation function, we have to evaluate the contributions

$$\begin{aligned}
\langle\psi(x)\bar{\psi}(x')\rangle_{\Delta n} &= \sum_m {}_{\mathrm{out}}\langle m+\Delta n|\psi(x)\bar{\psi}(x')|m\rangle_{\mathrm{in}} = \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \int \mathcal{D}A_{\bar{n},n}\mathcal{D}\bar{\psi}\mathcal{D}\psi\, \psi(x)\bar{\psi}(x')\mathrm{e}^{\mathrm{i}S_{\bar{n},n}}\\
&= \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!n!}\left(\prod_{\bar{\nu}=1}^{\bar{n}}\int_{VT} \mathrm{d}^4x_{0,\bar{\nu}}\mathrm{d}\Omega_{\bar{\nu}}J_{\bar{\nu}}\right)\left(\prod_{\nu=1}^{n}\int_{VT} \mathrm{d}^4x_{0,\nu}\mathrm{d}\Omega_{\nu}J_{\nu}\right)\mathrm{i}S(x,x')\\
&\times |\det(-\not{\partial}^{\mathrm{E}} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})|\Big|_{T^{\mathrm{E}}\to\mathrm{i}T}(\det{}_{A=0})^{-1/2}\\
&\times \mathrm{e}^{-S_{\mathrm{E}}(\bar{n}+n)}\mathrm{e}^{-\mathrm{i}(\bar{n}-n)(\alpha+\theta)}\varpi^{(\bar{n}+n)}(-\Theta)^{\bar{n}+n} .
\end{aligned} \tag{68}$$

Here, $|n\rangle_{\text{in/out}}$ are Heisenberg states at times $\mp T/2$, with well-defined Chern-Simons number, $\mathcal{D}A_{\bar{n},n}$ stands for the restriction of the path integrals to fluctuations about the configuration with $\bar{n}$ instantons with $\eta=-1$ and n with $\eta=+1$, and the classical Euclidean action is $S_{\rm E}=8\pi^2/g^2$ (before adding the topological term). Note that the classical action for the ϑ-dependent instanton solution is however ϑ-independent, i.e. $\mathrm{i}S[A^\vartheta]=-S^{\rm E}[A^{\rm E}]$, cf. Ref. [15]. This is also assumed for the topological contribution to the action. The collective coordinates corresponding to dilatational and gauge-orientation zero modes are integrated through $\mathrm{d}\Omega_{\bar{\nu},\nu}$, and $J_{\bar{\nu},\nu}$ are the Jacobians that arise when trading the zero modes for collective coordinates, which are derived for Euclidean space in Refs. [5, 26]. For the path integral in Minkowski spacetime, the Jacobians are purely imaginary because of the analytic continuation of the collective coordinate corresponding to time-translations [15]. Furthermore, all determinants are understood to be renormalized. In regards to the bosonic fluctuations, one can use here the results of Ref. [15], which show how the integral over the bosonic fluctuations on a thimble (i.e. an appropriately chosen contour for the bosonic path integral) about an analytically continued complex saddle, when the zero modes are separated, is related to the functional determinant evaluated at the corresponding Minkowskian saddle. The combinatorial factor $1/(\bar{n}!n!)$ is due to the fact that exchanging any two locations $x_{0,\bar{\nu}}$ or $x_{0,\nu}$ results in the same configuration. The contribution $Z_{\Delta n}$ from the configurations with Δn to the partition function, that is necessary for normalization, is computed as in Eq. (68), just with the factor $\psi(x)\bar{\psi}(x')$ deleted from the integrand:

$$
\begin{aligned}
Z_{\Delta n} =& \sum_m {}_{\rm out}\langle m+\Delta n|m\rangle_{\rm in} = \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \int \mathcal{D}A_{\bar{n},n}\mathcal{D}\bar{\psi}\mathcal{D}\psi\, \mathrm{e}^{\mathrm{i}S_{\bar{n},n}} \\
=& \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!n!}\left(-\textstyle\int \mathrm{d}\Omega\, J\, VT\,\Theta\,\varpi\,\mathrm{e}^{-S_{\rm E}}\right)^{(\bar{n}+n)} \left|\det(-\not{\partial}^{\rm E}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\right|\Big|_{T^{\rm E}\to\mathrm{i}T} \\
&\times(\det{}_{A=0})^{-1/2}\,\mathrm{e}^{-\mathrm{i}(\bar{n}-n)(\alpha+\theta)}\,.
\end{aligned}
\tag{69}
$$

Here, we have carried out the spacetime integrals over the instanton locations, resulting in powers of the spacetime volume. Since we are considering here real time, Δn can be interpreted as the net change in Chern-Simons number over the time T, i.e. each path integral associated with Δn corresponds to a transition between states with Chern-Simons number m and $m+\Delta n$, as suggested by the notation in the first line of Eq. (69). The factors $|\det(-\not{\partial}^{\rm E}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})|_{T^{\rm E}\to\mathrm{i}T}$ and $(\det_{A=0})^{-1/2}$ are common for all $Z_{\Delta n}$ and the correlation functions in backgrounds with any fixed Δn. They are thus total factors that cancel out in any physical quantities. To clean up notation, we will simply drop these factors below.

In order to evaluate the fermion correlation (68), we first notice that for dilute instantons in a fixed configuration, as discussed around Eq. (58), the correlation agrees with its form in the zero-instanton background almost everywhere, except near the locations of the anti-instantons and instantons.

Now for fixed x and x', each spacetime integral $\mathrm{d}x_{0,\bar{\nu}}$ and $\mathrm{d}x_{0,\nu}$ sweeps over the point $(x+x')/2$ once, thus leading to $\bar{n}$ contribution with $\eta=-1$ and n with $\eta=+1$. For a single of these integrals, e.g. for the location of a $\eta=-1$ instanton, this yields anomalous terms of the type

$$
\begin{aligned}
\int\limits_{VT}\mathrm{d}^4x_{0,\bar{\nu}}\;\mathrm{i}S(x,x') \approx& \int\limits_{VT}\mathrm{d}^4x_{0,\bar{\nu}}\left[\mathrm{i}S_{0\rm inst}(x,x')+\frac{\varphi_{0\rm L}(x-x_{0,\bar{\nu}})\varphi^\dagger_{0\rm L}(x'-x_{0,\bar{\nu}})}{m\mathrm{e}^{-\mathrm{i}\alpha}}+\cdots\right] \\
=& VT\left(\mathrm{i}S_{0\rm inst}(x,x')+\cdots\right)+m^{-1}\mathrm{e}^{\mathrm{i}\alpha}h(x,x')P_{\rm L}\,,
\end{aligned}
\tag{70}
$$

where the dots represent the contributions to the propagator from the zero modes of the (anti)-instantons whose centres were not integrated over (see Eq. (58)), and $h(x,x')$ is defined as a block-diagonal matrix (with two identical blocks) satisfying

$$h(x,x')P_{\mathrm{L}} = \int\limits_{VT} \mathrm{d}^4 x_{0,\bar\nu}\, \varphi_{0\mathrm{L}}(x-x_{0,\bar\nu})\varphi^\dagger_{0\mathrm{L}}(x'-x_{0,\bar\nu})\,, \tag{71}$$

$$h(x,x')P_{\mathrm{R}} = \int\limits_{VT} \mathrm{d}^4 x_{0,\bar\nu}\, \varphi_{0\mathrm{R}}(x-x_{0,\bar\nu})\varphi^\dagger_{0\mathrm{R}}(x'-x_{0,\bar\nu})\,. \tag{72}$$

Unfortunately, we do not find an analytic expression for this matrix-valued function that depends on the invariant distance $(x-x')^2$ only. Note though that this function is independent of VT as we take this spacetime volume to infinity. The overlap integral $h(x,x')$ as defined above depends on other collective coordinates of the instanton, e.g. the scale ρ. As such, insertions of $h(x,x')$ do not factor out of the integration over the collective coordinates. We choose then to approximate $h(x,x')$ by its average over the collective coordinates, defined as

$$\bar h(x,x') \equiv \frac{\int d\Omega\, h(x,x')}{\int d\Omega}. \tag{73}$$

This approximation allows to carry out all spacetime integrals over the instanton locations and collective coordinates. Neglecting contributions for which two or more of these locations coincide, the result is

$$\begin{aligned}
&\langle\psi(x)\bar\psi(x')\rangle_{\Delta n}\\
&=\sum_{\substack{\bar n,n\geq 0\\ n-\bar n=\Delta n}} \frac{1}{\bar n! n!}\Big[\bar h(x,x')\left(\frac{\bar n}{m\mathrm{e}^{-\mathrm{i}\alpha}}P_{\mathrm{L}}+\frac{n}{m\mathrm{e}^{\mathrm{i}\alpha}}P_{\mathrm{R}}\right)(VT)^{\bar n+n-1}+\mathrm{i}S_{0\mathrm{inst}}(x,x')\,(VT)^{\bar n+n}\Big]\\
&\times(\mathrm{i}\kappa)^{\bar n+n}(-1)^{n+\bar n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}\\
&=\left[\left(\mathrm{e}^{\mathrm{i}\alpha}I_{\Delta n+1}(2\mathrm{i}\kappa VT)P_{\mathrm{L}}+\mathrm{e}^{-\mathrm{i}\alpha}I_{\Delta n-1}(2\mathrm{i}\kappa VT)P_{\mathrm{R}}\right)\frac{\mathrm{i}\kappa}{m}\,\bar h(x,x')+I_{\Delta n}(2\mathrm{i}\kappa VT)\mathrm{i}S_{0\mathrm{inst}}(x,x')\right]\\
&\times(-1)^{\Delta n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}\,,
\end{aligned} \tag{74}$$

where

$$\mathrm{i}\kappa = \int\!\mathrm{d}\Omega\, J\ \Theta\, \varpi\, \mathrm{e}^{-S_{\mathrm{E}}}\,, \tag{75}$$

and $I_\alpha(x)$ is the modified Bessel function. Recall that the Jacobian J contains an imaginary factor i and that Θ is a positive real number so that κ is defined to be a positive number as well. Correspondingly, the contributions to the partition function are found to be

$$Z_{\Delta n} = I_{\Delta n}(2\mathrm{i}\kappa VT)\,(-1)^{\Delta n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}\,. \tag{76}$$

The total partition function, given by the transition amplitude from the vacuum $|\mathrm{vac}\rangle$ onto itself, is given by

$$Z = {}_{\mathrm{out}}\langle\mathrm{vac}|\mathrm{vac}\rangle_{\mathrm{in}} = \sum_{m,n} {}_{\mathrm{out}}\langle m|n\rangle_{\mathrm{in}} = \sum_{\Delta n=-\infty}^{\infty}\sum_m {}_{\mathrm{out}}\langle m+\Delta n|m\rangle_{\mathrm{in}} = \sum_{\Delta n=-\infty}^{\infty} Z_{\Delta n}. \tag{77}$$

Correspondingly, the fermion correlator in the vacuum (63) is given by

$$\langle\psi(x)\bar{\psi}(x')\rangle \equiv \frac{1}{Z}\,{}_{\rm out}\langle{\rm vac}|\psi(x)\bar{\psi}(x')|{\rm vac}\rangle_{\rm in} = \frac{\sum_{\Delta n=-\infty}^{\infty}\sum_n {}_{\rm out}\langle n+\Delta n|\psi(x)\bar{\psi}(x')|n\rangle_{\rm in}}{\sum_{\Delta n=-\infty}^{\infty} Z_{\Delta n}}$$
$$= \lim_{\substack{N\to\infty\\ N\in\mathbb{N}}}\lim_{VT\to\infty}\frac{\sum_{\Delta n=-N}^{N}\langle\psi(x)\bar{\psi}(x')\rangle_{\Delta n}}{\sum_{\Delta n=-N}^{N} Z_{\Delta n}} = {\rm i}S_{0{\rm inst}}(x,x') + {\rm i}\kappa\bar{h}(x,x')m^{-1}{\rm e}^{-{\rm i}\alpha\gamma^5}\,. \tag{78}$$

We have used here the limit $\lim_{x\to\infty} I_{\Delta n}({\rm i}x\,{\rm e}^{-{\rm i}0^+})/I_{\Delta n'}({\rm i}x\,{\rm e}^{-{\rm i}0^+}) = 1$. The factor ${\rm e}^{-{\rm i}0^+}$ is due to the rotation $T^{\rm E}\to {\rm i}{\rm e}^{-{\rm i}0^+}T$ so that the Jacobian J actually contains a factor of ${\rm i}{\rm e}^{-{\rm i}0^+}$. The limit however also holds for real positive arguments in the modified Bessel functions such that the steps presented here can also be applied in Euclidean space. Note that the fermion determinant contains a leading factor m that cancels with the explicit occurrence of m^{-1} and recall that the determinants in this expression are understood to be renormalized. The ordering of the limits follows from the fact that the winding numbers are only well-defined in the limit $VT\to\infty$. It is also of crucial relevance for the form of the final result because if we were not taking $VT\to\infty$ first, we would instead obtain

$$\sum_{\bar{n},n\geq 0}\frac{1}{\bar{n}!n!}\Big[\bar{h}(x,x')(\bar{n}\,m^{-1}{\rm e}^{{\rm i}\alpha}P_{\rm L} + n\,m^{-1}{\rm e}^{-{\rm i}\alpha}P_{\rm R})\,(VT)^{\bar{n}+n-1} + {\rm i}S_{0{\rm inst}}(x,x')\,(VT)^{\bar{n}+n}\Big]$$
$$\times(-{\rm i}\kappa)^{\bar{n}+n}{\rm e}^{{\rm i}\Delta n(\alpha+\theta)}$$
$$= \Big[-\Big({\rm e}^{-{\rm i}\theta}P_{\rm L} + {\rm e}^{{\rm i}\theta}P_{\rm R}\Big)\frac{{\rm i}\kappa}{m}\bar{h}(x,x') + {\rm i}S_{0{\rm inst}}(x,x')\Big]\,{\rm e}^{-2{\rm i}\kappa VT\cos(\alpha+\theta)}\,. \tag{79}$$

Analogously, taking the $VT\to\infty$ limit in the end, the total partition function would be

$$Z \to \sum_{n,\bar{n}}\frac{1}{n!\bar{n}!}(-{\rm i}\kappa VT)^{\bar{n}+n}{\rm e}^{-{\rm i}(\bar{n}-n)(\alpha+\theta)} = {\rm e}^{-2{\rm i}\kappa VT\cos(\alpha+\theta)}. \tag{80}$$

For the two-point function, we see that different phases are multiplying the left and right anomalous terms when compared to Eq. (78). One may notice here that in the limit $|\Delta n| \ll \bar{n}+n$, which gives the dominant contributions to the binomial distribution for $VT\to\infty$ [25], there are no relative chiral phases between the anomalous terms involving $\bar{h}$ and the term containing ${\rm i}S_{0{\rm inst}}(x,x')$. This would indicate that any CP-violating contribution from a background with $|\Delta n| \ll \bar{n}+n$, that can e.g. be measured by an observer in the same background, is suppressed by the volume. The fact that in Eq. (79) the CP-violation is enhanced follows from a cancellation of phases that is a consequence of the exchange of limits in Eq. (78). We comment on the relevance of the different phases appearing in Eqs. (78) and (79) in the following.

We observe that in Eq. (78) the chiral phase multiplying the anomalous term proportional to $\bar{h}$ is the same as the one that appears together with ${\rm i}S_{0{\rm inst}}$ (see Eq. (57)). Furthermore, the anomalous term has the expected exponential suppression compared to the contributions corresponding to regions that are not influenced by the instantons. As a consequence, this correlation function does not exhibit CP violation. The instanton effects are often approximated in terms of an effective operator [4, 5], which in our case, based on Eq. (78) reads

$$\mathcal{L}\to\mathcal{L} - \bar{\psi}(x)\Gamma{\rm e}^{{\rm i}\alpha\gamma^5}\psi(x)\,, \tag{81}$$

where at leading order in a gradient expansion Γ is a real number that can in principle be inferred from Eq. (78), in particular after an appropriate treatment of the dilatations, where the symmetry is broken radiatively. This corresponds to an effective mass with a chiral phase that is aligned with the one in the Dirac operator (10). Therefore, when using the operator (81) together with the Dirac mass in order to build an effective theory valid below the scale of chiral symmetry breaking, there is only one CP-odd phase that can be removed by a field redefinition. Consequently, the theory explains the absence of CP-violating observables, such as the vanishing permanent electric dipole moment of the neutron or the nonobservation of the decay of an η'-meson in two pions. This is to be compared with what one would infer from Eq. (79),

$$\mathcal{L} \to \mathcal{L} + \bar{\psi}(x)\Gamma \mathrm{e}^{-\mathrm{i}\theta\gamma^5}\psi(x)\,. \tag{82}$$

Here, the difference between the phase $-\theta$ and the phase α from a perturbative insertion of the mass m in a fermion line would indicate a CP-odd phase that cannot be removed by a field redefinition. We emphasize that for Eqs. (81) and (82), no assumption about the values of θ and α are made, which of course transform under chiral rotations of the fermion fields while leaving the sum $\alpha + \theta$ invariant. It should be noted that the phase in the operator in Eq. (81) is compatible with the following selection rule implied by the anomalous Ward identity: The theory should be invariant under a chiral transformation supplemented with changes in α, θ going as follows:

$$\psi \to \mathrm{e}^{\mathrm{i}\beta\gamma_5}\psi, \qquad \bar{\psi} \to \bar{\psi}\,\mathrm{e}^{\mathrm{i}\beta\gamma_5}, \qquad \alpha \to \alpha - 2\beta, \qquad \theta \to \theta + 2\beta, \tag{83}$$

where β is the parameter of the transformation. The previous selection rule is usually invoked as a justification of an effective operator involving the θ parameter as in Eq. (82); however, this is not the only possibility, and the result of (81) is equally compliant with the selection rule. We stress again that, given our results for the fermionic fluctuation determinants, our expressions capture the full dependence on the chiral angle α. It can also be observed that while Eq. (78) shows that the breaking of the axial U(1) symmetry due to the fermion mass is enhanced by the effect of the instantons in a way that is independent of the absolute value of the mass, this still leaves open the question of how the correlations and the low-energy effective theory behave in the massless limit.

The previous conclusions can be extended to correlation functions in theories with more fermion flavours. In a theory with N_f Dirac fermions ψ_j , $j = 1, \dots, N_f$, in the fundamental representation of the gauge group and with complex masses $m_j \mathrm{e}^{\mathrm{i}\alpha_j\gamma_5}$, one can consider correlation functions of the form

$$\langle\prod_{j=1}^{N}(\psi_{\sigma(j)}\bar{\psi}_{\sigma(j)})\rangle = \frac{1}{Z}\int \mathcal{D}A \prod_{k=1}^{N_f}\left(\mathcal{D}\bar{\psi}_k \mathcal{D}\psi_k\right)\prod_{j=1}^{N}(\psi_{\sigma(j)}\bar{\psi}_{\sigma(j)})\mathrm{e}^{\mathrm{i}S}\,, \tag{84}$$

where $\sigma = \{\sigma(1), \dots, \sigma(N)\}$ is a set containing N flavour indices (e.g. the list of all indices, a subset thereof, or other variants), and we have not specified spacetime indices or the different possible Lorentz contractions in order to simplify the notation. As before, we construct the correlation function by summing over contributions from topological sectors with fixed winding number Δn:

$$\begin{aligned}&\langle\prod_{j=1}^{N}(\psi_{\sigma(j)}\bar{\psi}_{\sigma(j)})\rangle_{\Delta n}\\ &= \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!n!}\left(\prod_{\bar{\nu}=1}^{\bar{n}}\int_{VT}\mathrm{d}^4x_{0,\bar{\nu}}\mathrm{d}\Omega_{\bar{\nu}}J_{\bar{\nu}}\right)\left(\prod_{\nu=1}^{\bar{n}}\int_{VT}\mathrm{d}^4x_{0,\nu}\mathrm{d}\Omega_{\nu}J_{\nu}\right)\prod_{j=1}^{N}\left(\mathrm{i}S_{\sigma(j)}\right)\\ &\times \mathrm{e}^{-S_{\mathrm{E}}(\bar{n}+n)}\mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)}\varpi^{(\bar{n}+n)}\,\bar{\Theta}^{(\bar{n}+n)}\,(-1)^{N_f(\bar{n}+n)}\,,\end{aligned} \tag{85}$$

where $\bar{\alpha}$ denotes the argument of the determinant of the fermionic mass matrix,

$$\bar{\alpha} = \sum_{j}^{N_f} \alpha_j \tag{86}$$

and

$$\bar{\Theta} = \prod_{j=1}^{N_f} \Theta_j \,, \tag{87}$$

where Θ_j is defined for each flavour in analogy with Eq. (61). Note that $\bar{\Theta}$ is also a positive real number.

The partition functions $Z_{\Delta n}$, on the other hand, are now given by

$$\begin{aligned} Z_{\Delta n} = &\sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!n!} \left(\textstyle\int \mathrm{d}\Omega\, J\, VT\, \bar{\Theta}\, \varpi\, \mathrm{e}^{-S_{\mathrm{E}}}\right)^{(\bar{n}+n)} (-1)^{N_f(\bar{n}+n)} \mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)} \\ \equiv &\sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!n!} (\mathrm{i}\kappa_{N_f} VT)^{\bar{n}+n} (-1)^{N_f\Delta n}\, \mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)} = I_{\Delta n}(2\mathrm{i}\kappa_{N_f} VT)\, (-1)^{N_f\Delta n}\, \mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)} \,, \end{aligned} \tag{88}$$

where we partly abbreviate the factors in the round bracket by $\mathrm{i}\kappa_{N_f}$.

Using propagators of the form of Eq. (58) and approximating nontrivial integrals over the translational coordinates $x_{0,\nu}, x_{0,\bar{\nu}}$ by their averages over the remaining collective coordinates, as in Eqs. (72), (73), we have the following types of contributions:

- terms with only propagators as in the zero-instanton background,
- "diagonal" terms, which are obtained by summing over terms in which all zero modes correspond to a common (anti-)instanton,
- "off-diagonal" contributions which mix zero modes from different (anti-)instantons.

For contributions with only propagators as in the zero-instanton background, the integrals over the centres are trivial and simply lead to $Z_{\Delta n} \prod_j \mathrm{i}S_{\sigma(j),0\mathrm{inst}}$, so that the ensuing contributions to the full correlator are simply given by products of these propagators. The "diagonal" contributions involve overlap integrals over varying numbers of zero-modes of a single (anti-)instanton. When summing over (anti-)instantons, one always gets a factor of n ($\bar{n}$), exactly as in the two-point function case analyzed before, resulting in contributions that go schematically as (for the case of instantons)

$$\begin{aligned} &\left(\prod_{m=1}^{p} \mathrm{i}S_{\sigma_p(m),0\mathrm{inst}}\right) \left(\prod_{j=1}^{q} m^{-1}_{\sigma_q(j)} \mathrm{e}^{-\mathrm{i}\alpha_{\sigma_q(j)}} P_{\mathrm{R}\sigma_q(j)}\right) \bar{h}_q \\ &\times \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{n}{\bar{n}!n!} (VT)^{\bar{n}+n-1} (\mathrm{i}\kappa_{N_f})^{\bar{n}+n} (-1)^{N_f\Delta n}\, \mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)} \\ &= \left(\prod_{m=1}^{p} \mathrm{i}S_{\sigma_p(m),0\mathrm{inst}}\right) \left(\prod_{j=1}^{q} m^{-1}_{\sigma_q(j)} \mathrm{e}^{-\mathrm{i}\alpha_{\sigma_q(j)}} P_{\mathrm{R}\sigma_q(j)}\right) \bar{h}_q \\ &\times (\mathrm{i}\kappa_{N_f})\, I_{\Delta n-1}(2\mathrm{i}\kappa_{N_f} VT)\, (-1)^{N_f\Delta n}\, \mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)} \,. \end{aligned}$$

In this equation $\sigma_{p/q} = \{\sigma_{p/q}(1), \ldots, \sigma_{p/q}(p/q)\}$ are subsets of the set σ defined above, with $p+q=N$, $\sigma_p \cup \sigma_q = \sigma$. $P_{\mathrm{R}\sigma_q(j)}$ are right-handed projectors for the flavour $\sigma_q(j)$, while $\bar{h}_q$ denotes a generalized tensor-valued overlap integral constructed from a product of q instanton zero-mode projectors, averaged over the collective coordinates of the instanton. As before, when computing contributions to the fermion correlation by taking the infinite volume limit, summing over Δn and dividing by the partition function, the phases proportional to $\bar{\alpha}+\theta$ drop out, and one ends up with contributions to the correlator of the form

$$\langle\prod_{j=1}^{N}(\psi_{\sigma(j)}\bar{\psi}_{\sigma(j)})\rangle \supset \left(\prod_{m=1}^{p} \mathrm{i}S_{\sigma_p(m),0\mathrm{inst}}\right)\left(\prod_{j=1}^{q} m^{-1}_{\sigma_q(j)}\mathrm{e}^{-\mathrm{i}\alpha_{\sigma_q(j)}}P_{\mathrm{R}\sigma_q(j)}\right)\bar{h}_q\,(\mathrm{i}\kappa_{N_f})\,. \tag{89}$$

As in the single-flavour case, all the phases of the correlators are determined by the chiral phases in the mass matrices, and similar results hold for the diagonal anti-instanton contributions. The contributions to the correlators can be captured by effective operators whose α_j-dependent phases are in accordance with the generalization of the selection rule of Eq. (83) for N_f flavours, which reads

$$\psi_j \to \mathrm{e}^{\mathrm{i}\beta\gamma_5}\psi_j, \qquad \bar{\psi}_j \to \bar{\psi}_j\,\mathrm{e}^{\mathrm{i}\beta\gamma_5}, \qquad \alpha_j \to \alpha_j - 2\beta, \qquad \theta \to \theta + 2N_f\beta\,. \tag{90}$$

In particular, the 't Hooft interactions with N_f flavours induced by (anti-)instantons correspond to diagonal contributions to correlators with $N=N_f$ pairs of fermions, $p=0$ and $q=N_f$, with the resulting effective vertices having the form

$$\mathcal{L} \to \mathcal{L} - \Gamma_{N_f}\mathrm{e}^{-\mathrm{i}\bar{\alpha}}\prod_{j=1}^{N_f}(\bar{\psi}_j P_{\mathrm{L}}\psi_j) - \Gamma_{N_f}\mathrm{e}^{\mathrm{i}\bar{\alpha}}\prod_{j=1}^{N_f}(\bar{\psi}_j P_{\mathrm{R}}\psi_j), \tag{91}$$

where at leading order in a gradient expansion the Γ_{N_f} are constant. Note how the dependence on the chiral phases is such that all of these can be removed by the same redefinitions that get rid of the phases in the tree-level mass terms. Once again, had we done the summation over Δn before taking the infinite volume limit, we would have obtained different phases, with $\bar{\alpha}$ replaced by $-\theta$. For these 't Hooft interactions, the $q=N_f$ factors of $m^{-1}_{\sigma_q(j)}$ in Eq. (89) are canceled with the factor of $\prod_{j=1}^{N_f} m_j$ associated with the fermionic zero modes implicit in $\kappa_{N_f} \propto \bar{\Theta}$. Diagonal correlators with $p=0$ but $N<N_f$ yield additional interaction vertices with fewer fermions, higher powers of m_i and phases compatible again with the selection rule, confirming the symmetry arguments put forth for example in the context of SU(2) instantons in Ref. [27]. Finally, the off-diagonal terms involve contributions to the fermionic propagators coming from different instantons. These can be classified according to the number of different (anti-)instantons involved and the number of propagators corresponding to each (anti-)instanton. Each class has an associated combinatorial factor for the number of terms in the class contained in the product of fermion propagators of the form of Eq. (58). For example, as we have seen, the diagonal class of single-(anti-)instanton contributions has an associated combinatorial factor of $n(\bar{n})$. Now for the off-diagonal term, suppose we consider a class where m different instantons are involved. This amounts to m combinations from a set of size n and gives a combinatorial factor $n!/(m!(n-m)!)$. In this case the integrals over the translational collective coordinates give now contributions proportional to

$$\begin{aligned}&\sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!m!(n-m)!}(VT)^{\bar{n}+n-m}(\mathrm{i}\kappa_{N_f})^{\bar{n}+n}(-1)^{N_f\Delta n}\mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)}\\ =&\frac{(\mathrm{i}\kappa_{N_f})^m}{m!}I_{\Delta n-m}(2\mathrm{i}\kappa_{N_f}VT)(-1)^{N_f\Delta n}\mathrm{e}^{\mathrm{i}\Delta n(\bar{\alpha}+\theta)}\,.\end{aligned} \tag{92}$$

Since $\kappa_{N_f} \propto \mathrm{e}^{-S_\mathrm{E}}$, we see that these contributions have a higher suppression factor and are expected to be subdominant. Nevertheless, taking the limit of $VT \to \infty$ before summing over Δn and dividing by the partition function, the dependence on θ drops from the corresponding contribution to the correlator. Analogous results hold for other contributions involving anti-instantons, or mixed instantons and anti-instantons: In general one obtains Bessel functions multiplied by extra factors of κ_{N_f} and inverse powers of VT. This makes the terms subleading but also in such a way that the θ-dependence disappears from the final contributions to the correlators.

4 More general correlation functions

The $2N_f$-point functions discussed in Section 3 correspond to expectation values of observables, up to their gauge-covariant nature and the fact that they transform under redefinitions of the fermion fields, in particular under chiral rotations of these. A gauge-invariant observable can be obtained e.g. by taking the trace of the gauge indices. We have obtained these correlations to tree-level accuracy in an expansion around multi-instanton backgrounds (based on additional approximations spelled out in Section 3). Here, we comment on how to obtain any correlation function in addition to the $2N_f$-point fermion correlation, where also loop corrections may be included.

For simplicity, we consider again the case of a single fermion flavour. To compute the expectation value of an observable $\mathcal{O}$ to some approximation, Eq. (68) generalizes to

$$
\begin{aligned}
\langle \mathcal{O}(z_1,\ldots,z_t)\rangle_{\Delta n} =& \sum_{\substack{\bar n,n\geq 0\\ n-\bar n=\Delta n}} \frac{1}{\bar n! n!}\left(\prod_{\bar\nu=1}^{\bar n}\int\limits_{VT} \mathrm{d}^4 x_{0,\bar\nu}\mathrm{d}\Omega_{\bar\nu} J_{\bar\nu}\right)\left(\prod_{\nu=1}^{n}\int\limits_{VT} \mathrm{d}^4 x_{0,\nu}\mathrm{d}\Omega_{\nu} J_{\nu}\right)\\
&\times \left|\det(-\partial\!\!\!/^{\mathrm{E}} - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\right|\Big|_{T^\mathrm{E}\to\mathrm{i}T} (\det{}_{A=0})^{-1/2}\, \mathrm{e}^{-S_\mathrm{E}(\bar n+n)}\varpi^{(\bar n+n)}(-\Theta)^{\bar n+n}\\
&\times \int \mathrm{d}^4 z'_1\cdots \mathrm{d}^4 z'_u \mathcal{F}\left(z'_1,\ldots,z'_u;z_1,\ldots,z_t\right)\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}\\
=& \sum_{\substack{\bar n,n\geq 0\\ n-\bar n=\Delta n}} \frac{1}{\bar n! n!}\int \mathrm{d}^4 z'_1\cdots \mathrm{d}^4 z'_u\\
&\Big[\left(\bar n\, \bar{\mathcal{G}}_{\bar 1}\left(z'_1,\ldots,z'_u;z_1,\ldots,z_t\right) + n\,\bar{\mathcal{G}}_1\left(z'_1,\ldots,z'_u;z_1,\ldots,z_t\right)\right)(VT)^{\bar n+n-1}\\
&+\mathcal{G}_{0\mathrm{inst}}\left(z'_1,\ldots,z'_u;z_1,\ldots,z_t\right)(VT)^{\bar n+n}\Big](\mathrm{i}\kappa)^{\bar n+n}(-1)^{n+\bar n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}\\
=& \int \mathrm{d}^4 z'_1\cdots \mathrm{d}^4 z'_u \left[\left(I_{\Delta n+1}(2\mathrm{i}\kappa VT)\bar{\mathcal{G}}_{\bar 1} + I_{\Delta n-1}(2\mathrm{i}\kappa VT)\bar{\mathcal{G}}_1\right)\mathrm{i}\kappa + I_{\Delta n}(2\mathrm{i}\kappa VT)\mathrm{i}\mathcal{G}_{0\mathrm{inst}}\right]\\
&\times(-1)^{\Delta n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}\,.
\end{aligned}
\tag{93}
$$

The function $\mathcal{F}$ can be represented by a sum of Feynman diagrams, i.e. as a sum of products of two-point Green's functions and their derivatives in the multi-instanton background. For the fermions, these Green's functions may be approximated by $\mathrm{i}S_{n,\bar n}$ given in Eq. (58), but other species, e.g. gauge bosons, can contribute as well. For these additional fields we assume that, in analogy to the fermionic propagators, their two-point functions can be approximated by the free contribution plus a sum over contributions peaking at the centres of each (anti-)instanton. Each of the two-point functions is evaluated at a given pair of the spacetime arguments of $\mathcal{F}$. (For gauge bosons and self-interacting scalars, these arguments may coincide according to the Feynman rules.) The integrations over the coordinates z'_i correspond to loop integrals. In the second step, we have carried out the integrations over the collective coordinates in analogy with Eq. (74). Organized in powers of VT, this defines the contributions $\mathcal{G}_{0\text{inst}}$ from the bulk of the spacetime volume where there are no instantons, as well as $\bar{\mathcal{G}}_1$ and $\bar{\mathcal{G}}_{\bar{1}}$ which are obtained for one instanton sweeping over $\mathcal{F}$. This gives $\bar{\mathcal{G}}_{\bar{1}/1}$ as generalized overlap integrals averaged over the collective coordinates Ω, involving products of free propagators times one or more contributions to two-point functions—either fermionic or bosonic—arising from a single (anti-)instanton. Contributions of lower order in VT, corresponding to more than one instanton sweeping over $\mathcal{F}$ at a time, are suppressed exponentially and have thus been omitted in Eq. (93). In the third step, we have carried out the summation and suppressed the spacetime arguments of $\mathcal{G}_{0\text{inst}}$, $\bar{\mathcal{G}}_1$ and $\bar{\mathcal{G}}_{\bar{1}}$. Note also that $\mathcal{O}$ in general has a spinor structure. In contrast to Eq. (74), for which this structure is presented, we do not explicitly show the chiral phases, which are $\mathrm{e}^{\pm \mathrm{i}\alpha}$ for left and right-chiral contributions, respectively, because the only phases in $\mathcal{G}_{0\text{inst}}$, $\bar{\mathcal{G}}_1$ and $\bar{\mathcal{G}}_{\bar{1}}$ can originate from the mass term.

In order to evaluate the expectation value by first taking $VT \to \infty$ and then summing over the topological sectors Δn, we note that the volume-dependence of the loop integrand can be isolated as

$$I_n(x) \sim \frac{\mathrm{e}^x}{\sqrt{2\pi x}} \quad \text{for} \quad |x| \to \infty \quad \text{and} \quad |\arg(x)| < \frac{\pi}{2}\,, \tag{94}$$

and we can apply the same arguments as in Section 3. (Recall that the time interval is to be understood as $Te^{-\mathrm{i}0^+}$, so that we can apply the asymptotic expansion of Eq. (94).) Taking limits in this order thus leads to

$$\begin{aligned}
&\langle \mathcal{O}(z_1,\ldots,z_t)\rangle \\
&= \lim_{\substack{N\to\infty \\ N\in\mathbb{N}}} \lim_{VT\to\infty} \frac{\sum_{\Delta n=-N}^{N} \langle \mathcal{O}(z_1,\ldots,z_t)\rangle_{\Delta n}}{\sum_{\Delta n=-N}^{N} Z_{\Delta n}} = \int \mathrm{d}^4 z_1' \cdots \mathrm{d}^4 z_u' \left[\bar{\mathcal{G}}_{\bar{1}} + \bar{\mathcal{G}}_1 + \mathcal{G}_{0\text{inst}}\right] .
\end{aligned} \tag{95}$$

Again, we observe that interferences from contributions from different topological sectors Δn cancel when normalizing with the partition function. The only phases for the terms in square bracket are $\mathrm{e}^{\pm \mathrm{i}\alpha}$, and they appear in accordance with the breaking of chiral symmetry by the mass term. However, unless additional CP-odd phases are introduced in the theory, the phase α can be removed by field redefinitions and is unobservable.

This cancellation does not hold when taking the limit $VT \to \infty$ after the summation over the topological sectors Δn, which leads to

$$\langle \mathcal{O}(z_1,\ldots,z_t)\rangle = \lim_{VT\to\infty} \lim_{\substack{N\to\infty \\ N\in\mathbb{N}}} \int \mathrm{d}^4 z_1' \cdots \mathrm{d}^4 z_u' \left[\bar{\mathcal{G}}_{\bar{1}} \mathrm{e}^{-\mathrm{i}(\theta+\alpha)} + \bar{\mathcal{G}}_1 \mathrm{e}^{\mathrm{i}(\theta+\alpha)} + \mathcal{G}_{0\text{inst}}\right] . \tag{96}$$

Here, in addition the phase $\theta + \alpha$ appears which is independent of field redefinitions, according to Eq. (83), and generally leads to CP-violating observables.

Under certain conditions, these general correlation functions can be obtained using the effective operators from Eqs. (81) and (82). To see this explicitly, we assume that the loop integrals are not ultraviolet sensitive in the sense that only contributions with $|(z_i' - z_j')^2| \gg \varrho^2$ are relevant. We can then assume the arguments of the Green's functions to be sufficiently separated such that we do not have to account for contributions where two of the Green's functions $\mathrm{i}S_{n,\bar{n}}$ are to be evaluated close to the same instanton. Recalling that $\mathcal{F}$ depends on the two-point fermionic Green's functions, we denote $\mathcal{F} = \mathcal{F}(\{\mathrm{i}S^{(i)}\}, \ldots)$ where the dots represents all other arguments. Furthermore, close to an (anti-)instanton we only collect the contributions from the corresponding fermionic zero-mode. In this case, within Eq. (93), we can identify

$$
\begin{aligned}
\mathcal{G}_0 =& \mathcal{F}(\{\mathrm{i}S^{(i)}\},...) \;\text{ where }\; \mathrm{i}S^{(i)} = \mathrm{i}S_{0\mathrm{inst}} \;\; \forall i\,, \\
\bar{\mathcal{G}}_{\bar{1}} =& \sum_j \mathcal{F}(\{\mathrm{i}S^{(i)}\},...) \text{ where } \mathrm{i}S^{(i)} = \frac{\bar{h}\,P_{\mathrm{L}}}{m\mathrm{e}^{-\mathrm{i}\alpha}} \;\text{ for } i=j \;\text{ and }\; \mathrm{i}S^{(i)} = \mathrm{i}S_{0\mathrm{inst}} \;\text{ for } i \neq j\,, \\
\bar{\mathcal{G}}_1 =& \sum_j \mathcal{F}(\{\mathrm{i}S^{(i)}\},...) \text{ where } \mathrm{i}S^{(i)} = \frac{\bar{h}\,P_{\mathrm{R}}}{m\mathrm{e}^{\mathrm{i}\alpha}} \;\text{ for } i=j \;\text{ and }\; \mathrm{i}S^{(i)} = \mathrm{i}S_{0\mathrm{inst}} \;\text{ for } i \neq j\,,
\end{aligned} \tag{97}
$$

where $\bar{h}$ is given in Eq. (73). Then, following Section 3, all anomalous contributions can be approximated to linear order in κ as

$$
\langle \mathcal{O}(z_1,\ldots,z_t)\rangle \approx \int \mathrm{d}^4 z_1' \cdots \mathrm{d}^4 z_u' \left[\mathcal{G}_0 + \mathcal{G}_1\right] . \tag{98}
$$

The term with $\mathcal{G}_0$ is just the contribution that would arise in a background without instantons, while the term with $\mathcal{G}_1$ represents the leading instanton-effects. When taking $VT \to \infty$ first, we are led to substitute

$$
\mathcal{G}_1 = \sum_j \mathcal{F}(\{\mathrm{i}S^{(i)}\},...) \text{ where } \mathrm{i}S^{(i)} = \frac{\mathrm{i}\kappa h}{m}\mathrm{e}^{-\mathrm{i}\alpha\gamma^5} \;\text{ for } i=j \;\text{ and }\; \mathrm{i}S^{(i)} = \mathrm{i}S_{0\mathrm{inst}} \;\text{ for } i \neq j\,, \tag{99}
$$

while, when summing over Δn first, we take

$$
\mathcal{G}_1 = \sum_j \mathcal{F}(\{\mathrm{i}S^{(i)}\},...) \text{ where } \mathrm{i}S^{(i)} = \frac{\mathrm{i}\kappa h}{m}\mathrm{e}^{\mathrm{i}\theta\gamma^5} \;\text{ for } i=j \;\text{ and }\; \mathrm{i}S^{(i)} = \mathrm{i}S_{0\mathrm{inst}} \;\text{ for } i \neq j\,. \tag{100}
$$

Now, we can indeed observe that the result (98) can be obtained by using effective operators of the form (81) or, respectively, of (82) to linear order. When aiming to go beyond linear order in κ, one should note however that any explicit dependence on θ can only enter via the global phases $\Delta n(\alpha+\theta)$ that appear for the path integrals over the individual topological sectors. When summing over Δn before taking $VT\to\infty$, the effective operator (82) can therefore be only used to linear order. Beyond linear order, one should go back to Eq. (93) as a starting point. The same applies when considering values of z_i that are not well separated, such that one cannot neglect contributions in which more than one Green's function are evaluated close to the same instanton. Similarly, using the 't Hooft vertices of Eqs. (91) in diagrams with ordinary propagators would only capture a restricted set of contributions of order κ in which N_f fermion propagators are evaluated close to the instanton. For higher-order in κ or for capturing contributions with more propagators close to the instanton, the use of the effective vertex cannot be justified.

While the construction of θ-vacua as in and out states requires the use of an infinite spacetime-volume, we note that nonetheless, topological sectors with fixed winding number Δn are well-defined within finite spacetimes with periodic boundary conditions [28]. The periodicity and finiteness remove the necessity of specifying vacuum boundary conditions of a certain Chern-Simons number. This precludes the interpretation of the path integral within a sector of fixed Δn as a transition amplitude between vacua with Chern-Simons numbers differing by Δn. Because of this, there is no principle (save for some correspondence with the infinite-volume limit) that requires certain weights for the contributions to the path integral from different Δn. We may note that the quantum equation of motions (that may also include an observer) are separately independent for each sector Δn in the periodic spacetime, i.e. Δn will appear fixed within each such sector. For an observer, it is possible to measure Δn e.g. through the correlation function (74). Interferences between the different sectors will therefore not be seen by observers defined through local quantum fields. Therefore, the predictions for the θ-vacuum in a boundless spacetime, where the limit $VT \to \infty$ is to be taken before the summation over Δn, coincide with what is seen in a large but finite periodic spacetime with $\Delta n = 0$. Under the finiteness assumption, the latter condition should be imposed in agreement with the observation that there is no spontaneous CP-violation, i.e. $\langle \Delta n \rangle = 0$ in the vacuum for any subvolume of physical spacetime.

5 Conclusions

This paper reports three main results. First, we show how the Green's function for a fermion in an instanton background can be constructed in terms of a spectral sum. While this is trivial e.g. for the case of a fermion with real mass in Euclidean space, the case with a complex mass as well as the Green's function in Minkowski spacetime require a more detailed discussion because the Dirac operator then does not have definite Hermiticity properties and the mass term is not proportional to an identity operator in spinor space. In Euclidean space, we find that the spectral sum can be constructed in terms of the eigenfunctions of the massless Dirac operator after an additional orthogonal transformation between the massless eigenvectors of opposite eigenvalues. Using the results of Ref. [15], we have argued that the spectral sum can also be carried out in Minkowski spacetime, despite the fact that the Dirac operator does not have definite Hermiticity even when multiplied by γ^0 because of the complex field configuration corresponding to the instanton saddle. The former results also allow us to explicitly verify that the Green's function has the correct structure that is expected from the anomalous violation of the chiral current.

The second main result is that the dependence of the determinant of the Dirac operator on the chiral phases of the fermion masses only arises from the contributions of the zero modes. This may be well-known and is immediately obvious when treating a complex mass term in Euclidean space as a perturbation to the massless limit. Here, we have shown explicitly that this also holds for the full spectrum of massive modes in Euclidean space and furthermore that this observation also holds when the spectrum is continued to Minkowski spacetime.

Finally, we have used the fermionic Green's function in an (anti)-instanton background in order to calculate correlation functions for fermions in multi-instanton backgrounds. For the case of the two-point function in a model with a single flavour, the result (78) shows that there is no relative phase between the mass term and the term associated with the anomalous violation of chiral symmetry. When the correlation function (78) is substituted for fermion lines in an expansion in terms of Feynman diagrams, no CP-violating results follow unless additional CP-odd phases are added to the theory. We have discussed that in order to arrive at Eq. (78), care has to be taken of the correct order of integrating over infinite volume and summing over the number of instantons up to infinity: The spacetime volume has to be taken to infinity for each path integral with boundary conditions determined by a fixed winding number Δn. The results for the two-point function have been extended to higher-order correlators in the presence of multiple flavours, where again the dependence on the θ-angle drops out of the final result, and the effective interactions associated with the correlators—including the usual 't Hooft interactions—end up depending on the chiral phases of the complex masses in a manner compatible with the selection rule imposed by the chiral anomaly. Again, CP violation does not ensue in the absence of additional CP-odd phases.

We emphasize that the results for the correlation functions presented here hold for massive fermions and leaves open the question of the behaviour in the massless case. The fact that taking the limit $m \to 0$ in e.g. Eq. (78) depends on the phase α requires further investigation. In particular, it may be indicated to carry out calculations on multi-instanton effects on the Green's functions in the presence of a chiral phase. Furthermore, it would be interesting to investigate whether the results for the chiral phase in the correlation function have a bearing on the CP-odd phases that appear in the low-energy effective theory.

Acknowledgements

Funding information WYA is supported by the FSR Postdoc incoming fellowship of UC Louvain. This work has also been supported in part by SFB 1258 of the Deutsche Forschungsgemeinschaft.

A Spectral decomposition of the free fermionic propagator in Minkowski spacetime

To illustrate the spectral decomposition and the ϑ-adjoint defined in Eq. (45), we use here the techniques of Section 2.3 to derive the free Minkowski propagator in Eq. (57). Throughout this section, all objects are assumed to be defined in Minkowski spacetime. The free propagator is the inverse of the operator

$$\mathrm{i}\partial\!\!\!/ - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5}\,, \tag{101}$$

and so we need to consider its eigenfunctions. One can construct a complete basis of continuum modes of the form

$$\psi_{\{k\}}(x) = \frac{1}{(2\pi)^2}\, f(k)\mathrm{e}^{-\mathrm{i}kx}\,, \tag{102}$$

where $f(k)$ is a spinor depending on the four-momentum k^μ. Imposing

$$(\mathrm{i}\partial\!\!\!/ - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\psi_{\{k\}}(x) = \xi_{\{k\}}\psi_{\{k\}}(x) \tag{103}$$

gives

$$(k\!\!\!/ - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})f(k) = \xi_{\{k\}}f(k)\,, \tag{104}$$

so that the spinors $f(k)$ are eigenvectors of the operator $k\!\!\!/ - m\mathrm{e}^{\mathrm{i}\alpha\gamma^5}$. We can explicitly obtain these eigenvectors and their corresponding eigenvalues. The latter are:

$$\xi_{\{k\},i} = \left\{-m_\mathrm{R} - \mathrm{i}\sqrt{m_\mathrm{I}^2 - k^2}, -m_\mathrm{R} - \mathrm{i}\sqrt{m_\mathrm{I}^2 - k^2}, -m_\mathrm{R} + \mathrm{i}\sqrt{m_\mathrm{I}^2 - k^2}, -m_\mathrm{R} + \mathrm{i}\sqrt{m_\mathrm{I}^2 - k^2}\right\}\,, \tag{105}$$

which can be understood from the Euclidean results for the continuum spectrum given in Eq. (39) and the relation between rotated and Euclidean eigenvalues given in Eq. (43). The eigenvectors corresponding to the eigenvalues in Eq. (105) are

$$f_1(k) = \begin{bmatrix} \frac{k^2+\mathrm{i}k^1}{\sqrt{2}\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}+m_\mathrm{I}\right)}} \\ \frac{\mathrm{i}\left(k^0-k^3\right)}{\sqrt{2}\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}+m_\mathrm{I}\right)}} \\ 0 \\ \frac{1}{\sqrt{2}}\sqrt{\frac{\sqrt{m_\mathrm{I}^2-k^2}+m_\mathrm{I}}{\sqrt{m_\mathrm{I}^2-k^2}}} \end{bmatrix}, \quad f_2(k) = \begin{bmatrix} \frac{\mathrm{i}\left(k^0+k^3\right)}{\sqrt{2}\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}+m_\mathrm{I}\right)}} \\ \frac{-k^2+\mathrm{i}k^1}{\sqrt{2}\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}+m_\mathrm{I}\right)}} \\ \frac{1}{\sqrt{2}}\sqrt{\frac{\sqrt{m_\mathrm{I}^2-k^2}+m_\mathrm{I}}{\sqrt{m_\mathrm{I}^2-k^2}}} \\ 0 \end{bmatrix}, \tag{106}$$

$$f_3(k) = \begin{bmatrix} -\frac{1}{\sqrt{2}}\frac{k^2+\mathrm{i}k^1}{\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}-m_\mathrm{I}\right)}} \\ -\frac{1}{\sqrt{2}}\frac{\mathrm{i}(k^0-k^3)}{\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}-m_\mathrm{I}\right)}} \\ 0 \\ \frac{1}{\sqrt{2}}\sqrt{\frac{\sqrt{m_\mathrm{I}^2-k^2}-m_\mathrm{I}}{\sqrt{m_\mathrm{I}^2-k^2}}} \end{bmatrix}, \quad f_4(k) = \begin{bmatrix} -\frac{1}{\sqrt{2}}\frac{\mathrm{i}\left(k^0+k^3\right)}{\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}-m_\mathrm{I}\right)}} \\ -\frac{1}{\sqrt{2}}\frac{-k^2+\mathrm{i}k^1}{\sqrt{\sqrt{m_\mathrm{I}^2-k^2}\left(\sqrt{m_\mathrm{I}^2-k^2}-m_\mathrm{I}\right)}} \\ \frac{1}{\sqrt{2}}\sqrt{\frac{\sqrt{m_\mathrm{I}^2-k^2}-m_\mathrm{I}}{\sqrt{m_\mathrm{I}^2-k^2}}} \\ 0 \end{bmatrix}. \tag{107}$$

These eigenvectors satisfy orthogonality with respect to a ϑ-adjoint inner product:

$$\tilde{f}_i(k) f_j(k) = \delta_{ij}\,, \tag{108}$$

with the tilde operation defined in accordance with our general arguments in Eq. (45) applied to $\vartheta = 0$:

$$\tilde{f}_i(k) = f_i(k)^\dagger|_{k_0 \to -k_0}\,. \tag{109}$$

Moreover, one can explicitly verify the completeness relation

$$\sum_{i=1}^{4} f_i(k)\tilde{f}_i(k) = \mathbb{I}_4\,. \tag{110}$$

We can extend this property now to the eigenfunctions (102) in position space. The ϑ-adjoint defined in Eq. (45) implies

$$\tilde{\psi}_{\{k\},j}(x) = \frac{1}{(2\pi)^2}\,\tilde{f}_j(k)\,\mathrm{e}^{\mathrm{i}kx}\,, \tag{111}$$

and we have the ϑ-adjoint inner products

$$\begin{aligned}&(\psi_{\{k\},i}(x),\psi_{\{k'\},j}(x))\\ &=\int \mathrm{d}^4x\,\tilde{\psi}_{\{k\},i}(x)\psi_{\{k'\},j}(x)=\frac{1}{(2\pi)^4}\int \mathrm{d}^4x\,\mathrm{e}^{\mathrm{i}(k-k')x}\tilde{f}_i(k)f_j(k)=\delta_{ij}\delta^4(k-k')\,,\end{aligned} \tag{112}$$

which imply orthogonality of the eigenfunctions. Similarly, one can derive the completeness relation

$$\sum_i\int \mathrm{d}^4k\,\psi_{\{k\},i}(x)\tilde{\psi}_{\{k\},i}(x')=\frac{1}{(2\pi)^4}\int \mathrm{d}^4k\,\mathrm{e}^{-\mathrm{i}k(x-x')}\sum_i f_i(k)\tilde{f}_i(k)=\delta^4(x-x')\mathbb{I}_4\,, \tag{113}$$

where we used Eq. (110). From the completeness and orthogonality it follows that we can write the Minkowskian free propagator as

$$S_0(x,x')=\sum_i\int \mathrm{d}^4p\,\frac{1}{\xi_{\{p\},i}}\,\psi_{\{p\},i}(x)\tilde{\psi}_{\{p\},i}(x')=\frac{1}{(2\pi)^4}\int \mathrm{d}^4p\,\mathrm{e}^{-\mathrm{i}p(x-x')}\sum_i\frac{1}{\xi_{\{p\},i}}\,f_i(p)\tilde{f}_i(p)\,. \tag{114}$$

Direct evaluation with the $\xi_i(p)$ in Eq. (105), the eigenvectors $f_i(p)$ in Eqs. (106) and the ϑ-adjoint of Eq. (109) gives again the result of Eq. (57):

$$S_0(x,x')=\int\frac{\mathrm{d}^4p}{(2\pi)^4}\,\mathrm{e}^{-\mathrm{i}p(x-x')}\,\frac{(\not{p}+m\mathrm{e}^{-\mathrm{i}\gamma^5})}{p^2-m^2+\mathrm{i}\epsilon}\,. \tag{115}$$

To end, let us note that the operator in Eq. (101) is Hermitian under the Dirac adjoint inner product

$$\langle\psi_{\{k\},i},\psi_{\{k'\},j}\rangle\equiv\int \mathrm{d}^4x\,\bar{\psi}_{\{k\},i}(x)\psi_{\{k'\},j}\,. \tag{116}$$

However, this does not enter in conflict with the fact that the eigenvalues in Eq. (105) are complex, because the eigenfunctions (102) have zero norm under the Dirac adjoint inner product, as can be verified by noting that the spinors $f_i(k)$ satisfy

$$\bar{f}_i(k)f_i(k)=0\,. \tag{117}$$

Moreover, the $f_i(k)$ are not orthogonal under the Dirac adjoint inner product, which again does not conflict with Hermiticity because the nonzero mixed products relate eigenvectors $f_i(k), f_j(k)$ with mutually conjugate eigenvalues. (Note that the eigenvalues in Eq. (105) come in conjugate pairs.) Hermiticity implies

$$\begin{aligned}&\langle\psi_{\{k\}i},(\mathrm{i}\not{\partial}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\psi_{\{k\}j}\rangle=\xi_{\{k\},j}\langle\psi_{\{k\}i},\psi_{\{k\}j}\rangle\\ =&\langle(\mathrm{i}\not{\partial}-m\mathrm{e}^{\mathrm{i}\alpha\gamma^5})\psi_{\{k\}i},\psi_{\{k\}j}\rangle=\xi^*_{\{k\},i}\langle\psi_{\{k\}i},\psi_{\{k\}j}\rangle\,,\end{aligned} \tag{118}$$

which allows nonzero mixed products $\langle\psi_{\{k\}i},\psi_{\{k\}j}\rangle$ as long as $\xi^*_{\{k\},i}=\xi_{\{k\},j}$. The previous properties imply that the Dirac adjoint product does not allow to define orthogonal projectors that resolve the identity, in contrast to the ϑ-adjoint inner product, from which one recovers the standard propagator.

References

[1] J. S. Bell and R. Jackiw, *A PCAC puzzle: $\pi^0 \to \gamma\gamma$ in the σ model*, Nuovo Cim. **A60**, 47 (1969), doi:10.1007/BF02823296.

[2] S. L. Adler, *Axial vector vertex in spinor electrodynamics*, Phys. Rev. **177**, 2426 (1969), doi:10.1103/PhysRev.177.2426.

[3] A. A. Belavin, A. M. Polyakov, A. S. Schwartz and Yu. S. Tyupkin, *Pseudoparticle Solutions of the Yang-Mills Equations*, Phys. Lett. **59B**, 85 (1975), doi:10.1016/0370-2693(75)90163-X.

[4] G. 't Hooft, *Symmetry Breaking Through Bell-Jackiw Anomalies*, Phys. Rev. Lett. **37**, 8 (1976), doi:10.1103/PhysRevLett.37.8.

[5] G. 't Hooft, *Computation of the Quantum Effects Due to a Four-Dimensional Pseudoparticle*, Phys. Rev. **D14**, 3432 (1976), doi:10.1103/PhysRevD.18.2199.3, 10.1103/PhysRevD.14.3432, [Erratum: Phys. Rev.D18,2199(1978)].

[6] F. R. Klinkhamer and N. S. Manton, *A Saddle Point Solution in the Weinberg-Salam Theory*, Phys. Rev. **D30**, 2212 (1984), doi:10.1103/PhysRevD.30.2212.

[7] V. A. Kuzmin, V. A. Rubakov and M. E. Shaposhnikov, *On the Anomalous Electroweak Baryon Number Nonconservation in the Early Universe*, Phys. Lett. **155B**, 36 (1985), doi:10.1016/0370-2693(85)91028-7.

[8] S. Weinberg, *The U(1) Problem*, Phys. Rev. **D11**, 3583 (1975), doi:10.1103/PhysRevD.11.3583.

[9] J. S. Schwinger, *Brownian motion of a quantum oscillator*, J. Math. Phys. **2**, 407 (1961), doi:10.1063/1.1703727.

[10] L. V. Keldysh, *Diagram technique for nonequilibrium processes*, Zh. Eksp. Teor. Fiz. **47**, 1515 (1964), [Sov. Phys. JETP20,1018(1965)].

[11] E. Witten, *Analytic Continuation Of Chern-Simons Theory*, AMS/IP Stud. Adv. Math. **50**, 347 (2011), 1001.2933.

[12] Y. Tanizaki and T. Koike, *Real-time Feynman path integral with Picard–Lefschetz theory and its applications to quantum tunneling*, Annals Phys. **351**, 250 (2014), doi:10.1016/j.aop.2014.09.003, 1406.2386.

[13] A. Cherman and M. Unsal, *Real-Time Feynman Path Integral Realization of Instantons* (2014), 1408.0012.

[14] A. Andreassen, D. Farhi, W. Frost and M. D. Schwartz, *Precision decay rate calculations in quantum field theory*, Phys. Rev. **D95**(8), 085011 (2017), doi:10.1103/PhysRevD.95.085011, 1604.06090.

[15] W.-Y. Ai, B. Garbrecht and C. Tamarit, *Functional methods for false vacuum decay in real time*, JHEP **12**, 095 (2019), doi:10.1007/JHEP12(2019)095, 1905.04236.

[16] Z.-G. Mou, P. M. Saffin and A. Tranberg, *Quantum tunnelling, real-time dynamics and Picard-Lefschetz thimbles*, JHEP **11**, 135 (2019), doi:10.1007/JHEP11(2019)135, 1909.02488.

[17] Z.-G. Mou, P. M. Saffin, A. Tranberg and S. Woodward, *Real-time quantum dynamics, path integrals and the method of thimbles*, JHEP **06**, 094 (2019), doi:10.1007/JHEP06(2019)094, 1902.09147.

[18] H. B. Nielsen and M. Ninomiya, *ADLER-BELL-JACKIW ANOMALY AND WEYL FERMIONS IN CRYSTAL*, Phys. Lett. **130B**, 389 (1983), doi:10.1016/0370-2693(83)91529-0.

[19] V. Domcke, Y. Ema, K. Mukaida and R. Sato, *Chiral Anomaly and Schwinger Effect in Non-Abelian Gauge Theories*, JHEP **03**, 111 (2019), doi:10.1007/JHEP03(2019)111, 1812.08021.

[20] V. Domcke, Y. Ema and K. Mukaida, *Chiral Anomaly, Schwinger Effect, Euler-Heisenberg Lagrangian, and application to axion inflation*, JHEP **02**, 055 (2020), doi:10.1007/JHEP02(2020)055, 1910.01205.

[21] M. A. Shifman, A. I. Vainshtein and V. I. Zakharov, *Instanton Density in a Theory with Massless Quarks*, Nucl. Phys. **B163**, 46 (1980), doi:10.1016/0550-3213(80)90389-2.

[22] G. 't Hooft, *How Instantons Solve the U(1) Problem*, Phys. Rept. **142**, 357 (1986), doi:10.1016/0370-1573(86)90117-1.

[23] S. Vandoren and P. van Nieuwenhuizen, *Lectures on instantons* (2008), 0802.1862.

[24] A. I. Vainshtein, V. I. Zakharov, V. A. Novikov and M. A. Shifman, *ABC's of Instantons*, Sov. Phys. Usp. **25**, 195 (1982), doi:10.1070/PU1982v025n04ABEH004533, [Usp. Fiz. Nauk136,553(1982)].

[25] D. Diakonov and V. Yu. Petrov, *A Theory of Light Quarks in the Instanton Vacuum*, Nucl. Phys. **B272**, 457 (1986), doi:10.1016/0550-3213(86)90011-8.

[26] C. W. Bernard, *Gauge Zero Modes, Instanton Determinants, and QCD Calculations*, Phys. Rev. **D19**, 3013 (1979), doi:10.1103/PhysRevD.19.3013.

[27] D. G. Cerdeño, P. Reimitz, K. Sakurai and C. Tamarit, *$B + L$ violation at colliders and new physics*, JHEP **04**, 076 (2018), doi:10.1007/JHEP04(2018)076, 1801.03492.

[28] H. Leutwyler and A. V. Smilga, *Spectrum of Dirac operator and role of winding number in QCD*, Phys. Rev. **D46**, 5607 (1992), doi:10.1103/PhysRevD.46.5607.