Calculation of QCD instanton determinant with arbitrary mass

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The precise quark mass dependence of the one-loop effective action in an instanton background has recently been computed [Phys. Rev. Lett. **94**, 072001 (2005).]. The result interpolates smoothly between the previously known extreme small and large mass limits. The computational method makes use of the fact that the single instanton background has radial symmetry, so that the computation can be reduced to a sum over partial waves of logarithms of radial determinants, each of which can be computed numerically in an efficient manner. The bare sum over partial waves is divergent and must be regulated and renormalized. In this paper we provide more details of this computation, including both the renormalization procedure and the numerical approach. We conclude with comparisons of our precise numerical results with a simple interpolating function that connects the small and large mass limits, and with the leading order of the derivative expansion.

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I. INTRODUCTION

The computation of fermion determinants in nontrivial background fields is an important challenge for both continuum and lattice quantum field theory. Explicit analytic results are known only for very simple backgrounds, and are essentially all variations on the original work of Heisenberg and Euler [1–4]. For applications in quantum chromodynamics (QCD), an important class of background gauge fields are instanton fields, as these minimize the Euclidean gauge action within a given topological sector of the gauge field. Furthermore, instanton physics has many important phenomenological consequences [5–9]. Thus, we are led to consider the fermion determinant, and the associated one-loop effective action, for quarks of mass m in an instanton background. Here, no exact results are known for the full mass dependence, although several terms have been computed analytically in the small mass [5,10,11] and large mass [11,12] limits. Recently, in [13], the present authors presented a new computation which is numerical, but essentially exact, that evaluates the one-loop effective action in a single instanton background, for any value of the quark mass (and for arbitrary instanton size parameter). The result is fully consistent with the known small and large mass limits, and interpolates smoothly between these limits. This could be of interest for the extrapolation of lattice results [14], obtained at unphysically large quark masses, to lower physical masses, and for various instanton-based phenomenology. Our computational method is simple and efficient, and can be adapted to many other determinant computations in which the background is sufficiently symmetric so that the problem can be reduced to a product of one-dimensional radial determinants. While this is still a very restricted set of background field configurations, it contains many examples of interest, the single instanton being one of the most obvious. It is well known how to compute determinants of *ordinary* differential operators [15–19]; but in higher-dimensional problems with *partial* differential operators, one must confront the renormalization problem since there are now an infinite number of 1-D determinants to deal with (even when the partial differential operator has a radial symmetry).

In this paper we present more details of the results of [13]. In Sec. II we define the renormalized effective action in the minimal subtraction scheme, as introduced by ’t Hooft [5], and summarize what is known about the small and large mass limits. In Sec. III we review how the single instanton background reduces the spectral problem to a set of radial problems, and indicate how to regularize the effective action. This reduces the computation to two parts, one of which is analytic and the other is numerical. The analytic part concerns the renormalization of the effective action, and for this we use a WKB expansion as is developed in our earlier paper [20]. We stress that this renormalization computation, which constitutes Sec. IV, is analytic and exact, even though we use a WKB expansion, since we show that only the first two orders of the WKB

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expansion contribute. Section V presents details of the numerical part of the computation and shows how to combine the numerical part of the computation with the renormalization part to obtain the finite renormalized effective action, which is plotted in Fig. 5. In Sec. VI we present a simple interpolating function that has been fit to our results, and we also compare our precise mass dependence with the mass dependence of the leading derivative expansion approximation, which was computed previously in [20]. The final section contains some concluding comments. In Appendix A we give some details (not fully given in [20]) which are needed in the approximate effective action calculation using the WKB phase-shift method. For this WKB analysis, the Schwinger proper-time framework [2] provides a natural way to implement the renormalization procedure consistently. Appendix B confirms that the same result is obtained in the regular and singular gauges for the instanton background.

II. RENORMALIZED EFFECTIVE ACTION IN A SELF-DUAL BACKGROUND

An instanton background field is self-dual, and self-dual gauge fields have the remarkable property that the Dirac and Klein-Gordon operators in such a background are isospectral; that is, they have identical spectra, apart from an extra degeneracy factor of 4 in the spinor case and zero modes present in the spinor case [5,21,22]. Since the one-loop effective action is proportional to the logarithm of the determinant of the respective operator, this has the immediate consequence that it is sufficient to consider the scalar effective action to learn also about the corresponding fermionic effective action, for any mass value m. In particular, for a quark in a background instanton field, the renormalized one-loop effective action of a Dirac spinor field of mass m (and isospin $\frac{1}{2}$), $\Gamma^F_{\rm ren}(A;m)$, can be related to the corresponding scalar effective action, $\Gamma^S_{\rm ren}(A;m)$, for a complex scalar of mass m (and isospin $\frac{1}{2}$) by [5,11,22]

$$\Gamma^F_{\rm ren}(A;m) = -2\Gamma^S_{\rm ren}(A;m) - \frac{1}{2}\ln\left(\frac{m^2}{\mu^2}\right), \tag{2.1}$$

where μ is the renormalization scale. The ln term in (2.1) corresponds to the existence of a zero eigenvalue in the spectrum of the Dirac operator for a single instanton background.

The one-loop effective action must be regularized. We choose Pauli-Villars regularization adapted to the Schwinger proper-time formalism, and later we relate this to dimensional regularization, as in the work of 't Hooft [5]. The Pauli-Villars regularized one-loop scalar effective action is [11,12]

$$\Gamma^S_\Lambda(A;m) = \ln\left[\frac{\mathrm{Det}(-D^2+m^2)}{\mathrm{Det}(-\partial^2+m^2)}\frac{\mathrm{Det}(-\partial^2+\Lambda^2)}{\mathrm{Det}(-D^2+\Lambda^2)}\right]. \tag{2.2}$$

where $D^2 \equiv D_\mu D_\mu$, with $D_\mu = \partial_\mu - iA_\mu(x)$. In (2.2), Λ is a heavy regulator mass. We consider an SU(2) single instanton in the regular gauge [5,23]:

$$\begin{aligned} A_\mu(x) &\equiv A^a_\mu(x)\frac{\tau^a}{2} = \frac{\eta_{\mu\nu a}\tau^a x_\nu}{r^2+\rho^2}, \\ F_{\mu\nu}(x) &\equiv F^a_{\mu\nu}(x)\frac{\tau^a}{2} = -\frac{2\rho^2\eta_{\mu\nu a}\tau^a}{(r^2+\rho^2)^2}, \end{aligned} \tag{2.3}$$

where $\eta_{\mu\nu a}$ are the standard 't Hooft symbols [5,8].

The regularized effective action (2.2) has the proper-time representation

$$\begin{aligned} \Gamma^S_\Lambda(A;m) &= -\int_0^\infty \frac{ds}{s}(e^{-m^2 s} - e^{-\Lambda^2 s}) \\ &\quad \times \int d^4x\, \mathrm{tr}\langle x|e^{-s(-\mathrm{D}^2)} - e^{-s(-\partial^2)}|x\rangle \\ &\equiv -\int_0^\infty \frac{ds}{s}(e^{-m^2 s} - e^{-\Lambda^2 s})F(s). \end{aligned} \tag{2.4}$$

The renormalized effective action, in the minimal subtraction scheme, is defined as [5,11]

$$\begin{aligned} \Gamma^S_{\rm ren}(A;m) &= \lim_{\Lambda\to\infty}\left[\Gamma^S_\Lambda(A;m) - \frac{1}{12}\frac{1}{(4\pi)^2}\ln\left(\frac{\Lambda^2}{\mu^2}\right)\right. \\ &\quad \left.\times \int d^4x\, \mathrm{tr}(F_{\mu\nu}F_{\mu\nu})\right] \\ &\equiv \lim_{\Lambda\to\infty}\left[\Gamma^S_\Lambda(A;m) - \frac{1}{6}\ln\left(\frac{\Lambda}{\mu}\right)\right], \end{aligned} \tag{2.5}$$

where we have subtracted the charge renormalization counterterm, and μ is the renormalization scale. By dimensional considerations, we may introduce the modified scalar effective action $\tilde\Gamma^S_{\rm ren}(m\rho)$, which is a function of $m\rho$ only, defined by

$$\Gamma^S_{\rm ren}(A;m) = \tilde\Gamma^S_{\rm ren}(m\rho) + \frac{1}{6}\ln(\mu\rho), \tag{2.6}$$

and concentrate on studying the $m\rho$ dependence of $\tilde\Gamma^S_{\rm ren}(m\rho)$. Then there is no loss of generality in our setting the instanton scale $\rho = 1$ henceforth.

It is known from previous works that in the small mass [5,10,11] and large mass [11,12] limits, $\tilde\Gamma^S_{\rm ren}(m)$ behaves as

$$\tilde\Gamma^S_{\rm ren}(m) = \begin{cases} \alpha(\frac{1}{2}) + \frac{1}{2}(\ln m + \gamma - \ln 2)m^2 + \ldots, & m\to 0 \\ -\frac{\ln m}{6} - \frac{1}{75m^2} - \frac{17}{735m^4} + \frac{232}{2835m^6} - \frac{7916}{148\,225m^8} + \cdots, & m\to\infty \end{cases} \tag{2.7}$$

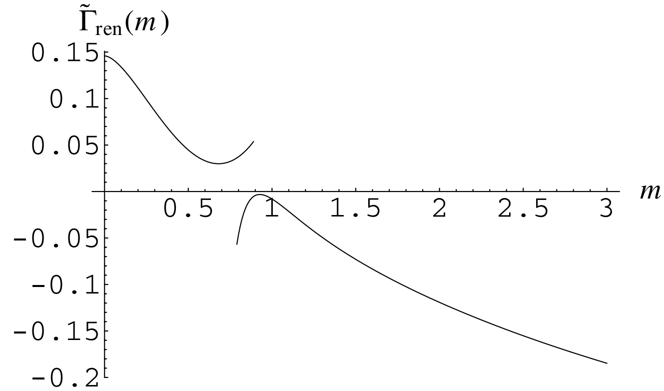

FIG. 1. Plot of the analytic small and large mass expansions for $\tilde{\Gamma}^S_{\rm ren}(m)$, from Eq. (2.7). Note the gap in the region $0.5 \leq m \leq 1$, in which the two expansions do not match up.

where

$$\alpha\left(\frac{1}{2}\right) = -\frac{5}{72} - 2\zeta'(-1) - \frac{1}{6}\ln 2 \simeq 0.145\,873\ldots, \quad (2.8)$$

and $\gamma \simeq 0.5772\ldots$ is Euler's constant [24]. The leading behavior of the small mass limit in (2.7) was first computed by 't Hooft [5], and the next corrections were computed in [10,11]. This small mass expansion is based on the fact that the massless propagators in an instanton background are known in closed form [25]. On the other hand, the large mass expansion in (2.7) can be computed in several ways. The $O(1/m^2)$ and $O(1/m^4)$ terms were computed in [12], while the next two terms were computed in [11]. A very direct approach is to use the small-s behavior of $F(s)$, the proper-time function appearing in (2.4), as given by the Schwinger-DeWitt expansion. In our case this expansion reads [11]

$$s \to 0+: F(s) \sim -\frac{1}{12} + \frac{1}{75}s + \frac{17}{735}s^2 - \frac{116}{2835}s^3 + \frac{3958}{44\,675}s^4 + \cdots, \quad (2.9)$$

and using this series with (2.4) immediately leads to the large m expansion for $\tilde{\Gamma}^S_{\rm ren}(m)$ in (2.7).

Equation (2.7) summarizes what is known analytically about the mass dependence of the renormalized one-loop effective action in an instanton background. This situation is represented in Fig. 1, which shows a distinct gap approximately in the region $0.5 \leq m \leq 1$, where the small and large mass expansions do not match up. In this paper we present a technique which computes $\tilde{\Gamma}^S_{\rm ren}(m)$ numerically for *any* value of the mass m. Our results interpolate smoothly between the analytic small and large mass limits depicted in Fig. 1.

III. RADIAL FORMULATION

Our computational approach makes use of the fact that the single instanton background (2.3) has radial symmetry [5]. This has the important consequence that the computation of the regularized one-loop effective action (2.4) can be reduced to a sum over partial waves of logarithms of determinants of radial ordinary differential operators. Each such radial determinant can be computed by a simple numerical method, described in Sec. V. The physical challenge is to renormalize the (divergent) sum over partial waves.

In the instanton background (2.3), with scale $\rho = 1$, the Klein-Gordon operator $-D^2$ for isospin $\frac{1}{2}$ particles can be cast in the radial form [5]

$$-D^2 \to \mathcal{H}_{(l,j)} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4l(l+1)}{r^2} + \frac{4(j-l)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2}\right], \quad (3.1)$$

where $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$, and $j = |l \pm \frac{1}{2}|$, and there is a degeneracy factor of $(2l+1)(2j+1)$ for each partial wave characterized by (l, j) values. [Note that $l(l+1)$ can be identified with the eigenvalue of $\vec{L}^2 \equiv L_a L_a$ for $L_a = -\frac{i}{2}\eta_{\mu\nu a}x_\mu\partial_\nu$, and $j(j+1)$ with the eigenvalue of $\vec{J}^2 \equiv (L_a + T_a)(L_a + T_a)$ for $T^a = \tau^a/2$]. In the absence of the instanton background, the free operator is

$$-\partial^2 \to \mathcal{H}^{\rm free}_{(l)} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4l(l+1)}{r^2}\right]. \quad (3.2)$$

This radial decomposition means that we can express the Pauli-Villars regularized effective action (2.2) also as

$$\Gamma^S_\Lambda(A;m) = \sum_{l=0,1/2,\ldots}(2l+1)(2l+2) \times \left\{\ln\left(\frac{\det[\mathcal{H}_{[l,l+(1/2)]}+m^2]}{\det[\mathcal{H}^{\rm free}_{(l)}+m^2]}\right) + \ln\left(\frac{\det[\mathcal{H}_{[l+(1/2),l]}+m^2]}{\det[\mathcal{H}^{\rm free}_{[l+(1/2)]}+m^2]}\right) - \ln\left(\frac{\det[\mathcal{H}_{[l,l+(1/2)]}+\Lambda^2]}{\det[\mathcal{H}^{\rm free}_{(l)}+\Lambda^2]}\right) - \ln\left(\frac{\det[\mathcal{H}_{[l+(1/2),l]}+\Lambda^2]}{\det[\mathcal{H}^{\rm free}_{[l+(1/2)]}+\Lambda^2]}\right)\right\}. \quad (3.3)$$

Here we have combined the radial determinants for $(l, j = l + \frac{1}{2})$ and $(l + \frac{1}{2}, j = (l + \frac{1}{2}) - \frac{1}{2})$, which have the common degeneracy factor $(2l+1)(2l+2)$, so that the sum over l and j reduces to a single sum over l. In our actual analysis, as explained in detail below, we need to consider only a truncated sum over l with the expression (3.3), and hence possible ambiguities as regards effecting the infinite sum over l become irrelevant.

In Sec. V we present a simple and efficient numerical technique for computing each of the radial determinants appearing in (3.3). But to extract the renormalized effective action we need to be able to consider the $\Lambda \to \infty$ limit in conjunction with the infinite sum over l. This can be achieved as follows. Split the l sum in (3.3) into two parts as:

$$\Gamma^S_\Lambda(A;m) = \sum_{l=0,1/2,\ldots}^{L} \Gamma^S_{\Lambda,(l)}(A;m) + \sum_{l=L+(1/2)}^{\infty} \Gamma^S_{\Lambda,(l)}(A;m) \tag{3.4}$$

where L is a large but finite integer. In the first sum, which is finite, the cutoff Λ may be safely removed since for any given finite l [15,19],

$$\lim_{\Lambda\to\infty}\left(\frac{\det[\mathcal{H}_{[l,l+(1/2)]} + \Lambda^2]}{\det[\mathcal{H}^{\rm free}_{(l)} + \Lambda^2]}\right) = 1, \qquad \lim_{\Lambda\to\infty}\left(\frac{\det[\mathcal{H}_{[l+(1/2),l]} + \Lambda^2]}{\det[\mathcal{H}^{\rm free}_{[l+(1/2)]} + \Lambda^2]}\right) = 1. \tag{3.5}$$

Thus, the first sum in (3.4) may be written without the regulator Λ as

$$\sum_{l=0,1/2,\ldots}^{L} \Gamma^S_l(A;m) = \sum_{l=0,1/2,\ldots}^{L} (2l+1)(2l+2) \times \left\{\ln\left(\frac{\det[\mathcal{H}_{[l,l+(1/2)]} + m^2]}{\det[\mathcal{H}^{\rm free}_{(l)} + m^2]}\right) + \ln\left(\frac{\det[\mathcal{H}_{[l+(1/2),l]} + m^2]}{\det[\mathcal{H}^{\rm free}_{[l+(1/2)]} + m^2]}\right)\right\}. \tag{3.6}$$

This sum can be computed numerically, and we find [see Sec. V] that for any mass m it is quadratically divergent as $L \to \infty$. This divergence is canceled by a divergence of the second sum in (3.4) in the large L limit, as we show in the next section.

IV. WKB ANALYSIS AND RENORMALIZATION

In the second sum in (3.4) we cannot take the large L and large Λ limits blindly, as each leads to a divergence. However, we show in this section that the Λ divergence is precisely of the counterterm form in the renormalized action in (2.5), and that the large L divergence is such that it precisely cancels the large L divergences from the large L limit of the sum in (3.6). Thus we obtain a finite renormalized effective action.

The advantage of this technique is that the large Λ and large L divergences of the second sum in (3.4) can be computed *analytically*, using the WKB approximation for the corresponding determinants. The WKB approach to radial determinants was derived in [20] up to third order in the WKB approximation, and the relevant results are reviewed below, and in Appendix A. It turns out that in the large Λ and large L limits we only need up to the second order in WKB. The large L limit of the second sum in (3.4) can then be analyzed using the Euler-Maclaurin summation formula [26].

It is convenient to express the second piece by the proper-time representation

$$\sum_{l=L+(1/2)}^{\infty} \Gamma^S_{\Lambda,(l)}(A;m) = \int_0^\infty ds\left[-\frac{1}{s}(e^{-m^2 s} - e^{-\Lambda^2 s})F_L(s)\right], \tag{4.1}$$

with

$$F_L(s) = \int_0^\infty dr\left(\sum_{l=L+(1/2)}^{\infty} f_l(s,r)\right), \tag{4.2}$$

$$f_l(s,r) = (2l+1)(2l+2) \times [f_{[l,l+(1/2)]}(s,r) + f_{[l+(1/2),l]}(s,r)]. \tag{4.3}$$

Here the term $\int_0^\infty dr f_l(s,r)$, obviously related to $\Gamma^S_{\Lambda,(l)}(A;m)$, can be found using the scattering phase shifts of the Schrödinger problem with the radial Hamiltonian in (3.1). Also, in considering the above infinite sum over partial-wave terms, it is now crucial to have the contribution from partial-wave $(l, j = l + \frac{1}{2})$ and that from partial-wave $(l + \frac{1}{2}, l)$ treated together as a package, as indicated in (4.3). For details on this, readers may consult Appendix A. We here only note that, for large l, the WKB approximation becomes exact and so in the large L limit we can use the WKB approximation (to an appropriate order) for $F_L(s)$. According to the WKB expressions derived in Appendix A, it is found that, for each l, $f_l(s,r)$ has a local expansion in terms of the Langer-modified [27] potential, $\tilde{V}_{(l,j)}(r)$, and the corresponding Langer-modified free potential, $\tilde{V}_l(r)$:

$$\tilde{V}_{(l,j)}(r) \equiv \frac{4(l+\frac{1}{2})^2}{r^2} + \frac{4(j-l)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2}, \tag{4.4}$$

$$\tilde{V}_l(r) \equiv \frac{4(l+\frac{1}{2})^2}{r^2}. \tag{4.5}$$

Specifically, the first-order WKB result for $f_l(s,r)$ is obtained by using the form

$$f^{(1)}_{(l,j)}(s,r) = \frac{1}{2\sqrt{\pi s}}\exp[-s\tilde{V}_{(l,j)}(r)] - \frac{1}{2\sqrt{\pi s}} \times \exp[-s\tilde{V}_l(r)] \tag{4.6}$$

in the right-hand side of (4.3), and the second-order WKB by using

$$f^{(2)}_{(l,j)}(s,r) = \frac{1}{2\sqrt{\pi s}}\left(\frac{s}{4r^2} - \frac{s^2}{12}\frac{d^2\tilde{V}_{(l,j)}}{dr^2}\right)\exp[-s\tilde{V}_{(l,j)}(r)] - \frac{1}{2\sqrt{\pi s}}\left(\frac{s}{4r^2} - \frac{s^2}{12}\frac{d^2\tilde{V}_{l}}{dr^2}\right)\exp[-s\tilde{V}_{l}(r)]. \tag{4.7}$$

The corresponding expression for the third order of WKB is also given in Appendix A, but this result is not needed for our present purposes.

An important observation (which holds true to any order in the WKB expansion) is that the l dependence in $f_{(l,j)}(s,r)$ has the form of a polynomial in l multiplied by an exponential in which l appears quadratically. Thus, if we use the Euler-Maclaurin expansion [26] for (4.2)

$$\sum_{l=L+(1/2)}^{\infty} f_l = 2\int_L^\infty dl f(l) - \frac{1}{2}f(L) - \frac{1}{24}f'(L) + \ldots \tag{4.8}$$

all terms in this expansion, including the integral term, can be computed analytically. The integral term yields an error function [24]

$$\int_L^\infty dl \exp[-al^2 - 2bl] = \sqrt{\frac{\pi}{4a}}e^{b^2/a}\,\mathrm{Erfc}\left(\frac{aL+b}{\sqrt{a}}\right), \tag{4.9}$$

where $\mathrm{Re}(a) > 0$. We here remark that it is important to perform the l sum prior to considering the r integration. For more details on the issue of the integration order, see Appendix A.

To compute the sum in (4.1) we still need to perform the proper-time integral over s as well as the radial integral over r appearing in the WKB expression (4.2). To achieve this, we adopt the following procedure. First, we trade the regulator mass Λ for a dimensional regularization parameter ϵ, by demanding that

$$\int_0^\infty ds\left[-\frac{1}{s}(e^{-m^2 s} - e^{-\Lambda^2 s})F_L(s)\right] = \int_0^\infty ds\left[-\frac{1}{s}(e^{-m^2 s}s^\epsilon)F_L(s)\right]. \tag{4.10}$$

Then, from the facts that $F_L(s) \sim F(s)$ as $s \to 0+$, and $F(s) = \frac{1}{12} + O(s)$ for small s, we see that (4.10) requires

$$-\frac{1}{6}\ln\left(\frac{\Lambda}{m}\right) = -\frac{1}{12\epsilon} + \frac{1}{12}(\gamma + 2\ln m) + O(\epsilon). \tag{4.11}$$

Thus, the correspondence between ϵ and Λ is

$$\epsilon \leftrightarrow \frac{1}{\gamma + 2\ln\Lambda}. \tag{4.12}$$

We now proceed to do the proper-time and radial integrals as follows. First, for L very large, it becomes convenient to rescale variables as $s \to y/L^2$ and $r \to x\sqrt{y}$. Second, we expand all terms (except the $e^{-m^2 s}$ factor) in decreasing powers of large L. Then the y integral can be performed in closed form, yielding incomplete gamma functions [24]. These can be further expanded for large L, after which the x (that is, the radial) integral can be done. It is straightforward to perform these operations using MATHEMATICA. To zeroth order in ϵ, the results for the first and second order of WKB are given below. For the first-order WKB term, the result is

$$\int_0^\infty dr\int_0^\infty ds\left[-\frac{1}{s}(e^{-m^2 s}s^\epsilon)\right]\left(\sum_{l=L+(1/2)}^{\infty} f^{(1)}_l(s,r)\right) = \frac{1}{24\epsilon} + 2L^2 + 4L - \frac{\ln L}{2}\left(\frac{1}{6} + m^2\right) + \frac{119}{72} - \frac{\ln 2}{12} + \frac{\psi(\frac{1}{2})}{24} + \frac{m^2}{2}(1 - 2\ln 2 + \ln m) - \frac{1+6m^2}{12L} + O\left(\frac{1}{L^2}\right), \tag{4.13}$$

where $\psi(\frac{1}{2}) = -\gamma - 2\ln 2$. For the second-order WKB term, the result is

$$\int_0^\infty dr\int_0^\infty ds\left[-\frac{1}{s}(e^{-m^2 s}s^\epsilon)\right]\left(\sum_{l=L+(1/2)}^{\infty} f^{(2)}_l(s,r)\right) = \frac{1}{24\epsilon} - \frac{\ln L}{12} + \frac{1}{9} - \frac{\ln 2}{12} + \frac{\psi(\frac{1}{2})}{24} - \frac{1}{12L} + O\left(\frac{1}{L^2}\right). \tag{4.14}$$

The third-order WKB term gives a contribution of at most $O(1/L^2)$, and has no ϵ pole. Similarly, it can be shown that all higher-order WKB terms have no ϵ pole, and vanish for large L.

We can thus compute the large L limit by considering only the relevant parts of the first two WKB expressions in (4.13) and (4.14). Inserting the identification between ϵ and Λ in (4.12), we obtain

$$\sum_{l=L+(1/2)}^{\infty}\Gamma^S_{\Lambda,(l)}(A;m) \sim \frac{1}{6}\ln\Lambda + 2L^2 + 4L - \left(\frac{1}{6} + \frac{m^2}{2}\right)\ln L + \left[\frac{127}{72} - \frac{1}{3}\ln 2 + \frac{m^2}{2} - m^2\ln 2 + \frac{m^2}{2}\ln m\right] + O\left(\frac{1}{L}\right). \tag{4.15}$$

We can now identify the physical role of the various terms in (4.15). The first term is the expected logarithmic counterterm which is subtracted in (2.5), and explains the origin of the $\frac{1}{6}\ln\mu$ term in (2.6). The next three terms give quadratic, linear and logarithmic divergences in L. We shall show in the next section that these divergences cancel corresponding divergences in the first sum in (3.4), which were found in our numerical data. It is a highly nontrivial check on this WKB computation that these divergent terms have the correct coefficients to cancel these divergences. Note that the $\ln L$ coefficient, and the finite term, are mass dependent.

Thus, the minimally subtracted renormalized effective action $\tilde{\Gamma}^S_{\rm ren}(m)$, defined in (2.6), is

$$\tilde{\Gamma}^S_{\rm ren}(m) = \lim_{L\to\infty}\left\{\sum_{l=0,1/2,\ldots}^{L}\Gamma_l^S(A;m) + 2L^2 + 4L - \left(\frac{1}{6}+\frac{m^2}{2}\right)\ln L + \left[\frac{127}{72} - \frac{1}{3}\ln 2 + \frac{m^2}{2} - m^2\ln 2 + \frac{m^2}{2}\ln m\right]\right\}, \quad (4.16)$$

where the first sum is to be computed numerically from the partial-wave expansion in (3.6).

V. NUMERICAL CALCULATION

In this section we describe the numerical technique for computing the radial determinants which enter the partial-wave expansion in (3.6). These one-dimensional determinants can be computed efficiently using the following result [15–19]. Suppose $\mathcal{M}_1$ and $\mathcal{M}_2$ are two second-order ordinary differential operators on the interval $r\in[0,\infty)$, with Dirichlet boundary conditions assumed. Then the ratio of the determinants of $\mathcal{M}_1$ and $\mathcal{M}_2$ is given by

$$\left(\frac{\det\mathcal{M}_1}{\det\mathcal{M}_2}\right) = \lim_{R\to\infty}\left(\frac{\psi_1(R)}{\psi_2(R)}\right) \quad (5.1)$$

where $\psi_i(r)$ (for $i=1,2$) satisfies the initial value problem

$$\mathcal{M}_i\psi_i(r) = 0, \quad \text{with } \psi_i(0)=0 \quad \text{and} \quad \psi'(0)=1. \quad (5.2)$$

Since an initial value problem is very simple to solve numerically, this theorem provides an efficient way to compute the determinant of an ordinary differential operator. Note, in particular, that no direct information about the spectrum (either bound or continuum states, or phase shifts) is required in order to compute the determinant.

We can simplify the numerical computation further. Note that for the free massive Klein-Gordon partial-wave operator, $\mathcal{H}^{\rm free}_{(l)} + m^2$ [with $\mathcal{H}^{\rm free}_{(l)}$ given in (3.2)], the solution to (5.2) is the modified Bessel function [24]

$$\psi^{\rm free}_{(l)}(r) = \frac{I_{2l+1}(mr)}{r}. \quad (5.3)$$

This solution grows exponentially fast at large r, as do the numerical solutions to (5.2) for the operators $\mathcal{H}_{(l,j)} + m^2$, with $\mathcal{H}_{(l,j)}$ specified in (3.1). Thus, it is numerically better to consider the ordinary differential equation satisfied by the *ratio* of the two functions

$$\mathcal{R}_{(l,j)}(r) = \frac{\psi_{(l,j)}(r)}{\psi^{\rm free}_{(l)}(r)}. \quad (5.4)$$

This quantity has a finite value in the large r limit, which is just the ratio of the determinants as in (5.1). The boundary conditions for the ratio function are

$$\mathcal{R}_{(l,j)}(0) = 1; \qquad \mathcal{R}'_{(l,j)}(0) = 0. \quad (5.5)$$

A similar idea of considering the ratio function was used by Baacke and Lavrelashvili in their analysis of metastable vacuum decay [28].

It is worthwhile making a brief side comment about the boundary conditions at $r=0$. The two functions on the right-hand side of (5.4) do not necessarily satisfy the boundary conditions at $r=0$ in (5.2). For example, when $l=0$, $\psi^{\rm free}_{(l=0)}(r)$ does not vanish at $r=0$. And in the massless case this issue is more serious. However, since only the ratio is important, one can introduce an ultraviolet regulator by imposing the boundary conditions in (5.2) at $r=a$, for a small but nonzero. Then the free solution satisfying the boundary conditions is a linear combination of the two modified Bessel functions $I_{2l+1}(mr)/r$ and $K_{2l+1}(mr)/r$. It is straightforward to show that the differential equation governing the ratio function, and the asymptotic ($r\to\infty$) value of the ratio function are independent of a as $a\to 0$.

In fact, since we are ultimately interested in the logarithm of the determinant, it is more convenient (and more stable numerically) to consider the logarithm of the ratio, i.e.,

$$S_{(l,j)}(r) \equiv \ln\mathcal{R}_{(l,j)}(r), \quad (5.6)$$

which satisfies the differential equation

$$\frac{d^2S_{(l,j)}}{dr^2} + \left(\frac{dS_{(l,j)}}{dr}\right)^2 + \left(\frac{1}{r} + 2m\frac{I'_{2l+1}(mr)}{I_{2l+1}(mr)}\right)\frac{dS_{(l,j)}}{dr} = U_{(l,j)}(r), \quad (5.7)$$

with boundary conditions

$$S_{(l,j)}(r=0) = 0, \qquad S'_{(l,j)}(r=0) = 0. \quad (5.8)$$

The "potential" term $U_{(l,j)}(r)$ in (5.7) is given by

$$U_{(l,j)}(r) = \frac{4(j-l)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2}. \quad (5.9)$$

To illustrate the computational method, in Fig. 2 we plot $S_{[l,l+(1/2)]}(r)$ and $S_{[l+(1/2),l]}(r)$ for various values of l, with mass value $m=1$ (which is in the region in which neither

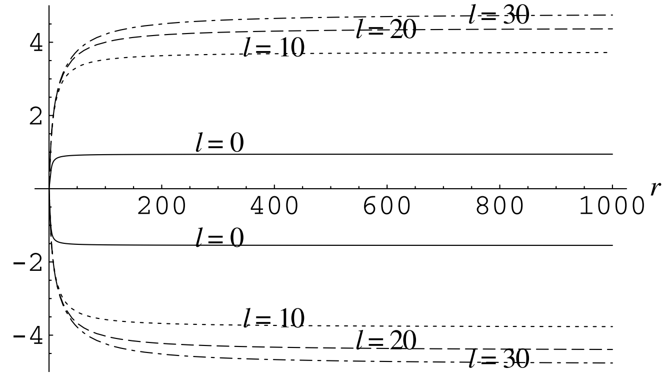

FIG. 2. Plots of the r dependence of $S_{[l,l+(1/2)]}(r)$ and $S_{[l+(1/2),l]}(r)$, solutions of the nonlinear differential equation in (5.7), for $m = 1$, and for $l = 0, 10, 20, 30$. The upper curves are for $S_{[l,l+(1/2)]}(r)$, while the lower ones are for $S_{[l+(1/2),l]}(r)$. Note that the curves quickly reach an asymptotic large-r constant value, and also notice that the contributions from $S_{[l,l+(1/2)]}(r = \infty)$ and $S_{[l+(1/2),l]}(r = \infty)$ almost cancel one another when summed.

the large nor small mass expansions is accurate). Note that the curves quickly reach an asymptotic large-r constant value, and also notice that the contributions from $S_{[l,l+(1/2)]}(r = \infty)$ and $S_{[l+(1/2),l]}(r = \infty)$ almost cancel one another when summed. This behavior is generic for all values of mass m.

To obtain very high precision for $S_{(l,j)}(r = \infty)$ in the numerical computation, it proves useful to make a further numerical modification. For large r, a good first approximation to $S_{(l,j)}(r)$ is provided by neglecting the first two terms on the left-hand side of the differential equation in (5.7). Thus we define a new function $T_{(l,j)}(r)$ by

$$S_{(l,j)}(r) = \int_0^r dr' \left(\frac{U_{(l,j)}(r')}{W_l(r')} \right) + T_{(l,j)}(r), \tag{5.10}$$

$$W_l(r) = \frac{1}{r} + 2m \frac{I'_{2l+1}(mr)}{I_{2l+1}(mr)}. \tag{5.11}$$

This new function $T_{(l,j)}(r)$ satisfies the modified equation

$$\frac{d^2 T_{(l,j)}}{dr^2} + \left(\frac{dT_{(l,j)}}{dr} \right)^2 + \left(W_l(r) + 2 \frac{U_{(l,j)}(r)}{W_l(r)} \right) \frac{dT_{(l,j)}}{dr} = -\left(\frac{U_{(l,j)}(r)}{W_l(r)} \right)^2 - \frac{d\left(\frac{U_{(l,j)}(r)}{W_l(r)}\right)}{dr} \tag{5.12}$$

with the boundary conditions: $T_{(l,j)}(0) = T'_{(l,j)}(0) = 0$. Numerical values for the quantities defined in (5.11) provide greater accuracy at large r, and are also better for large l. In fact, we can iterate this type of transformation as many times as we wish. For our computation we achieved excellent numerical precision by iterating this transformation twice.

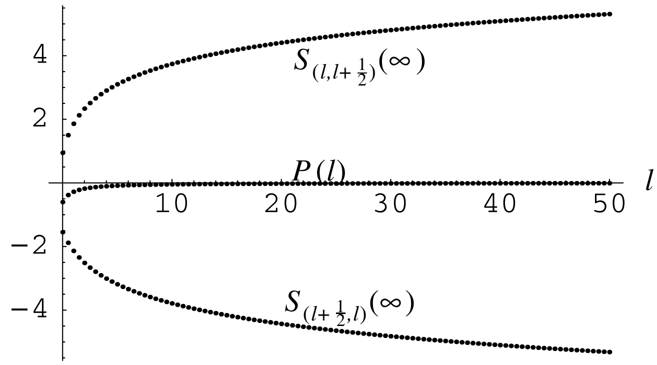

FIG. 3. Plot of $S_{[l,l+(1/2)]}(r = \infty)$, $S_{[l+(1/2),l]}(r = \infty)$, and their sum $P(l)$, defined in (5.13), for $m = 1$. Note that $S_{[l,l+(1/2)]}(r = \infty)$ and $S_{[l+(1/2),l]}(r = \infty)$ almost cancel, with their sum $P(l)$ vanishing at large l. See also Fig. 4.

The large r values of $S_{[l,l+(1/2)]}(r)$ and $S_{[l+(1/2),l]}(r)$ can be extracted with very good precision (we integrated out to $r = 10^8$). Notice that the asymptotic values of $S_{[l,l+(1/2)]}(r)$ and $S_{[l+(1/2),l]}(r)$ very nearly cancel one another, as illustrated in Fig. 3. This behavior occurs for all m, and becomes more accurate as l increases. In fact, for a given mass, it is found that, as a function of l, $S_{[l,l+(1/2)]}(r = \infty)$ grows like $\ln l$ while $S_{[l+(1/2),l]}(r = \infty)$ decreases like $-\ln l$. This divergence cancels in the sum, resulting in the behavior:

$$P(l) \equiv S_{[l,l+(1/2)]}(r = \infty) + S_{[l+(1/2),l]}(r = \infty) \sim O\left(\frac{1}{l}\right), \quad l \to \infty. \tag{5.13}$$

This behavior is illustrated in Fig. 4, which is a blowup of the $P(l)$ data in Fig. 3.

Recall from (3.6) that the first numerical sum in (4.16) is in fact a sum over $P(l)$, with degeneracy factors:

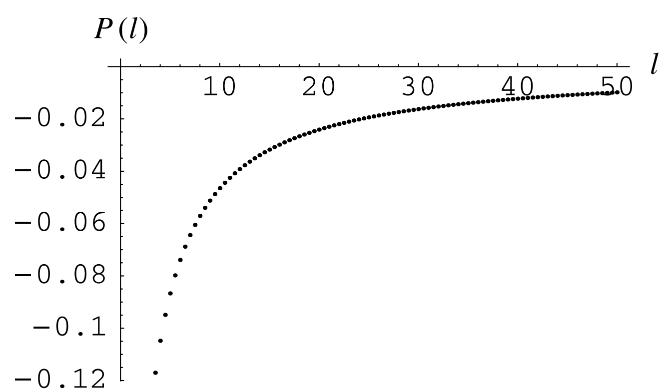

FIG. 4. Plot of the l dependence of $P(l)$, for $m = 1$. [This is a blowup of the $P(l)$ data from Fig. 3.] $P(l)$ behaves like $O(\frac{1}{l})$ for large l. Note that this implies that the sum over l in (5.14) has quadratic divergences in the large L limit.

$$\sum_{l=0,1/2,\ldots}^{L} \Gamma_l^S(A;m) = \sum_{l=0,1/2,\ldots}^{L} (2l+1)(2l+2)P(l). \quad (5.14)$$

Thus, we can rewrite our final expression (4.16) for the minimally subtracted renormalized effective action $\tilde{\Gamma}^S_{\rm ren}(m)$ as

$$\tilde{\Gamma}^S_{\rm ren}(m) = \lim_{L\to\infty}\left\{\sum_{l=0,1/2,\ldots}^{L}(2l+1)(2l+2)P(l) + 2L^2 + 4L - \left(\frac{1}{6}+\frac{m^2}{2}\right)\ln L + \left[\frac{127}{72} - \frac{1}{3}\ln 2 + \frac{m^2}{2} - m^2\ln 2 + \frac{m^2}{2}\ln m\right]\right\}. \quad (5.15)$$

The first sum is over terms that are computed numerically, as described above. The rest represents renormalization terms which have been computed using minimal subtraction and WKB.

Since the degeneracy factor $(2l+1)(2l+2)$ is quadratic, the large l behavior of $P(l)$ indicated in (5.13) [and plotted in Fig. 4] shows that in the large L limit, the sum (5.14) has potentially divergent terms going like L^2, L and $\ln L$, as well as terms finite and vanishing for large L. Remarkably, we find that these divergent terms are exactly canceled by the divergent large L terms found in the previous section for the second sum in (3.4). Thus, the renormalized effective action $\tilde{\Gamma}^S_{\rm ren}(m)$ calculated using (5.15) is finite, converges for large L, and can be computed for any mass m. We found excellent convergence with $L = 50$ in our numerical data, combined with Richardson extrapolation [26]. In Fig. 5 we plot these results for $\tilde{\Gamma}^S_{\rm ren}(m)$, and compare them with the analytic small and large mass expansions in (2.7). The agreement is spectacular. Thus, our expression (5.15) provides a simple and numerically precise interpolation between the large mass and small mass regimes.

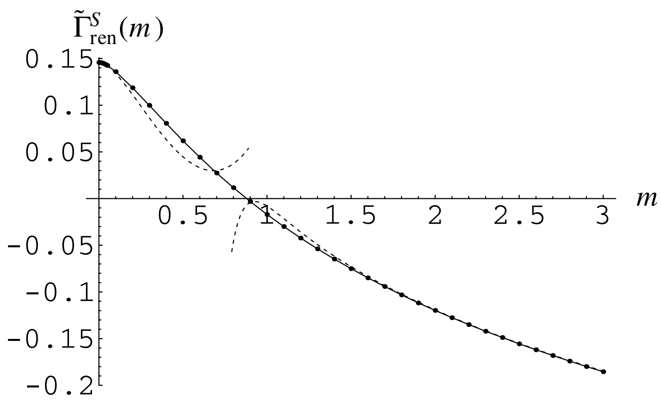

FIG. 5. Plot of our numerical results for $\tilde{\Gamma}^S_{\rm ren}(m)$ from (5.15), compared with the analytic extreme small and large mass limits [dashed curves] from (2.7). The dots denote numerical data points from (5.15), and the solid line is a fit through these points. The agreement with the analytic small and large mass limits is very precise.

As an interesting check, our formula (5.15) provides a very simple computation of 't Hooft's leading small mass result. In the $m \to 0$, (5.7) becomes

$$\frac{d^2 S_{(l,j)}}{dr^2} + \left(\frac{dS_{(l,j)}}{dr}\right)^2 + \left(\frac{4l+3}{r}\right)\frac{dS_{(l,j)}}{dr} = U_{(l,j)}(r). \quad (5.16)$$

One can find the solution of this equation in analytic form:

$$S_{[l,l+(1/2)]}(r) = \ln\left[\frac{2l+1}{2l+2}\right] + \ln\left[\sqrt{1+r^2} + \frac{1}{2l+1}\frac{1}{\sqrt{1+r^2}}\right] \quad (5.17)$$

$$S_{[l+(1/2),l]}(r) = -\ln[\sqrt{1+r^2}]. \quad (5.18)$$

As $r \to \infty$, each quantity diverges but the sum, $P(l)$, has a finite value

$$P(l) = \ln\left[\frac{2l+1}{2l+2}\right]. \quad (5.19)$$

Then it follows that

$$\begin{aligned}\tilde{\Gamma}^S_{\rm ren}(m=0) &= \lim_{L\to\infty}\left\{\sum_{l=0,1/2,\ldots}^{L}(2l+1)(2l+2)\ln\left(\frac{2l+1}{2l+2}\right) + 2L^2 + 4L - \frac{1}{6}\ln L + \frac{127}{72} - \frac{1}{3}\ln 2\right\} \\ &= -\frac{17}{72} - \frac{1}{6}\ln 2 + \frac{1}{6} - 2\zeta'(-1) \\ &= \alpha\left(\frac{1}{2}\right) = 0.145\,873\ldots \end{aligned} \quad (5.20)$$

which agrees precisely with the leading term (2.8) in the small mass limit in (2.7).

VI. COMPARISON WITH OTHER RESULTS

Since this is the first computation of the full mass dependence of the one-loop effective action in an instanton background, there is not much with which we can compare, except the small and large mass limits (2.7), which agree very well. There are, however, two other comparisons worth making. The first is with a modified Padé interpolating fit proposed in [11], which is consistent with the two leading terms in each of the known analytic small and large mass limits given in (2.7):

$$\tilde{\Gamma}^S_{\rm ren}(m) \sim -\frac{1}{6}\ln m + \frac{\frac{1}{6}\ln m + \alpha - (3\alpha+\beta)m^2 - \frac{1}{5}m^4}{1 - 3m^2 + 20m^4 + 15m^6}, \quad (6.1)$$

with $\alpha \equiv \alpha(1/2) \sim 0.145\,873$ and $\beta = \frac{1}{2}(\ln 2 - \gamma) \sim 0.057\,97$. Based on the numerical data found in the present paper, we can fit the exact mass dependence in Fig. 5 with an expanded form of this interpolating function. Let us assume the form

$$\tilde{\Gamma}^{S}_{\rm ren}(m) \sim -\frac{1}{6}\ln m + \frac{\frac{1}{6}\ln m + \alpha - (3\alpha + \beta)m^2 + A_1 m^4 - A_2 m^6}{1 - 3m^2 + B_1 m^4 + B_2 m^6 + B_3 m^8}. \quad (6.2)$$

One may easily check that the leading two terms of the small mass expansion of this expression (6.2) is the same as the small mass expansion in (2.7). Then, comparing the four leading terms of the large mass expansion of (6.2) with the large mass expansion of (2.7) fixes the coefficients B_1, B_2, B_3 to be

$$B_1 = 25\left(\frac{592\,955}{21\,609}A_2 + \frac{255}{49}A_1 + 9\alpha + 3\beta\right),$$
$$B_2 = -75\left(\frac{85}{49}A_2 + A_1\right), \qquad B_3 = 75A_2. \quad (6.3)$$

There remain two free parameters, A_1 and A_2, unfixed in (6.2). We can choose them so that the Padé approximant in (6.2) best fits the numerical data found in the previous section. This is a straightforward numerical exercise, and we find the best fit is given by

$$A_1 = -13.4138, \qquad A_2 = 2.645\,87. \quad (6.4)$$

In Fig. 6, we compare these approximations with the precise numerical data. Note that the fit based on (6.2) [solid line] is extremely precise, so we can use (6.2) as a simple analytic expression approximating the full mass dependence of the effective action, over the entire range of mass values. This is analogous to modified Padé fits used in chiral extrapolation of lattice data [14], and has also been explored for Heisenberg-Euler effective actions [29]. This form will also be useful if one wishes to capture the full ρ dependence (for a given quark mass value) of the scalar effective action $\tilde{\Gamma}^{S}_{\rm ren}(m)$ via (2.6) [and then also of the fermion effective action $\tilde{\Gamma}^{F}_{\rm ren}(m)$ via (2.1)].

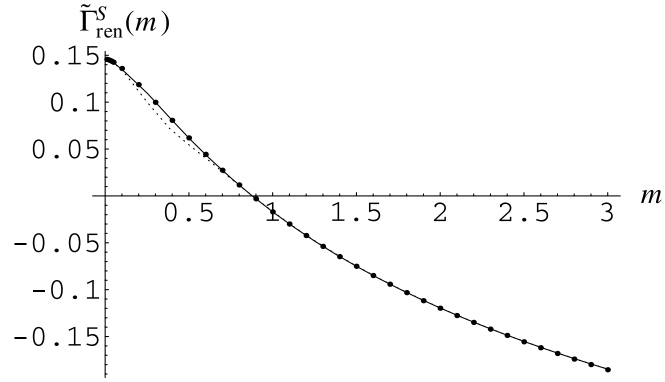

FIG. 6. Plot of "Padé" approximations of the effective action. The dotted line is the interpolation in (6.1) proposed in [11], while the solid line is the approximation in (6.2) which is an interpolating function fit to the exact mass dependence found in this paper. The solid dots are the exact numerical data.

Another comparison we can make is to the derivative expansion approximation. This approximation was already studied in [20], where it was noted that it was remarkably close to the extreme small and large mass limits in (2.7). Now that we have computed the full mass dependence of $\tilde{\Gamma}^{S}_{\rm ren}(m)$, it is worth revisiting this comparison. Recall that the philosophy of the derivative expansion is to compute the one-loop effective action for a covariantly constant background field, which can be done exactly, and then perturb around this constant background solution. The leading-order derivative expansion for the effective action is obtained by first taking the (exact) expression for the effective Lagrangian in a covariantly constant background, substituting the space-time dependent background, and then integrating over space-time. For an instanton background, which is self-dual, we base our derivative expansion approximation on a covariantly constant and self-dual background [4,30]. This leads to the following simple integral representation for the leading derivative expansion approximation to the effective action [20]:

$$\tilde{\Gamma}^{S}_{\rm ren}(A;m)]_{\rm DE} = -\frac{1}{14}\int_0^\infty \frac{dx\,x}{e^{2\pi x} - 1}\left\{-84 + 14\ln\left(1 + \frac{48x^2}{m^4}\right) + 7\sqrt{3}\frac{m^2}{x}\arctan\left(\frac{4\sqrt{3}x}{m^2}\right) + 768\frac{x^2}{m^4}\,{}_2F_1\left(1, \frac{7}{4}, \frac{11}{4}; -\frac{48x^2}{m^4}\right)\right\} - \frac{1}{6}\ln m. \quad (6.5)$$

Figure 7 shows a comparison of this leading derivative expansion expression with the exact numerical data. In the range covered, the agreement is surprisingly good for such a crude approximation.

VII. CONCLUDING REMARKS

In this paper we have presented the details of a computation of the fermion determinant in an instanton background for all values of the quark mass. The agreement with the known analytic expressions in the small and large mass limits is excellent. As another application of our result, we can reinstate the dependence on ρ, the instanton scale parameter, simply by replacing m by $m\rho$. Then, given a quark field of fixed mass m, the fermion determinant as a function of instanton size ρ can be studied. For phenomenological applications, this can now be simply described with better than 1% numerical accuracy by using the interpolating function (6.2) for $\tilde{\Gamma}^S_{\rm ren}$, together with our formulas (2.1) and (2.6). The resulting interpolating expression for the fermion determinant in an instanton background is

$$e^{-\Gamma^F_{\rm ren}} = \frac{m}{\mu}(\mu\rho)^{1/3}\exp\left\{-\frac{1}{3}\ln m\rho + \frac{\frac{1}{3}\ln(m\rho) + 2\alpha - (6\alpha + 2\beta)(m\rho)^2 + 2A_1(m\rho)^4 - 2A_2(m\rho)^6}{1 - 3(m\rho)^2 + B_1(m\rho)^4 + B_2(m\rho)^6 + B_3(m\rho)^8}\right\}. \tag{7.1}$$

This expression assumes minimal subtraction for the renormalized coupling entering the tree-level contribution. To obtain the corresponding expression for $e^{-\Gamma^F_{\rm ren}}$ in other renormalization schemes, one needs to perform additional finite renormalizations, as discussed in Refs. [11,31]. Notice that such one-loop finite renormalization terms $\Delta\Gamma^F_{\rm finite}$ can have dependence on the quark mass m (but not on ρ), and the lack of manifest decoupling for large quark mass in the expression (7.1) is a renormalization artifact [11]. We also remark that in instanton-based QCD phenomenology one may well choose the quark mass value m in (7.1) to be different from the Lagrangian (or current) quark mass, taking instead some effective mass value [32]. Our formula (7.1) can be used for discussing instanton effects in gauge theories with compact extra dimensions as well [33].

The computational method we described is versatile and can be adapted to a large class of previously insoluble computations of one-loop functional determinants in nontrivial backgrounds in various dimensions of space-time, as long as the spectral problem of the given system can be reduced to that of partial waves. One may especially consider using analogous methods for the computation of quantum corrections to the soliton energy in field theories. Several examples along this direction are currently under investigation.

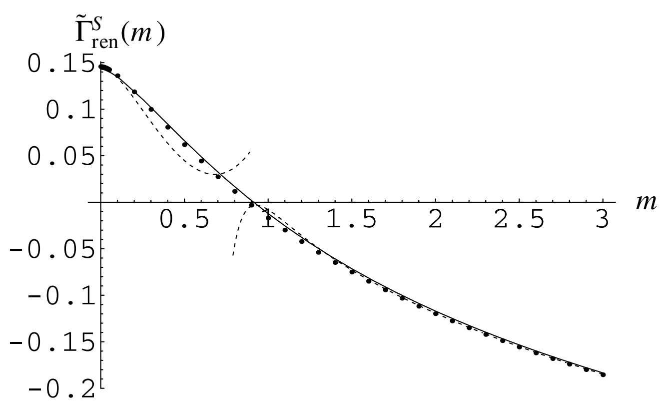

FIG. 7. Plot of $\tilde{\Gamma}^S(m)$, comparing the leading derivative expansion approximation (solid line) with the precise numerical answers (dots). The dashed lines show the small and large mass limits from (2.7).

ACKNOWLEDGMENTS

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APPENDIX A: ONE-LOOP EFFECTIVE ACTION BY THE WKB PHASE-SHIFT METHOD

WKB theory is a powerful tool for obtaining a global approximation to the solution of a second-order ordinary differential equation [26,34]. Hence one expects that it can be utilized for the approximate calculation of a one-dimensional functional determinant [35,36]. In the case of higher-dimensional functional determinants, which are usually needed in the one-loop effective action calculation of field theory, one can still try to use this WKB theory if the relevant partial differential operator becomes separable (as is often the case with rotationally invariant background fields). In the latter case, however, no useful result can be derived from such analysis if one does not have an unambiguous renormalization procedure that goes with the WKB theory. In fact, the usual leading-order WKB theory is not sufficient for the determinant calculation if a consistent renormalization demands the contribution from higher-order WKB approximation to be included. We shall see below that this is the case.

The renormalization problem mentioned above has been solved in our earlier paper [20], by including needed higher-order WKB contributions within the Schwinger proper-time representation [2] for the effective action. Also achieved there is a generalization of the Schwinger-DeWitt small proper-time expansion [37,38] to the appropriate expression for arbitrary proper-time value (in the case of rotationally invariant background fields only) so that one can have an approximation to the full effective action. In this appendix we shall briefly summarize this development and also provide further technical details on the formulas stated in [20].

In the proper-time representation (2.4) for the effective action, it is the function

$$F(s) = \int d^4x \, \mathrm{tr}\langle x|(e^{-s(-D^2)} - e^{-s(-\partial^2)})|x\rangle, \quad \text{(A1)}$$

which contains the important information. Given a rotationally invariant background field, we may utilize the phase-shift analysis with scattering solutions of the "Hamiltonian" $\mathcal{H} \equiv -D^2$ to rewrite the expression (A1). To that end we will put the system in a large spherical box of radius R (with a Dirichlet or Neumann boundary condition at $r = R$), thus making the spectrum discrete [5]. In a single instanton background, in particular, we may then consider the quantum mechanical scattering solution for each partial wave, that is,

$$\mathcal{H}_{(l,j)}\psi(r) \equiv \left\{ -\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4l(l+1)}{r^2} + \frac{4(j-l)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2} \right\}\psi(r) = k^2\psi(r). \quad \text{(A2)}$$

The corresponding free Schrödinger equation yields

$$\mathcal{H}^{\text{free}}_{(l)}\psi_0(r) \equiv \left\{ -\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4l(l+1)}{r^2} \right\}\psi_0(r) = k^2\psi_0(r). \quad \text{(A3)}$$

We are interested in the solution of (A2) and (A3) that vanishes as r^{2l} for $r \to 0$. Then, for large r, $\psi_0(r)$ behaves as

$$\psi_0(r) \sim Cr^{-3/2}\cos[k_0(n)(r+a)], \quad \text{(A4)}$$

where

$$k_0(n+1) - k_0(n) = \frac{\pi}{R} + O\left(\frac{1}{R^2}\right), \quad \text{(A5)}$$

(for nonnegative integer n), and a is a certain constant which is not important. On the other hand, we may write the large-r asymptotic behavior of the solution to (A2) in the form

$$\psi(r) \sim Cr^{-3/2}\cos[k(n)(r+a) + \eta(k(n))], \quad \text{(A6)}$$

where $\eta(k(n))$ denotes the appropriate scattering phase shift [the related scattering matrix is give by $S(k) = e^{2i\eta(k)}$]. Here, because of the boundary condition at $r = R$, we may demand the discretized momentum $k(n)$ to be related to $k_0(n)$ above according to

$$k(n)(R+a) + \eta(k(n)) = k_0(n)(R+a). \quad \text{(A7)}$$

From (A7) we conclude that

$$k_0(n) = k(n) + \frac{\eta(k(n))}{R} + O\left(\frac{1}{R^2}\right). \quad \text{(A8)}$$

If $[k^{l,j}(n)]^2$ and $[k_0^l(n)]^2$ denote the energy eigenvalues associated with the Schrödinger equations (A2) and (A3), respectively, the function $F(s)$ give by (A1) can be represented as

$$F(s) = \sum_{l=0,1/2,\cdots}\sum_j (2l+1)(2j+1) \times \sum_n \{e^{-s[k^{l,j}(n)]^2} - e^{-s[k_0^l(n)]^2}\}, \quad \text{(A9)}$$

including the degeneracy factor $(2l+1)(2j+1)$ for the (l, j) partial wave. But, because of (A8), we find for large R

$$\{e^{-s[k^{l,j}(n)]^2} - e^{-s[k_0^l(n)]^2}\} = e^{-s[k^{l,j}(n)]^2} \times \left\{\frac{2k^{l,j}(n)\eta_{l,j}(k(n))}{R}s + O\left(\frac{1}{R^2}\right)\right\}. \quad \text{(A10)}$$

Using (A10) in (A9) gives rise to

$$F(s) \sim \sum_{l=0,1/2,\cdots}\sum_j (2l+1)(2j+1) \times \sum_n 2(\Delta k)e^{-s[k^{l,j}(n)]^2}\frac{2k^{l,j}(n)\eta_{l,j}(k(n))}{\pi}s, \quad \text{(A11)}$$

where $\Delta k \equiv \frac{\pi}{R}$, and then, replacing the sum $\sum_n$ by an integral for $R \to \infty$, we obtain the following formula:

$$F(s) = \frac{2s}{\pi}\sum_{l=0,1/2,\cdots}\sum_j (2l+1)(2j+1) \times \int_0^\infty dke^{-k^2s}k\eta_{l,j}(k). \quad \text{(A12)}$$

With (A12) some caution must be exercised in dealing with the infinite partial-wave sum. Actually, in the instanton background we are considering, the nature of the scattering problem as defined by (A2) and (A3) does not allow us to consider the l sum and j sum in (A12) in a completely independent manner. The point is that, as one looks at the given forms of $\mathcal{H}_{(l,j)}$ and $\mathcal{H}^{\text{free}}_{(l)}$, their small-$r$ behaviors match for a given l value; but it is the j value that governs the large-r behavior of the potential entering $\mathcal{H}_{(l,j)}$, while j does not appear in $\mathcal{H}^{\text{free}}_{(l)}$ at all. To obtain a convergent expression from (A12), it is necessary [20] to consider the $(l, j = l + \frac{1}{2})$ and $(l + \frac{1}{2}, j = l)$ partial-wave contributions, both of which have the same degeneracy factor of $(2l+1)(2l+2)$, together as one package. With this understanding, the expression (A12) can now be cast in the form

$$F(s) = \frac{2s}{\pi}\sum_{l=0,1/2,\cdots}(2l+1)(2l+2) \times \int_0^\infty dke^{-k^2s}k[\eta_{l,l+(1/2)}(k) + \eta_{l+(1/2),l}(k)]. \quad \text{(A13)}$$

If one has complete phase shifts for all partial waves at hand, one may use this formula (A13) to calculate the function $F(s)$ and then the one-loop effective action as well. But, in the massive case, the exact phase shifts cannot be obtained analytically. Therefore, in [20], we proposed to use the WKB expressions for the phase shifts, together with our formula (A13). This method is elaborated below.

First, we need the results of Dunham [34] for higher-order WKB approximations to the scattering phase shifts. If the Schrödinger equation is written in the form

$$\left\{\frac{d^2}{dx^2} + Q(x)\right\}\Psi(x) = 0, \tag{A14}$$

the phase shift in the leading WKB approximation is given by

$$\eta^{(1)} = \frac{1}{2}\left[\oint \sqrt{Q(x)}dx - (\text{“free”})\right], \tag{A15}$$

where the integration path goes around the turning point r_1 [i.e., the point where $Q(x)$ vanishes] in the complex plane, and crosses the real axis at $r = r_0$ (with $r_0 < r$) and $r = r_2$ (with r_2 taken to positive infinity). The choice of r_0 has no effect on the value of the integral, and (“free”) in (A15) represents the same integral but with $Q(x)$ of the free Schrödinger equation. Dunham also derived the formulas in the second- and third-order WKB approximations:

$$\eta^{(2)} = -\frac{1}{2}\left[\oint \frac{1}{48}\frac{Q''(x)}{Q(x)^{3/2}}dx - (\text{“free”})\right], \tag{A16}$$

$$\eta^{(3)} = \frac{1}{2}\left[\oint\left(\frac{1}{768}\frac{Q^{(4)}(x)}{Q(x)^{5/2}} - \frac{7}{1536}\frac{[Q''(x)]^2}{Q(x)^{7/2}}dx\right) - (\text{“free”})\right]. \tag{A17}$$

One cannot use Dunham’s formula directly with the *radial* Schrödinger equation in (A2) and (A3). The latter should be transformed appropriately, following Langer [27]. Thus, writing $r = e^x$ and introducing the function

$$\Psi(x) = r\psi(r)|_{r=e^x} = e^x\psi(r = e^x), \tag{A18}$$

we recast (A2) as

$$\frac{d^2\Psi(x)}{dx^2} + e^{2x}\left\{k^2 - \frac{4(l+\frac{1}{2})^2}{e^{2x}} - \frac{4(j-l)(j+l+1)}{e^{2x}+1} + \frac{3}{(e^{2x}+1)^2}\right\}\Psi(x) = 0. \tag{A19}$$

Since this is of the form (A14), we can get the relevant scattering phase shifts simply by setting

$$Q_{(l,j)}(x) = e^{2x}\left\{k^2 - \frac{4(l+\frac{1}{2})^2}{e^{2x}} - \frac{4(j-l)(j+l+1)}{e^{2x}+1} + \frac{3}{(e^{2x}+1)^2}\right\}, \tag{A20}$$

and also, in connection with the free equation (A3),

$$Q_l(x) = e^{2x}\left\{k^2 - \frac{4(l+\frac{1}{2})^2}{e^{2x}}\right\}. \tag{A21}$$

Then, using the original variable $r = e^x$ and integrating by parts, the desired WKB expressions for the phase shifts assume the form

$$\eta^{(1)}_{l,j} = \frac{1}{2}\oint\sqrt{k^2 - \tilde{V}_{(l,j)}(r)}dr - (\text{“free”}), \tag{A22}$$

$$\eta^{(2)}_{l,j} = \frac{1}{2}\oint\left\{\frac{1}{8r^2}\frac{1}{(k^2 - \tilde{V}_{(l,j)}(r))^{1/2}} + \frac{1}{48}\frac{d^2\tilde{V}_{(l,j)}(r)}{dr^2}\frac{1}{(k^2 - \tilde{V}_{(l,j)}(r))^{3/2}}\right\}dr - (\text{“free”}), \tag{A23}$$

$$\eta^{(3)}_{l,j} = \frac{1}{2}\oint\left\{-\frac{5}{128r^4}\frac{1}{(k^2 - \tilde{V}_{(l,j)}(r))^{3/2}} - \frac{1}{128r^2}\times\frac{d^2\tilde{V}_{(l,j)}(r)}{dr^2}\frac{1}{(k^2 - \tilde{V}_{(l,j)}(r))^{5/2}} - \frac{7}{1536}\times\left(\frac{d^2\tilde{V}_{(l,j)}(r)}{dr^2}\right)^2\frac{1}{(k^2 - \tilde{V}_{(l,j)}(r))^{7/2}} - \frac{1}{768}\times\frac{d^4\tilde{V}_{(l,j)}(r)}{dr^4}\frac{1}{(k^2 - \tilde{V}_{(l,j)}(r))^{5/2}}\right\}dr - (\text{“free”}), \tag{A24}$$

where $\tilde{V}_{(l,j)}(r)$ is the so-called Langer modification [27] of the potential

$$\tilde{V}_{(l,j)}(r) \equiv \frac{4(l+\frac{1}{2})^2}{r^2} + \frac{4(j-l)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2}, \tag{A25}$$

and the term referred to (free) denotes the integral expression appearing before but with $\tilde{V}_{(l,j)}(r)$ replaced by

$$\tilde{V}_l(r) \equiv \frac{4(l+\frac{1}{2})^2}{r^2}. \tag{A26}$$

Note that $Q_{(l,j)}(x) = r^2\{k^2 - \tilde{V}_{(l,j)}(r)\}|_{r=e^x}$, and $Q^0_l(x) = r^2\{k^2 - \tilde{V}_l(r)\}|_{r=e^x}$.

Using the results (A22)–(A24) in (A13), we can simplify the expression by carrying out the k integration. First, consider the leading-order WKB. The first contour integral in (A22) can be changed to the integral along the real axis over the interval $(r_1(k), \infty)$, where $r_1(k)$ is a turning point, i.e., $[k^2 - \tilde{V}_{(l,j)}(r_1(k))] = 0$. On the other hand, k integral in (A13) runs from 0 to ∞. We may here change the order of integration, that is, perform the k integral prior to considering the r integration: in this case, the integration range for k would be over the interval $(k_1(r), \infty)$, where $k_1(r)$ represents the value specified by the condition $[k_1(r)^2 - \tilde{V}_{(l,j)}(r)] = 0$ for a given value of r. Similar consideration may be given to the second contour integral in (A23), the free part. Then, observing that we obtain from the first contour integral

$$\int_{\sqrt{\tilde{V}_{(l,j)}}}^{\infty} dk \frac{2s}{\pi} e^{-k^2 s} k \sqrt{k^2 - \tilde{V}_{(l,j)}(r)} = \frac{1}{2} \oint dk \frac{2s}{\pi} e^{-k^2 s} k \sqrt{k^2 - \tilde{V}_{(l,j)}(r)} = \frac{e^{-s\tilde{V}_{(l,j)}(r)}}{2\sqrt{\pi}\sqrt{s}}, \quad \text{(A27)}$$

(and similarly the form $e^{-s\tilde{V}_l(r)}/2\sqrt{\pi}\sqrt{s}$ from the second contour integral), we are led to the following leading-order WKB expression for $F(s)$:

$$F^{(1)}(s) = \sum_{l=0,1/2,\cdots} (2l+1)(2l+2) \times \int_0^\infty dr [f^{(1)}_{[l,l+(1/2)]}(s,r) + f^{(1)}_{[l+(1/2),l]}(s,r)], \quad \text{(A28)}$$

$$f^{(1)}_{(l,j)}(s,r) = \frac{e^{-s\tilde{V}_{(l,j)}(r)}}{2\sqrt{\pi}\sqrt{s}} - \frac{e^{-s\tilde{V}_l(r)}}{2\sqrt{\pi}\sqrt{s}}. \quad \text{(A29)}$$

We use similar procedures to simplify the contributions coming from the second- and third-order WKB phase shifts in (A23) and (A24). For this, a particularly useful relation is

$$\frac{1}{2} \oint dk \frac{2s}{\pi} e^{-k^2 s} \frac{k}{[k^2 - \tilde{V}(r)]^{n+(1/2)}} = \frac{e^{-s\tilde{V}(r)} s^{n+(1/2)} \Gamma(-n+\frac{1}{2})}{\pi}, \qquad (n = 0, 1, 2, \cdots). \quad \text{(A30)}$$

As a result, we obtain the higher-order WKB expressions for $F(s)$, i.e., $F^{(2)}(s)$ and $F^{(3)}(s)$, which may be expressed again by the form (A28) but with

$$f^{(2)}_{(l,j)}(s,r) = \frac{e^{-s\tilde{V}_{(l,j)}(r)}}{2\sqrt{\pi}\sqrt{s}} \left\{ \frac{s}{4r^2} - \frac{s^2}{12} \frac{d^2\tilde{V}_{(l,j)}(r)}{dr^2} \right\} - \frac{e^{-s\tilde{V}_l(r)}}{2\sqrt{\pi}\sqrt{s}} \left\{ \frac{s}{4r^2} - \frac{s^2}{12} \frac{d^2\tilde{V}_l(r)}{dr^2} \right\} \quad \text{(A31)}$$

$$\begin{aligned} f^{(3)}_{(l,j)}(s,r) = {} & \frac{e^{-s\tilde{V}_{(l,j)}(r)}}{2\sqrt{\pi}\sqrt{s}} \left\{ \frac{5s^2}{32r^4} - \frac{s^3}{48r^2} \frac{d^2\tilde{V}_{(l,j)}(r)}{dr^2} + \frac{7s^4}{1440} \left(\frac{d^2\tilde{V}_{(l,j)}(r)}{dr^2} \right)^2 - \frac{s^3}{288} \frac{d^4\tilde{V}_{(l,j)}(r)}{dr^4} \right\} \\ & - \frac{e^{-s\tilde{V}_l(r)}}{2\sqrt{\pi}\sqrt{s}} \left\{ \frac{5s^2}{32r^4} - \frac{s^3}{48r^2} \frac{d^2\tilde{V}_l(r)}{dr^2} + \frac{7s^4}{1440} \left(\frac{d^2\tilde{V}_l(r)}{dr^2} \right)^2 - \frac{s^3}{288} \frac{d^4\tilde{V}_l(r)}{dr^4} \right\}. \end{aligned} \quad \text{(A32)}$$

In connection with using the formula (A28), our discussion will not be complete without being clear about the *order* between executing the infinite series sum over l and performing the (improper) radial integral. This is a subtle point, and one possible way to settle the issue unambiguously would be to check explicitly which order gives rise to the known small-s behavior for the function $F(s)$ correctly. As was asserted in [20], doing the l sum before the r integration yields the correct result. If instead one performs the r integration first and then considers the l sum, it gives a result differing from the correct small-s expression of $F(s)$ by $\frac{1}{4s}$. [Note that, although we used the WKB series for the calculation, the thus-found difference is an exact result since the order-dependent ambiguity is purely a high-energy phenomenon and the WKB series can be trusted in the high-energy limit.] In view of this remark, the correct formula to be used in the WKB analysis of the effective action should read

$$F(s) = \int_0^\infty dr \sum_{l=0,1/2,\cdots} (2l+1)(2l+2) \times [f_{[l,l+(1/2)]}(s,r) + f_{[l+(1/2),l]}(s,r)]. \quad \text{(A33)}$$

The result of using this formula for the fermion determinant in a single instanton background is presented in [20].

APPENDIX B: THE INSTANTON DETERMINANT IN THE SINGULAR GAUGE

In this appendix we address the question of the gauge invariance of the determinant or the effective action. The proper-time representation of the effective action in (2.4) is written in terms of covariant derivatives and is clearly gauge invariant. However, to formulate the partial-wave expansion, as discussed in Sec. III, we chose a particular gauge (2.3). Thus the partial-wave expansion used in the main text does not possess manifest gauge invariance. In this appendix we verify gauge independence by showing that we obtain precisely the same result in a different gauge. Since our computational method relies on the radial symmetry of the background field, we are restricted in which gauge we can choose. The choice in (2.3) is often called the "regular" gauge. But an instanton background also has radial symmetry in the so-called "singular" gauge:

$$A^{\text{sing}}_\mu(x) \equiv A^a_\mu(x)\frac{\tau^a}{2} = \frac{\bar{\eta}_{\mu\nu a}\tau^a x_\nu \rho^2}{r^2(r^2+\rho^2)} \quad \text{(B1)}$$

in the singular gauge. In (B1), $\bar{\eta}_{\mu\nu a}$ differs from $\eta_{\mu\nu a}$ in (2.3) only by the sign in the components with μ or ν equal to 4 [5,7,8]. The gauge field in the singular gauge has singular behavior in the vicinity of $r = 0$. One may worry about the validity of the radial approach in the main text in the singular gauge because of this. However, it turns out that it is not so singular. Physically, the reason for this is the conformal invariance of the instanton background [5,7,8].

The differential operator $-D^2$ in the instanton background (B1) in the singular gauge can be written as, setting $\rho = 1$,

$$-D^2_{\rm sing} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4L^2}{r^2} + \frac{4(J^2 - L^2 - T^2)}{r^2(r^2+1)} + \frac{4T^2}{r^2(r^2+1)^2} \right]. \tag{B2}$$

In the region of $r \sim 0$, the potential term in (B2) has $1/r^2$ singular behavior. But the last two singular terms proportional to T^2 combine into $T^2/(r^2+1)^2$, which is regular. We decompose $1/(r^2(r^2+1))$ into $1/r^2 - 1/(r^2+1)$; i.e., into singular and regular parts. The singular part, $(J^2 - L^2)/r^2$ combines with the orbital part L^2/r^2. We can cast (B2) in the form

$$-D^2_{\rm sing} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4J^2}{r^2} + \frac{4(L^2 - J^2)}{(r^2+1)} - \frac{4T^2}{(r^2+1)^2} \right]. \tag{B3}$$

This should be compared with the corresponding operator in the regular gauge [see (3.1)]:

$$-D^2_{\rm reg} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4L^2}{r^2} + \frac{4(J^2 - L^2)}{(r^2+1)} - \frac{4T^2}{(r^2+1)^2} \right]. \tag{B4}$$

Note that these two have the same form except that J^2 and L^2 are interchanged. Therefore, in the partial-wave analysis the radial Hamiltonian (for isospin $\frac{1}{2}$) can be written as

$$\mathcal{H}^{\rm sing}_{(l,j)} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4j(j+1)}{r^2} + \frac{4(l-j)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2} \right]. \tag{B5}$$

There is a one-to-one correspondence between the eigenvalues for the sector (j, l) in the singular gauge and those for the sector (l, j) in the regular gauge, and they have the same multiplicities, $(2j+1)(2l+1)$.

The regularized one-loop effective action in the singular gauge can be written as

$$\Gamma^S_\Lambda(A_{\rm sing}; m) = \sum_{l=0,1/2,\ldots} (2l+1)(2l+2) \times \left\{ \ln\left(\frac{\det[\mathcal{H}^{\rm sing}_{[l,l+(1/2)]} + m^2]}{\det[\mathcal{H}^{\rm free}_{[l+(1/2)]} + m^2]}\right) + \ln\left(\frac{\det[\mathcal{H}^{\rm sing}_{[l+(1/2),l]} + m^2]}{\det[\mathcal{H}^{\rm free}_{(l)} + m^2]}\right) - \ln\left(\frac{\det[\mathcal{H}^{\rm sing}_{[l,l+(1/2)]} + \Lambda^2]}{\det[\mathcal{H}^{\rm free}_{[l+(1/2)]} + \Lambda^2]}\right) - \ln\left(\frac{\det[\mathcal{H}^{\rm sing}_{[l+(1/2),l]} + \Lambda^2]}{\det[\mathcal{H}^{\rm free}_{(l)} + \Lambda^2]}\right) \right\}. \tag{B6}$$

Here we have combined the radial determinants for $(l, j = l + \frac{1}{2})$ and $(l + \frac{1}{2}, j = (l + \frac{1}{2}) - \frac{1}{2})$, as in Sec. III, and we have arranged the free determinants appropriately. But from the above arguments, we know that

$$\mathcal{H}^{\rm sing}_{(l,l')} = \mathcal{H}^{\rm reg}_{(l',l)}. \tag{B7}$$

Hence the singular gauge expression in (B6) is identical with the regular gauge expression in (3.3). So the Pauli-Villars regularized one-loop effective action has the same value in the singular gauge and in the regular gauge, and therefore the renormalized effective action (2.5), and the modified effective action (2.6), has the same value in each gauge.

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