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The rotator spectrum in the delta-regime of the O(n) effective field theory in 3 and 4 dimensions

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Abstract

The low lying spectrum of the O(n) effective field theory is calculated in the delta-regime in 3 and 4 space-time dimensions using lattice regularization to NNL order. It allows, in particular, to determine, using numerical simulations in different spatial volumes, the pion decay constant F in QCD with 2 flavours or the spin stiffness ρ for an antiferromagnet in $d = 2 + 1$ dimensions.

1 Introduction

The low energy phenomena in systems with spontaneously broken symmetry are governed by the dynamics of the Goldstone bosons. This can be described by an effective field theory, and the calculations could be performed by chiral perturbation theory (ChPT) [1, 2]. The effective action contains low energy constants (LEC) determined by the underlying microscopic theory. The physical quantities can be systematically expanded in powers of momenta, or (as in the case of our interest here) inverse box size. In numerical simulations one can place the system into a space-time box of size $L_t \times L_s^{d-1}$ and study the dependence of different quantities on the box size. Comparing the data with theoretical predictions one can determine the corresponding LEC's.

There are important cases when the order parameter of the spontaneous symmetry breaking is an $\mathrm{O}(n)$ vector. These include QCD with two light quarks (4d O(4) case), and antiferromagnetic layers (3d O(3) case).

The different regimes of such systems in a finite box have been systematized by Leutwyler [3]. In particular, for the case of no explicit symmetry breaking (zero quark mass in QCD) one can distinguish the ϵ-regime ("cubic geometry"), where $L_t \sim L_s$, and the δ-regime ("cylindrical geometry") where $L_t \gg 1/m(L_s) \sim F^2 L_s^3 \gg L_s$. (Note that the expansion parameter of ChPT in this case is $1/(F^2 L_s^2)$ and must be small enough.)

In this work we calculate the low lying spectrum in a finite spatial box in the $\mathrm{O}(n)$ effective theory (i.e. we consider the δ-regime) with no explicit symmetry breaking, in 3 and 4 space time dimensions, using lattice regularization. It has been shown in [3] that in the leading order the spectrum is given by the quantum mechanical $\mathrm{O}(n)$ rotator with moment of inertia $\Theta = (n-1)/2 \cdot F^2 L_s^3$ (the "angular momentum" being the $\mathrm{O}(n)$ isospin). In the case of QCD the constant F is the pion decay constant. The next-to-leading (NL) order term of the expansion in $1/(F^2 L_s^2)$ has been calculated in [4]. In the calculation one considered an infinitely long lattice in the time direction, separating the spatially constant slow modes and the fast modes, and integrating out the latter. The resulting effective Lagrangian for the slow modes is then that of an $\mathrm{O}(n)$ rotator, with a modified moment of inertia. The NLO correction turned out to be large: at $L_s = 2.5\,\mathrm{fm}$ it is still $\sim 40\%$. Therefore it was important to calculate the NNLO term. This has been done recently for the 4d, O(4) case by P. Hasenfratz [5] by a method similar to the one used in [4], except that in [5] dimensional regularization (DR) was used. The NNLO term contains two new LEC's, Λ_1 and Λ_2, and is estimated to be -5% at $L_s = 2.5\,\mathrm{fm}$.

Since the calculation using DR with the time-dependent slow modes was quite involved, we have chosen to calculate the same quantity by a different method, following the calculation of the small-volume mass gap in 2d $\mathrm{O}(n)$ non-linear sigma-model by Lüscher, Weisz, Wolff [6], using lattice regularization, and we considered both the 3d and 4d cases for general $\mathrm{O}(n)$.

As mentioned above, the effective theory has also been successfully applied in condensed matter physics. In particular one can perform numerical simulations in the microscopic theory of the spin $\frac{1}{2}$ antiferromagnetic Heisenberg model and measure different quantities (like staggered susceptibility, etc.) with an impressive precision [7, 8]. Comparing these with the results of the effective field theory one can obtain the LEC's (spin stiffness, etc) to high accuracy of order 10^{-3} (for a recent paper see [9]). Given the high accuracy, in this case even a small NNLO term could have an important effect.

The rest of the paper is organized as follows. Section 2 discusses the different terms in the effective action needed to this order, section 3 recapitulates the method of [6] to obtain the perturbative expansion for the mass gap. In section 4 we describe the numerous checks of our calculations, and section 5 gives the general expression for the mass gap. The numerical values and the renormalization of the couplings for $d = 4$ and $d = 3$ dimensions are given in sections 6 and 7, respectively. Section 8 contains our conclusions. Some further details of the calculations are delegated to the Appendices.

2 The effective action

We consider the following effective action in 3 and 4 space-time dimensions

$$A = A_2 + A_4 + \dots\,, \tag{2.1}$$

where the leading term is

$$A_2 = \frac{1}{2\lambda_0^2} \sum_x \partial_\mu \mathbf{S}_x \cdot \partial_\mu \mathbf{S}_x, \quad x = (x_0, \mathbf{x}), \quad \mathbf{S}_x^2 = 1. \tag{2.2}$$

Here ∂_μ denotes the standard forward lattice derivative, and the A_4 part containing 4-derivative terms will be specified later. Note that we do not consider here an explicit $\mathrm{O}(n)$ symmetry breaking term.

The non-linear sigma model given by A_2 is non-renormalizable in $d > 2$ dimensions hence one has to consider A as an effective low energy action, with corresponding (infinitely many) low energy constants (LEC). The mass gap (and the energy of lowest states) in a box L_s^{d-1} can be expanded in inverse powers of the box size L_s, and to a given order in $1/L_s$ only finite number of LEC's appear. For our case of NNLO corrections we need only terms up to four derivatives in $d = 4$.

The action (2.1) in $d = 3$ describes e.g. the low energy behaviour of the antiferromagnetic spin $\frac{1}{2}$ quantum Heisenberg model, while in $d = 4$, and $n = 4$ it is the effective action of QCD with two massless quarks.

The dimensionless lattice coupling λ_0 in eq. (2.2) is expressed through the dimensionful lattice bare parameters of the corresponding theories as

$$\lambda_0^2 = \frac{1}{\rho_0 a}\,, \qquad \text{for } d = 3\,, \tag{2.3}$$

$$\lambda_0^2 = \frac{1}{F_0^2 a^2}\,, \qquad \text{for } d = 4\,, \tag{2.4}$$

where ρ_0 and F_0 denote the bare spin stiffness and bare pion decay constant, respectively, and a is the lattice spacing.[1] We parametrize the spin vector with the "pion" fields

$$\mathbf{S} = \left(\lambda_0 \vec{\pi}, \sqrt{1-\lambda_0^2\vec{\pi}^2}\right), \quad \vec{\pi} = \left(\pi^1, \pi^2, \ldots, \pi^{n-1}\right). \tag{2.5}$$

The pion fields reflect the perturbative fluctuations around the magnetization axis. We expand in the $\vec{\pi}$-fields keeping the volume $V_d = L_t \times L_s^{d-1}$ finite assuming a cylindrical geometry, $L_t \gg L_s$. As long as the volume is finite there is a slowly moving global mode which corresponds to the direction of the magnetization. This mode is treated nonperturbatively in the the path integral [10].

The partition function takes the form

$$Z = \mathcal{N} \prod_n \int d\vec{\pi}_n\, \delta\left(\frac{1}{V_d}\sum_x \vec{\pi}_x\right) \mathrm{e}^{-A_{\mathrm{eff}}[\vec{\pi}]} \tag{2.6}$$

where

$$A_{\mathrm{eff}}[\vec{\pi}] = A[\vec{\pi}] + A_{\mathrm{measure}}[\vec{\pi}] + A_{\mathrm{zero}}[\vec{\pi}]. \tag{2.7}$$

The first term is the action of (2.1) (expressed in terms of $\vec{\pi}$-fields). The second term is caused by the measure from the change to $\vec{\pi}$-variables

$$A_{\mathrm{measure}}[\vec{\pi}] = \sum_x \ln\left(1-\lambda_0^2\vec{\pi}_x^2\right)^{\frac{1}{2}}. \tag{2.8}$$

The irrelevant factor $\mathcal{N}$ and the last term together with the delta function arise when we separate the global zero mode and integrate it out in the path integral,

$$A_{\mathrm{zero}}[\vec{\pi}] = -(n-1)\ln\sum_x \left(1-\lambda_0^2\vec{\pi}_x^2\right)^{\frac{1}{2}}. \tag{2.9}$$

As a consequence of the delta function in (2.6) we must leave out the $p = (0, \mathbf{0})$ zero mode in the momentum decomposition of $\vec{\pi}$.

[1] In most expressions we use the convention "$a = 1$", but restore the a factors when it is useful for understanding.

For the $d = 4$ case at NNLO we also need the A_4 term in eq. (2.1). The most general 4-derivative interaction consistent with the lattice symmetries is given by (see e.g. [11])

$$A_4 = \sum_{i=2}^{5} \frac{g_4^{(i)}}{4} \left(A_4^{(i)} - c^{(i)} \sum_x \partial_\mu \mathbf{S}_x \cdot \partial_\mu \mathbf{S}_x \right), \tag{2.10}$$

where

$$A_4^{(1)} = \sum_x \partial_\mu \partial_\mu^* \mathbf{S}_x \cdot \partial_\nu \partial_\nu^* \mathbf{S}_x, \tag{2.11}$$

$$A_4^{(2)} = \sum_x (\partial_\mu \mathbf{S}_x \cdot \partial_\mu \mathbf{S}_x)^2, \tag{2.12}$$

$$A_4^{(3)} = \sum_x (\partial_\mu \mathbf{S}_x \cdot \partial_\nu \mathbf{S}_x)^2, \tag{2.13}$$

$$A_4^{(4)} = \sum_x \sum_\mu (\partial_\mu \mathbf{S}_x \cdot \partial_\mu \mathbf{S}_x)^2 - \frac{1}{d+2} \left(A_4^{(2)} + 2A_4^{(3)} \right), \tag{2.14}$$

$$A_4^{(5)} = A_4^{(5a)} - \frac{1}{d+2} \left(2A_4^{(5b)} + A_4^{(5c)} \right), \tag{2.15}$$

and

$$A_4^{(5a)} = \sum_x \sum_\mu \partial_\mu \partial_\mu^* \mathbf{S}_x \cdot \partial_\mu \partial_\mu^* \mathbf{S}_x, \tag{2.16}$$

$$A_4^{(5b)} = A_4^{(1)}, \tag{2.17}$$

$$A_4^{(5c)} = \sum_x \partial_\mu \partial_\mu \mathbf{S}_x \cdot \partial_\nu \partial_\nu \mathbf{S}_x. \tag{2.18}$$

We use the standard forward (∂) and backward (∂^*) lattice derivatives. Some comments are in order here:

- The interaction $A_4^{(1)}$ is redundant at the order of our calculation. Transforming variables in the path integral as $\mathbf{S} \to (\mathbf{S}+\alpha\Box\mathbf{S})/|\mathbf{S}+\alpha\Box\mathbf{S}|$ the leading action exhibits a contribution proportional to $A_4^{(1)}$. Choosing the parameter α we can absorb the contributions of this interaction [12].

- In ChPT of QCD with $N_f = 2$ flavours (in Minkowski space) the standard notation for the low energy constants is l_i [13]. Following [12] for the O(n) case (in Euclidean space) we use the convention $g_4^{(i)}/4$ for the couplings. They are related by

$$g_4^{(2)} = -4l_1\,, \quad g_4^{(3)} = -4l_2\,. \tag{2.19}$$

  The minus sign comes from going from Minkowski to Euclidean space. Note also that the convention for numbering the operators is different.

- The operators 4 and 5 are absent in dimensional regularization. They are needed to restore Lorentz symmetry on the lattice and their coefficients are fixed by this requirement. The subtracted pieces stem from the fact that we construct first the symmetric, traceless 4-index tensors, and take the sum $\sum_\mu t_{\mu\mu\mu\mu}$ [11].

- According to equation (2.10) we subtract a term proportional to the leading action A_2 from each of the 4-derivative interactions. The coefficients $c^{(i)}$ serve to remove the power-like divergence $1/a^4$ from the contribution of the corresponding operator. The subtracted operators renormalize then multiplicatively. This is discussed later.

3 Correlation function

We extract the mass gap from the correlation function

$$C(t) = \frac{1}{V_s^2} \sum_{\mathbf{x},\mathbf{y}} \langle \mathbf{S}_{x_0,\mathbf{x}} \cdot \mathbf{S}_{y_0,\mathbf{y}} \rangle , \quad t = |y_0 - x_0| \, , \tag{3.1}$$

where $V_s = L_s^{d-1}$ is the spatial volume. We follow closely the method of ref.[6] developed to obtain the small-volume mass gap $m(L_s)$ for the 2d $\mathrm{O}(n)$ nonlinear sigma-model.

We apply perturbation theory at fixed finite cylindrical volume $L_t \times L_s^{d-1}$ and following [6] we impose free boundary conditions in the time directions[2]. This guarantees that we project onto states with zero isospin (and zero total momentum) at the two boundaries. Except for the ground state all these states ("scattering states") have energies $\gtrsim 4\pi/L_s$. The correlation function drops off as

$$C(t) = A\mathrm{e}^{-m(L_s)t} + \mathcal{O}\left(\mathrm{e}^{-\frac{4\pi}{L_s}t}\right) \, , \tag{3.2}$$

where $m(L_s) = E_1 - E_0$ is the mass gap, the difference between the lowest energies in the $l = 1$ and $l = 0$ isospin sectors. For small λ_0 the mass gap is $m(L_s) \propto \lambda_0^2/V_s$ hence for $\lambda_0^2 \ll V_s/L_t$ the system is nearly completely polarized – the spins fluctuate only slightly around the direction of the total magnetization. Therefore for fixed L_s, L_t one can use perturbation theory in λ_0 to calculate the correlation function[3]

$$C(t) = 1 + \sum_{i=0}^{\infty} \left(\lambda_0^2\right)^{i+1} C_i\left(\frac{t}{L_s}\right) \, . \tag{3.3}$$

Inserting the expansion of the mass gap $m(L_s)$ into eq. (3.2) one concludes that the coefficients $C_i(t/L_s)$ are (up to exponentially decreasing terms) polynomials of order $i+1$ in

[2] with periodic b.c. in the spatial directions

[3] The notations are analogous to those of ref. [6], except that there a symmetric set-up with $x_0 = -\tau$, $y_0 = \tau$, $t = 2\tau$ is used.

the time t

$$C_i\left(\frac{t}{L_s}\right) = \sum_{k=0}^{i+1} C_{ik} \cdot \left(\frac{t}{L_s}\right)^k + \mathcal{O}\left(\mathrm{e}^{-\frac{4\pi}{L_s}t}\right) . \tag{3.4}$$

As seen from eq. (3.2) (neglecting the exponentially small terms in t) the expansion of $\log C(t)$ is linear in t, the higher order terms in t should cancel. To obtain the mass gap to NNLO only the coefficients C_{00}, C_{01}, C_{10}, C_{11}, and C_{21} are needed, while C_{12}, C_{22}, and C_{23} are useful to check the absence of t^2 and t^3 terms in $\log C(t)$.

Observe that the use of free b.c. in the time direction is essential here. Using periodic b.c. also in this direction, the transitions $l \to l+1$ between states of higher isospins with energies $E_l \approx l(l+n-2)\lambda_0^2/(2V_s)$ would also contribute to the perturbative expansion of $C(t)$, making the method unpractical for the determination of the mass gap.

Note that the method of ref. [6] is essentially an ϵ-regime expansion in a very elongated cylindrical volume, since the spins are strongly correlated over the whole length L_t. The correlation length $\xi_t(L_s) = 1/m(L_s)$, defined for an infinitely long cylindrical volume becomes much larger for $\lambda_0 \to 0$ than any finite L_t . For the "truly δ-regime" calculation one should study the dynamics of the spatially constant slow modes, which is described by the quantum mechanical rotator [3, 4, 5]. Of course, the two approaches should lead to the same result for the mass gap, but one meets different technical difficulties in these two approaches.

4 Procedure and checks

It is straightforward to derive the Feynman rules and to write down the corresponding Feynman diagrams. After that we separate the different t^n contributions analytically from each graph. This step is practically the same for $d = 2$ and $d > 2$. Evaluating the diagrams numerically provides a good check for separating the different powers of t. There are also other checks for the final results:

- The consistency relations mentioned in section 3 are satisfied.
- The NLO result is known for general dimensions [4].
- The NNLO result for $d = 2$ can be compared to the results of Lüscher and Weisz [14, 15]
- We also considered the same problem with Dirichlet-free boundary conditions. (This should obviously give the same result for the mass, but the corresponding transition

amplitudes are different.) We checked the result numerically for $d = 2$, including the 4-derivative contributions.

- Since the 4-derivative contributions were not calculated previously on the lattice for the 2d case, we compared the corresponding contributions to direct Monte-Carlo simulations for $d = 2$, $L_s = 3$ at sufficiently small λ_0 values.
- We solved the problem for $n = 2$ parametrizing the fields as $\mathbf{S}(x) = (\cos\phi(x), \sin\phi(x))$, including the 4-derivative contributions.

5 The mass gap at finite lattice spacing

Restoring the lattice spacing a the mass gap reads

$$m(L_s) = \frac{n_1 \lambda_0^2 a^{d-2}}{2L_s^{d-1}} \left[1 + \lambda_0^2 c_2(a/L_s) + \lambda_0^4 c_3(a/L_s) + \lambda_0^4 \sum_{i=2}^{5} g_4^{(i)} d_3^{(i)}(a/L_s) \right] + \mathcal{O}(\lambda_0^8) \quad (5.1)$$

The n-dependence of the coefficients is given by

$$c_2 = c_{21} + c_{22} n_1 \,, \quad (5.2)$$

$$c_3 = c_{31} + c_{32} n_1 + c_{33} n_1^2 \,, \quad (5.3)$$

$$d_3^{(i)} = d_{31}^{(i)} + d_{32}^{(i)} n_1, \qquad i = 2, 3, 4, 5 \,. \quad (5.4)$$

where we introduced the abbreviation

$$n_1 \equiv n - 1 \,. \quad (5.5)$$

The above coefficients are expressed as lattice sums over spatial momenta and are given in appendix B.

6 Results for $d = 4$

The expressions occurring in the previous section depend on the ratio a/L_s only. In four space-time dimensions one has

$$c_{2k}(a/L_s) = c_{2k0} + c_{2k1} \frac{a^2}{L_s^2} + \mathcal{O}\left(\frac{a^4}{L_s^4}\right) \,, \quad k = 1, 2 \,, \quad (6.1)$$

$$c_{3k}(a/L_s) = c_{3k0} + c_{3k1} \frac{a^2}{L_s^2} + c_{3k2} \frac{a^4}{L_s^4} + c_{3k3} \frac{a^4}{L_s^4} \log \frac{L_s}{a} + \mathcal{O}\left(\frac{a^6}{L_s^6}\right) \,, \quad k = 1, 2, 3 \,, \quad (6.2)$$

$$d_{3k}^{(i)}(a/L_s) = D_{3k}^{(i)} + E_{3k}^{(i)} \frac{a^4}{L_s^4} + \mathcal{O}\left(\frac{a^6}{L_s^6}\right) \,, \quad i = 2, 3, 4, 5; \quad k = 1, 2 \,. \quad (6.3)$$

In eq. (5.1) these coefficients are multiplied by $\lambda_0^2 = 1/F_0^2 a^2$ and $\lambda_0^4 = 1/F_0^4 a^4$, respectively. Therefore the omitted terms correspond to lattice artifacts. The resulting terms with power-like and logarithmic singularities in a will be absorbed by the renormalization of the lattice bare parameters. The numerical values of the coefficients are listed in Tables 1-3 in appendix C.

6.1 Discussion on the numerical values of appendix C

We have calculated the lattice sums in appendix B to a quadruple precision for different lattice sizes and fitted the a/L_s-dependence. In order to find out a reliable set of terms one can vary the minimum value of L_s and include fewer or more higher powers like a^6/L_s^6, a^8/L_s^8, etc. The coefficients should be stable under such variations, and we can estimate the precision of the values, which was 10 digits or better. Note, that we know the coefficients of the logarithmic terms from DR, hence fixing these parameters in the fit allows to determine the remaining ones to better accuracy.

The coefficient $c_{211} = -c_{221}$ is the shape coefficient $\beta_1^{(3)}$ for a three dimensional cubic box, given in [12]. The NLO finite size effect was first calculated in [4].

The logarithms originate from the double sums in (B.6) and (B.7). To obtain the leading L_s-dependence we expand them for small $\mathbf{k_1}$, $\mathbf{k_2}$,

$$c_{31} = \frac{1}{2V_s^2} \sum_{\mathbf{k_1 k_2}}'' \frac{s_1^2}{(s_1+s_2+s_3)s_1 s_2 s_3} + \dots \tag{6.4}$$

$$c_{32} = -\frac{1}{2V_s^2} \sum_{\mathbf{k_1 k_2}}'' \frac{s_1^2}{(s_1+s_2+s_3)s_1 s_2 s_3} + \dots\,, \tag{6.5}$$

where we expanded in $s_i \equiv \sinh \mu_i$. (See appendix A for notations.) The leading singularities of the double sums are related to those in the sum

$$\begin{aligned}\Delta \equiv \sum_x \Box_0 G(x) G(x)^2 = \\ = \frac{1}{4V_s^2} \sum_{\mathbf{k_1 k_2}}'' \frac{(1+\mathrm{e}^{-\mu_1-\mu_2-\mu_3})(\cosh\mu_1 - 1)}{(1-\mathrm{e}^{-\mu_1-\mu_2-\mu_3})\sinh\mu_1 \sinh\mu_2 \sinh\mu_3} - \frac{1}{4}\mathcal{S}_1^2 - \frac{1}{8V_s}\mathcal{S}_2 \\ = \frac{1}{4V_s^2} \sum_{\mathbf{k_1 k_2}}'' \frac{s_1^2}{(s_1+s_2+s_3)s_1 s_2 s_3} + \dots\,.\end{aligned} \tag{6.6}$$

Therefore, one has

$$c_{31} = 2\Delta + \dots\,, \tag{6.7}$$

$$c_{32} = -2\Delta + \dots\,. \tag{6.8}$$

According to the calculation in DR [5] the logarithmic part of Δ is given by

$$\int dx\, \Box_0 G(x) G(x)^2 = -\frac{10}{3}\frac{q}{16\pi^2}\frac{\log L_s}{L_s^4} + \dots\,, \tag{6.9}$$

where $q = 0.837536910696$ (cf. (C.1)). The coefficient of the logarithmic term in c_{31} is, therefore, -0.0353584296400 in agreement with the direct fits given in Table 2 in appendix C.

6.2 Renormalization for $d = 4$

The additive renormalization of the 4-derivative operators in eq. (2.10) are removed by setting

$$c^{(i)} = \frac{2}{F_0^2 a^4}\left(D_{31}^{(i)} + n_1 D_{32}^{(i)}\right)\,, \quad i = 2, 3, 4, 5. \tag{6.10}$$

The singular part of the a-dependence of the mass gap can be removed by the renormalization of the bare lattice parameters as

$$\frac{1}{F_0^2} = \frac{1}{F^2}\left[1 + \frac{b_1}{F^2 a^2} + \frac{b_2}{F^4 a^4} + \mathcal{O}\left(\frac{1}{F_0^6 a^6}\right)\right] \tag{6.11}$$

$$g_4^{(i)} = g_{40}^{(i)} + g_{41}^{(i)} \log aM = g_{41}^{(i)} \log aM_i, \quad i = 2, 3\,, \tag{6.12}$$

where M is a scale[4]. Like in DR we introduce the individual scales M_2 and M_3. Note that $g_4^{(4)}$ and $g_4^{(5)}$ do not need renormalization to this order. The coefficients in eq. (6.11) are expressed through the infinite volume limits of coefficients in eqs. (5.2), (5.3) as

$$b_1 = -c_2(0) = G(1, \mathbf{0}) - n_1 G(0) = -\frac{1}{2d} - (n-2)G(0)\,, \tag{6.13}$$

$$b_2 = -c_3(0) + 2c_2(0)^2\,. \tag{6.14}$$

Their numerical values for $d = 4$ are

$$b_1 = 0.029933390231 - 0.154933390231\, n_1\,, \tag{6.15}$$

$$b_2 = 0.001425585601 - 0.019893440100\, n_1 + 0.024004355409\, n_1^2\,. \tag{6.16}$$

Note that there are several nontrivial relations that should be satisfied to be able to absorb the singular cutoff dependence into the renormalized couplings – these are satisfied numerically to the expected accuracy, providing an additional check.

The renormalization of $g_4^{(2)}$ and $g_4^{(3)}$ agrees with the result of ChPT in dimensional regularization [2], taking into account eq. (2.19)[5]. On the lattice (with Euclidean action)

[4] In order to avoid confusion with DR we do not use Λ or μ.

[5] In ref. [2] only the $n = 4$ result is given but it is straightforward to restore the general n dependence.

we have

$$g_{41}^{(2)} = \frac{1}{16\pi^2}\left(\frac{14}{3} - 2n_1\right), \tag{6.17}$$

$$g_{41}^{(3)} = -\frac{1}{16\pi^2}\frac{8}{3}. \tag{6.18}$$

Note that, in contrast to the DR, the pion decay constant F_0 renormalizes on the lattice. The NLO coefficient b_1 in (6.11) has been calculated earlier in [4].

ChPT in the p-regime with lattice regularization was studied earlier by Shushpanov and Smilga [16] for the 4d O(4) case, who obtain, besides other 1- and 2-loop results, also the renormalization of F_0 to NLO. However, their result disagrees with ours – they obtain (for $n = 4$) $b_1 = -2G(0)$, i.e. the $-1/(2d)$ term of eq. (6.13) is missing. It is easy to verify its presence for the O(2) case in the same way as done in [16] (from the current-current correlator) when one uses the parametrization by the angular variable. In this case the action is given by $\lambda_0^{-2}\sum_{x,\mu}(1-\cos(\lambda_0\partial_\mu\phi(x)))$ while the conserved current is $A_\mu(x) = \lambda_0^{-2}\sin(\lambda_0\partial_\mu\phi(x))$. In this case one gets $b_1 = -1/(2d)$, as expected.

6.3 The moment of inertia

The isospin dependence of the lowest excitations up to (and including) NNLO corrections are given by the rotator spectrum [17, 5], i.e. by

$$E_l = \frac{l(l+2)}{2\Theta}, \quad l = 0, 1, 2, \ldots . \tag{6.19}$$

where Θ is the moment of inertia. We have also calculated the $E_2 - E_0$ gap with the method presented here, and found agreement with this expectation. The moment of inertia is given by

$$\begin{aligned}\Theta = L_s^3 F^2 \Bigg[1 &+ \frac{1}{F^2 L_s^2} 0.225784959441\,(n-2) \\ &+ \frac{1}{F^4 L_s^4}(-0.0692984943 + 0.0101978424\,n) \\ &- \frac{1}{F^4 L_s^4} 0.007071685925\,[(3n-10)\log M_2 L_s + 2n\log M_3 L_s] \\ &- \frac{g_4^{(4)}}{F^4 L_s^4}[-0.55835794046\,(n+1)] \\ &- \frac{g_4^{(5)}}{F^4 L_s^4}[0.55771822866 - 1.11639602502\,n] + \mathcal{O}\left(\frac{1}{F^6 L_s^6}\right)\Bigg].\end{aligned} \tag{6.20}$$

The scales M_2 and M_3 are related to the corresponding scales Λ_1, Λ_2 in dimensional regularization (cf. eq. (2.19)). However, to get this relation, and the values of the coefficients $g_4^{(4)}$ and $g_4^{(5)}$ (needed to restore Lorentz symmetry) one needs to relate the lattice regularization to the dimensional one. This step remains still to be done. The resulting uncertainty is a term const$/(F^4 L_s^4)$. The remaining terms are in agreement with the result of ref. [5] where the calculation was performed in DR for the $n = 4$ case.

7 Results for $d = 3$

In three space-time dimensions the coefficients of (5.2)-(5.4) depend on a/L_s as

$$c_{2k}(a/L_s) = c_{2k0} + c_{2k1}\frac{a}{L_s} + \ldots\,, \quad k = 1, 2\,, \tag{7.1}$$

$$c_{3k}(a/L_s) = c_{3k0} + c_{3k1}\frac{a}{L_s} + c_{3k2}\frac{a^2}{L_s^2} + \ldots\,, \quad k = 1, 2, 3\,, \tag{7.2}$$

$$d_{3k}^{(i)}(a/L_s) = D_{3k}^{(i)} + \mathcal{O}\left(\frac{a^3}{L_s^3}\right)\,, \quad i = 2, 3, 4, 5; \quad k = 1, 2\,. \tag{7.3}$$

The corresponding values are given in Tables 4-6 in appendix C.

7.1 Renormalization and the moment of inertia for $d = 3$

The 4-derivative interactions only contribute to order $1/L_s^3$. (Note that the corresponding couplings $g_4^{(i)}$ are dimensionful, in contrast to $d = 4$). They are also not needed for the renormalization here. Because the theory is non-renormalizable, it is expected that they are necessary to absorb divergences at higher orders. The spin stiffness renormalizes as

$$\frac{1}{\rho_0} = \frac{1}{\rho}\left(1 + \frac{b_1}{\rho a} + \frac{b_2}{\rho^2 a^2} + \ldots\right)\,. \tag{7.4}$$

The corresponding coefficients are still given by eqs. (6.13),(6.14) while their numerical values are

$$b_1 = 0.0860643431920 - 0.252731009859\, n_1\,, \tag{7.5}$$

$$b_2 = 0.0102138509611 - 0.0659002864141\, n_1 + 0.0638729633447\, n_1^2 \tag{7.6}$$

and the moment of inertia is

$$\Theta = \rho L_s^2 \left[1 + \frac{n-2}{\rho L_s}0.310373220693 - \frac{n-2}{\rho^2 L_s^2}0.000430499941 + \mathcal{O}\left(\frac{1}{L_s^3}\right)\right]. \tag{7.7}$$

The coefficient of the NNLO term has been estimated a long time ago from finite temperature simulations in the spin $\frac{1}{2}$ quantum Heisenberg model [8] and the result cited there is not consistent with our calculations. The discrepancy of parameters obtained from those finite-temperature data with other high precision measurements (about two per mille, but statistically significant) has been observed already in [9] and it was attributed to unaccounted finite-temperature corrections. A new measurement [18] of the staggered susceptibility at much lower temperatures agrees with our very small coefficient of the $\propto 1/L_s^2$ term.

8 Summary

We calculated the mass gap in the O(n) effective field theory in a cubic spatial box of size L_s for 3 and 4 space-time dimensions to NNLO, using lattice regularization. The renormalization of the bare lattice couplings is performed, however, the connection of the 4-derivative couplings with the $\overline{\mathrm{MS}}$ scheme is not established yet. This affects only the const$/F^4L_s^4$ term in the NNLO term in $d=4$ (relevant to QCD with two massless quarks), not the logarithmic terms, where we reproduced the result of [5]. Note that the effect of including a small explicit symmetry breaking (a small quark mass) has been done to LO in [3], and to NLO recently in [19]. In $d=3$ (relevant for 2+1 dimensional spin $\frac{1}{2}$ quantum Heisenberg model) our calculation is complete to NNL order since the 4-derivative operators do not contribute to this order.

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A The propagator

We expand the leading action in the $\vec{\pi}$-fields and write it as

$$A_2 = \frac{F^2}{2}\sum_x \partial_\mu \mathbf{S}_x \cdot \partial_\mu \mathbf{S}_x = \frac{1}{2}\sum_{x,y}\rho(x,y)\vec{\pi}_x\vec{\pi}_y + \mathcal{O}\left(\pi^4\right). \tag{A.1}$$

The kernel $\rho(x,y)$ decomposes into the spatial and time direction

$$\rho(x,y) = \sum_{\mu=1}^{d-1}\rho_s(x_\mu - y_\mu) + \rho_0(x_0,y_0). \tag{A.2}$$

The spatial kernel $\rho_s(x)$ is up to the sign the standard one-dimensional lattice Laplace operator

$$\rho_s(x) = 2\delta_{x,0} - \delta_{x,1} - \delta_{x,L_s-1}, \quad x = 0, 1, \ldots, L_s - 1, \tag{A.3}$$

and periodically continued for $x \geq L_s$ and $x < 0$. It is convenient to write $\rho_0(x_0, y_0)$ for free boundary conditions in matrix form

$$\rho_0 = \begin{pmatrix} 1 & -1 & 0 & \ldots & 0 & 0 & 0 \\ -1 & 2 & -1 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & -1 & 2 & -1 \\ 0 & 0 & 0 & \ldots & 0 & -1 & 1 \end{pmatrix}. \tag{A.4}$$

Consider the partial Fourier transform of the kernel

$$\tilde{\rho}(x_0, y_0, \mathbf{k}) = \sum_{\mathbf{x}} \rho(x_0, y_0, \mathbf{x} - \mathbf{y}) \mathrm{e}^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} = \rho_0(x_0, y_0) + \delta_{x_0,y_0} \tilde{\rho}_s(\mathbf{k}), \tag{A.5}$$

where

$$\tilde{\rho}_s(\mathbf{k}) = \sum_{i=1}^{d-1} 4\sin^2(k_i/2) \equiv 4\sinh^2(\mu(\mathbf{k})/2). \tag{A.6}$$

This equation defines $\mu(\mathbf{k})$ which is denoted by μ in the following. It will be useful to separate the $\mathbf{k} = \mathbf{0}$ contribution in the propagator

$$\begin{aligned} G(x, y) \equiv G(x_0, y_0, \mathbf{x} - \mathbf{y}) &= \frac{1}{V_s} \sum_{\mathbf{k}} G(x_0, y_0; \mu(\mathbf{k})) \mathrm{e}^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} \\ &= \frac{1}{V_s} g_0(x_0, y_0) + G_1(x, y) = G_0(x_0, y_0) + G_1(x, y). \end{aligned} \tag{A.7}$$

The 1-dimensional massless propagator is the inverse of ρ_0 in (A.4) with the zero mode left out (the boundaries are at $t = \pm T$)

$$g_0(x_0, y_0) = -\frac{1}{2}|x_0 - y_0| + \frac{1}{2(2T+1)}(x_0^2 + y_0^2) + \frac{T(T+1)}{3(2T+1)}. \tag{A.8}$$

and

$$G_1(x, y) = \frac{1}{V_s} \sum_{\mathbf{k}}{}' G(x_0, y_0; \mu) \mathrm{e}^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}. \tag{A.9}$$

The primed sum symbol means that the $\mathbf{k} = \mathbf{0}$ zero mode is excluded. The function $G(t, t'; \mu)$ is the massive propagator for the 1d case with free b.c.:

$$\begin{aligned} G(t, t'; \mu) = &\frac{1}{2\sinh\mu\,(1 - \mathrm{e}^{-2\mu(2T+1)})} \\ &\left\{ \mathrm{e}^{-\mu|t-t'|} + \mathrm{e}^{-\mu(4T+2-|t-t'|)} + \mathrm{e}^{-\mu(2T+1+t+t')} + \mathrm{e}^{-\mu(2T+1-t-t')} \right\}. \end{aligned} \tag{A.10}$$

This function is exponentially small for $|t-t'| \gg L_s$. In the limit $T \to \infty$ and when both time arguments are finite the propagator is simplified,

$$G(t,t';\mu) \approx \frac{\mathrm{e}^{-\mu|t-t'|}}{2\sinh\mu}. \tag{A.11}$$

The $\propto t^n$ dependence of a Feynman graph for $C(t)$ comes from the time-like part $G_0(x_0,y_0)$ in (A.7).

B Analytic results

B.1 Contributions from the leading action

We introduce the notations

$$\mathcal{S}_n = \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1}{\sinh^n\mu}\,, \tag{B.1}$$

$$\mathcal{E}_n = \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1-\mathrm{e}^{-\mu}}{\sinh^n\mu}\,, \tag{B.2}$$

$$\mathcal{C}_n = \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{\cosh\mu - 1}{\sinh^n\mu}\,. \tag{B.3}$$

The coefficients read:

$$c_{21}(a/L_s) = \frac{1}{2V_s} - \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{\mathrm{e}^{-\mu}}{2\sinh\mu}\,, \tag{B.4}$$

$$c_{22}(a/L_s) = \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1}{2\sinh\mu}\,, \tag{B.5}$$

$$\begin{aligned} c_{31}(a/L_s) = \frac{1}{2V_s^2} - \frac{1}{12}\mathcal{S}_1 + \frac{1}{12V_s}(-10\mathcal{S}_1 - 3\mathcal{E}_3 + 6\mathcal{E}_2 + 12\mathcal{E}_1) \\ + \frac{1}{4}\mathcal{E}_1(\mathcal{C}_3 + 2\mathcal{E}_1 - 2\mathcal{S}_1) - \frac{1}{4(d-1)}\mathcal{C}_3\mathcal{C}_1 \\ + \frac{1}{48V_s^2}\sum_{\mathbf{k_1k_2}}{}'' \frac{1}{(1-\mathrm{e}^{-\mu_1-\mu_2-\mu_3})\sinh\mu_1\sinh\mu_2\sinh\mu_3}\big[\mathrm{e}^{\mu_1+\mu_2} \\ +10\mathrm{e}^{\mu_1-\mu_2} - 13\mathrm{e}^{-\mu_1} + 14\mathrm{e}^{-2\mu_1-\mu_2} - 11\mathrm{e}^{-\mu_1-\mu_2} - \mathrm{e}^{-2\mu_1-2\mu_2-\mu_3}\big]\,, \end{aligned} \tag{B.6}$$

$$
\begin{aligned}
c_{32}(a/L_s) = \frac{1}{4}(\mathcal{S}_2 - \mathcal{E}_3) + \frac{1}{24V_s}(15\mathcal{S}_2 + 2\mathcal{S}_1 + 10\mathcal{E}_1) \\
+ \frac{1}{24}(\mathcal{E}_1 - \mathcal{S}_1)(11\mathcal{S}_1 + \mathcal{E}_1) - \frac{1}{6}\mathcal{S}_1^2 - \frac{1}{12}\mathcal{S}_1\mathcal{C}_1 - \frac{1}{4}\mathcal{C}_1\mathcal{C}_3 \\
+ \frac{1}{24(d-1)}(\mathcal{C}_1 + 6\mathcal{S}_1 - 6\mathcal{C}_3)\mathcal{C}_1 \\
+ \frac{1}{96V_s^2}\sum_{\mathbf{k_1 k_2}}{}'' \frac{1}{(1-\mathrm{e}^{-\mu_1-\mu_2-\mu_3})\sinh\mu_1\sinh\mu_2\sinh\mu_3}\big[\mathrm{e}^{2\mu_1} \\
+ 12 - 13\mathrm{e}^{-2\mu_1} - 9\mathrm{e}^{-\mu_1-\mu_2+\mu_3} + 8\mathrm{e}^{-\mu_1-\mu_2-\mu_3} + \mathrm{e}^{-\mu_1-\mu_2-3\mu_3} \\
-4\mathrm{e}^{-2\mu_1-2\mu_2} + 4\mathrm{e}^{-2\mu_1-2\mu_2-2\mu_3}\big] \;,
\end{aligned} \tag{B.7}
$$

(The double prime in the sum over $\mathbf{k_1}$, $\mathbf{k_2}$ means the condition that $\mathbf{k_1} \neq \mathbf{0}$, $\mathbf{k_2} \neq \mathbf{0}$, and $\mathbf{k_3} = \mathbf{k_1} - \mathbf{k_2} \neq \mathbf{0}$.)

$$
c_{33}(a/L_s) = -\frac{1}{24V_s^2} + \left(\frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1}{2\sinh\mu}\right)^2 . \tag{B.8}
$$

B.2 Contributions from the next-to-leading action

In this section we give the contributions of the 4-derivative interactions, without the contribution of the subtracted terms proportional to $c^{(i)}$ in equation (2.10). The effect of these terms is discussed in the renormalization chapter. The contributions of the interactions 2,3,4 depend only on the expression

$$
\Omega_0 \doteq \partial_0^u \partial_0^v G_{uv}\Big|_{v=u} = \frac{1}{V_s} + \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1-\mathrm{e}^{-\mu}}{\sinh\mu} = \frac{1}{V_s} + \mathcal{E}_1. \tag{B.9}
$$

They are given by

$$d_{31}^{(2)} = -2\Omega_0 \tag{B.10}$$
$$d_{31}^{(3)} = -1 - \Omega_0 \tag{B.11}$$
$$d_{31}^{(4)} = -\frac{2d}{d+2}\left(\Omega_0 - \frac{1}{d}\right) \tag{B.12}$$
$$d_{32}^{(2)} = -1 \tag{B.13}$$
$$d_{32}^{(3)} = -\Omega_0 \tag{B.14}$$
$$d_{32}^{(4)} = -\frac{d}{d+2}\left(\Omega_0 - \frac{1}{d}\right) . \tag{B.15}$$

The contribution of the fifth operator is more complicated. Using the labels introduced in section 2 we write

$$
d_{3i}^{(5)} = d_{3i}^{(5a)} - \frac{1}{d+2}\left[2d_{3i}^{(5b)} + d_{3i}^{(5c)}\right] , \quad i = 1, 2. \tag{B.16}
$$

We obtain

$$d_{31}^{(5a)} = -\frac{1}{V_s} - \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{(4+3\mathrm{e}^{-\mu}+\mathrm{e}^{-2\mu})\mathrm{e}^{-2\mu}}{(1+\mathrm{e}^{-\mu})^3} + \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1}{2\sinh^3\mu}\sum_{i=1}^{d-1}(1-\cos\mathbf{k_i})^2 \,, \quad \text{(B.17)}$$

$$d_{32}^{(5a)} = -\frac{1}{2V_s} - \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{(3+\mathrm{e}^{-\mu})\mathrm{e}^{-2\mu}}{(1+\mathrm{e}^{-\mu})^3} - \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{\cosh\mu}{2\sinh^3\mu}\sum_{i=1}^{d-1}(1-\cos\mathbf{k_i})^2 \,, \quad \text{(B.18)}$$

$$d_{31}^{(5b)} = -\frac{1}{V_s} - \frac{1}{V_s}\sum_{\mathbf{k}}{}' \mathrm{e}^{-\mu} \,, \quad \text{(B.19)}$$

$$d_{32}^{(5b)} = -\frac{1}{2} \,, \quad \text{(B.20)}$$

$$\begin{aligned} d_{31}^{(5c)} = &-\frac{1}{V_s} + \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{(3-8\mathrm{e}^{-\mu}-4\mathrm{e}^{-2\mu}+\mathrm{e}^{-4\mu})\mathrm{e}^{-\mu}}{(1+\mathrm{e}^{-\mu})^3} \\ &- \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{(2-\mathrm{e}^{-\mu}-2\mathrm{e}^{-2\mu}-\mathrm{e}^{-3\mu})\mathrm{e}^{-\mu}}{(1+\mathrm{e}^{-\mu})^2\sinh\mu}\sum_{i=1}^{d-1}(1-\cos\mathbf{k_i})^2 \\ &+ \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1}{2\sinh^3\mu}\left[\left|\sum_{i=1}^{d-1}\mathrm{e}^{i\mathbf{k_i}}(1-\cos\mathbf{k_i})\right|^2 - (\cosh\mu-1)^2\right] \,, \quad \text{(B.21)} \end{aligned}$$

$$\begin{aligned} d_{32}^{(5c)} = &-\frac{1}{2V_s} - \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{1-3\mathrm{e}^{-\mu}+13\mathrm{e}^{-2\mu}-\mathrm{e}^{-3\mu}-2\mathrm{e}^{-4\mu}}{2(1+\mathrm{e}^{-\mu})^3} \\ &- \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{(1-2\mathrm{e}^{-\mu}-\mathrm{e}^{-2\mu})\mathrm{e}^{-\mu}}{(1+\mathrm{e}^{-\mu})^2\sinh\mu}\sum_{i=1}^{d-1}(1-\cos\mathbf{k_i})^2 \\ &- \frac{1}{V_s}\sum_{\mathbf{k}}{}' \frac{\cosh\mu}{2\sinh^3\mu}\left[\left|\sum_{i=1}^{d-1}\mathrm{e}^{i\mathbf{k_i}}(1-\cos\mathbf{k_i})\right|^2 - (\cosh\mu-1)^2\right] \,. \quad \text{(B.22)} \end{aligned}$$

C Numerical values

C.1 Numerical values for $d = 4$

The values for the coefficients occurring in equation (6.1) and the following are collected in Tables 1-3 where we introduced the notations

$$\begin{aligned} q &= 0.837536910696\,, & r &= 0.9764866840\,, \\ v_0 &= -0.03163189123\,, & v_1 &= 0.01546809528\,. \end{aligned} \tag{C.1}$$

k	c_{21k}	c_{22k}
0	-0.029933390231	0.154933390231
1	0.225784959441	-0.225784959441

Table 1: Coefficients at NLO, $d = 4$.

k	c_{31k}	c_{32k}	c_{33k}
0	0.000366430100	0.001342713582	0.024004355408
1	-0.013517018599	0.083480277057	-0.069963258459
2	0.0961483532	-0.051187951	0.108634522
3	-0.035358429639	0.035358429639.	0

Table 2: Coefficients at NNLO, $d = 4$.

k	$D_{3k}^{(2)}$	$E_{3k}^{(2)}$	$D_{3k}^{(3)}$	$E_{3k}^{(3)}$	$D_{3k}^{(4)}$	$E_{3k}^{(4)}$	$D_{3k}^{(5)}$	$E_{3k}^{(5)}$
1	$-\frac{1}{2}$	$-2q$	$-\frac{5}{4}$	$-q$	0	$-\frac{4q}{3}$	v_0	$-\frac{5}{4}q + \frac{1}{2}r$
2	-1	0	$-\frac{1}{4}$	$-q$	0	$-\frac{2q}{3}$	v_1	$-\frac{3}{4}q - \frac{1}{2}r$

Table 3: Coefficients for the 4-derivative contributions at NNLO, $d = 4$.

C.2 Numerical values for $d = 3$

The values for the coefficients occurring in equation (7.1) and the following are given in Tables 4-6.

k	c_{21k}	c_{22k}
0	-0.086064343192	0.252731009859
1	0.310373220693	-0.310373220693

Table 4: Coefficients at NLO, $d = 3$.

k	c_{31k}	c_{32k}	c_{33k}
0	0.004600291377	-0.021104227057	0.063872963344
1	-0.053424134767	0.210306009764	-0.156881874998
2	0.095901036182	-0.192232572305	0.096331536123

Table 5: Coefficients at NNLO, $d = 3$.

k	$D_{3k}^{(2)}$	$D_{3k}^{(3)}$	$D_{3k}^{(4)}$	$D_{3k}^{(5)}$
1	$-\frac{2}{3}$	$-\frac{4}{3}$	0	0.038725856392
2	-1	$-\frac{1}{3}$	0	0.008715670880

Table 6: Coefficients for the 4-derivative contributions at NNLO, $d = 3$.

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