Matching effective chiral Lagrangians with dimensional and lattice regularizations

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ABSTRACT: We compute the free energy in the presence of a chemical potential coupled to a conserved charge in effective O(n) scalar field theory (without explicit symmetry breaking terms) to NNL order for asymmetric volumes in general *d*-dimensions, using dimensional (DR) and lattice regularizations. This yields relations between the 4-derivative couplings appearing in the effective actions for the two regularizations, which in turn allows us to translate results, e.g. the mass gap in a finite periodic box in d = 3 + 1 dimensions, from one regularization to the other. Consistency is found with a new direct computation of the mass gap using DR. For the case n = 4, d = 4 the model is the low-energy effective theory of QCD with $N_f = 2$ massless quarks. The results can thus be used to obtain estimates of low energy constants in the effective chiral Lagrangian from measurements of the low energy observables, including the low lying spectrum of $N_f = 2$ QCD in the δ -regime using lattice simulations, as proposed by Peter Hasenfratz.

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Contents

1	Introduction	1
2	The free energy on the lattice2.1The effective lattice action2.2Perturbative expansion2.3The chemical potential2.3.1Computation of F_1 up to $O(g_0^2)$ 2.3.2Computation of F_2 up to $O(g_0^2)$ 2.3.3Summary2.4Renormalization on the lattice2.4.1Case $d = 2$	3 3 5 7 8 9 10 11 11
	2.4.2 Case $d = 3$	13
	2.4.3 Case $d = 4$	14
3	The free energy with dimensional regularization 3.1 The effective action 3.2 Perturbative expansion 3.3 The chemical potential 3.4 Summary 3.5 Case $n = 2$ 3.6 Case $d = 2$ 3.7 Case $d = 3$ 3.8 Case $d = 4$ Matching the effective actions for $d = 2$ and $d = 4$	17 17 17 18 21 22 22 23 24 25
4	4.1 Case $d = 2$	25
	4.2 Case $d = 4$	27
5	The mass gap	29
6	Conclusions	32
\mathbf{A}	The terms $B_4^{(i)}$ and $C_4^{(i)}$	33
в	Some lattice momentum sums	34
С	Correlators appearing in F_r with lattice regularization C.1 Correlators appearing in $F_{1,0}$ and $F_{1,1}$ C.2 Correlators appearing in $F_{2,0}$ and $F_{2,1}$ C.3 Computation of F_3 up to O (g_0^2) C.3.1 Computation of $F_{3,1}^{(i)}$	36 36 38 39

D	C.5	r_{5} up to $O(g_{0})$	42 42
	C.5	C.4.1 Computation of $F_{4,1}^{(i)}$ Computation of F_5 up to $O(a_2^2)$	41 42
	C.4	Computation of F_4 up to ${ m O}\left(g_0^2 ight)$	40

1 Introduction

Quantum Chromodynamics (QCD) is a candidate theory of the strong interactions and there is good evidence that in this theory with massless quarks chiral flavor symmetry is spontaneously broken. The low energy phenomena in systems with spontaneously broken symmetry are governed by the dynamics of the Goldstone bosons (pions in the case of QCD). This can be described by an effective field theory, and the calculations can be performed by chiral perturbation theory χ PT [1, 2].

The interplay between χPT and QCD has been extremely fruitful. In early times of lattice simulations of QCD when light dynamical quarks could not be simulated efficiently, χPT was used to extrapolate the data to smaller pion masses m_{π} . Lately, since simulations at physical pion masses became feasible, one can use lattice data to obtain the parameters in the chiral Lagrangian, the pion decay constant F_{π} and the low energy constants (LEC's), from the underlying microscopic theory QCD more precisely than from phenomenology.

Both χ PT computations and lattice simulations of QCD can be done in special environments where physical experiments cannot be envisaged. One can study the dependence on parameters (such as quark masses), and one can place the system into a space-time box of size $L_t \times L_s^{d-1}$ and study the dependence of physical quantities on the box size L_s of the order a few fermi. Leutwyler was the first to systematize the different regimes of QCD in a finite box [3]. One special environment is the so called δ -regime where the system is in a periodic spatial box of sides L_s and $m_{\pi}L_s$ is small (i.e. small or zero quark mass) whereas $F_{\pi}L_s$ is large.

In 2009 Hasenfratz [4] pointed out that promising observables in the δ -regime are the low lying stable masses. Firstly measuring low lying stable masses to good precision is among the easiest numerical tasks. Secondly the finite box size introduces an infra-red cutoff which allows to study the chiral limit in a first stage and switching on the symmetry breaking terms later.

For massless two-flavor QCD the relevant χPT has $SU(2) \times SU(2) \simeq O(4)$ symmetry. It has been shown by Leutwyler [3] that in the leading order of χPT , with general (unbroken) O(n) symmetry (and d = 4), the spectrum is given by a quantum mechanical rotator $E(l) = l(l+2)/(2\Theta)$, l = 0, 1, 2, ..., the "angular momentum" being the O(n) isospin, with moment of inertia $\Theta = 1/(F^2L_s^3)$ fixed by the decay constant F (in the chiral limit).

The next-to-leading order (NLO) term of the expansion in $1/(F^2L_s^2)$ has been calculated in [5]. The level spectrum is to this order still governed solely by F, so an evaluation of this spectrum on the lattice potentially gives a good initial estimate of F. Since the NLO correction turned out to be large, however, it was important to calculate the NNLO term; furthermore the chiral logs and the LEC's l_1, l_2 (in the 4-derivative terms in the effective action) first appear at this order.

Two independent results for the NNLO correction have been presented. The first is by Hasenfratz [4] using dimensional regularization (DR). His procedure, which was quite involved, was to consider a volume infinite in the time direction, and to separate the degrees of freedom in the δ -regime into (spatially constant) slow and fast modes. The latter are then integrated out (treated in PT) resulting in an effective Lagrangian for the slow modes, an O(n) rotator with a modified moment of inertia, whose energy excitations are much smaller than those of the standard Goldstone boson excitations carrying finite momenta $\geq 2\pi/L_s$.

The second computation was by Niedermayer and Weiermann [6] using lattice regularization; it involved generalizing the computation of the small-volume mass gap in the 2d O(n) non-linear sigma-model by Lüscher, Weisz, and Wolff [7] to higher dimensions d > 2.

Of course the physical content of a QFT is independent of regularization. The matching of UV regularizations of renormalizable asymptotically free theories can be obtained by determining the ratio of Λ -parameters which just involves a 1-loop calculation. Here we have an effective QFT and the matching of different regularizations in such theories is, as far as we know, still a relatively untouched problem. In particular the results of the two NNLO computations referred to above could not be quantitatively compared, apart from the chiral logs, since relations between the couplings of the 4-derivative terms in the effective Lagrangians were unknown. In this paper we have closed this gap.

Here we compute the change in the free energy due to a chemical potential coupled to a conserved charge in the non-linear O(n) sigma model with two regularizations, lattice regularization (with standard action) in sect. 2 and DR in sect. 3. The computation is performed in a general *d*-dimensional volume with periodic boundary conditions in all directions. The volume is left asymmetric. This freedom allows us for d = 4 in sect. 4 to establish two independent relations among the 4-derivative couplings appearing in the effective actions of the two regularizations. These relations in turn allow us to convert results for physical quantities computed by the lattice regularization to those involving scales introduced in DR. Computations on the lattice, although algebraically more involved than analogous continuum computations, have the advantage that they are conceptually "fool-proof". Computations with DR are however often tricky starting at two loops.

In particular one of the relations referred to above allow us to convert the result of the mass gap computed on the lattice in [6] to DR (in sect. 5). Unfortunately the outcome of this does not agree with the result of Hasenfratz [4]. We thus recomputed the mass gap with DR and thereby obtained a result in complete agreement with that translated from the lattice. We are thus quite confident that it is correct.

The sums and integrals which appear in our computation, in particular the two-loop massless sunset diagram, are treated in a separate accompanying paper [8].

In this paper we do not consider explicit O(n) symmetry breaking. In QCD the effect of including a small explicit symmetry breaking (a small quark mass) has been done to LO in [3], and to NLO by Weingart [9, 10]. In a recent paper Matzelle and Tiburzi [11] study the effect of small symmetry breaking in the QM rotator picture, and extend the results for small non-zero temperatures.

There are other important physical systems where the order parameter of the spontaneous symmetry breaking is an O(n) vector. In particular in condensed matter physics, anti-ferromagnetic layers are described by O(3) for d = 3. Here the NNLO computation is complete to order $1/L_s^2$; for details and comparisons to experiment see ref. [5].

2 The free energy on the lattice

In this section we work with a hyper-cubic *d*-dimensional lattice of volume $V = L_t \times L_s^{d_s}$, $d_s = d - 1$. Define the aspect ratio $\ell \equiv L_t/L_s$.

The dynamical variables are spins $S_a(x)$, a = 1, ..., n of unit length $\mathbf{S}(x)^2 = 1$ with periodic boundary conditions in all directions $\mathbf{S}(x + L_t \hat{\mathbf{0}}) = \mathbf{S}(x) = \mathbf{S}(x + L_s \hat{k})$, $k = 1, ..., d_s$, where $\hat{\mu}$ is the unit vector in the μ -direction. We will often set the lattice spacing a to 1 and will restore it again only in selected equations.

2.1 The effective lattice action

The effective lattice action \mathcal{A} is a sum over terms

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

where the classical continuum limit of A_{2r} has 2r derivatives. In this paper we will only consider the expansion up to and including four derivatives.

For A_2 we take the standard lattice action:

$$A_2 = \frac{1}{2g_0^2} \sum_{x\mu} \partial_\mu \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) = -\frac{1}{g_0^2} \sum_{x\mu} \mathbf{S}(x) \cdot \mathbf{S}(x+\hat{\mu}) + \text{const}, \qquad (2.2)$$

where g_0 is the bare coupling and ∂_{μ} is the lattice difference operator (we will also need the backward difference operator ∂^*_{μ})

$$\partial_{\mu}f(x) = f(x+\hat{\mu}) - f(x), \qquad (2.3)$$

$$\partial^*_{\mu} f(x) = f(x) - f(x - \hat{\mu}).$$
 (2.4)

The most general form of the four derivative terms is given by [5]

$$A_{4} = \sum_{i=1}^{5} \frac{g_{4}^{(i)}}{4} \left[A_{4}^{(i)} - c^{(i)} \sum_{x\mu} \partial_{\mu} \mathbf{S}(x) \cdot \partial_{\mu} \mathbf{S}(x) \right] , \qquad (2.5)$$

where

$$A_4^{(1)} = \sum_x \Box \mathbf{S}(x) \cdot \Box \mathbf{S}(x) , \qquad (2.6)$$

$$A_4^{(2)} = \sum_{x\mu\nu} \left[\partial_\mu \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) \right] \left[\partial_\nu \mathbf{S}(x) \cdot \partial_\nu \mathbf{S}(x) \right] \,, \tag{2.7}$$

$$A_4^{(3)} = \sum_{x\mu\nu} \left[\partial_\mu \mathbf{S}(x) \cdot \partial_\nu \mathbf{S}(x) \right] \left[\partial_\mu \mathbf{S}(x) \cdot \partial_\nu \mathbf{S}(x) \right] , \qquad (2.8)$$

$$A_4^{(4)} = A_4^{(4a)} - \frac{1}{d+2} \left(A_4^{(2)} + 2A_4^{(3)} \right) , \qquad (2.9)$$

$$A_4^{(5)} = A_4^{(5a)} - \frac{1}{d+2} \left(2A_4^{(5b)} + A_4^{(5c)} \right) , \qquad (2.10)$$

and

$$A_4^{(4a)} = \sum_{x\mu} (\partial_\mu \mathbf{S}_x \cdot \partial_\mu \mathbf{S}_x)^2 \,, \tag{2.11}$$

$$A_4^{(5a)} = \sum_{x\mu} \Box_\mu \mathbf{S}(x) \cdot \Box_\mu \mathbf{S}(x), \qquad (2.12)$$

$$A_4^{(5b)} = A_4^{(1)} , (2.13)$$

$$A_4^{(5c)} = \sum_{x\mu\nu} \partial_\mu \partial_\mu \mathbf{S}(x) \cdot \partial_\nu \partial_\nu \mathbf{S}(x) , \qquad (2.14)$$

where

$$\Box_{\mu} \equiv \partial_{\mu} \partial_{\mu}^{*}, \qquad \Box = \sum_{\mu} \Box_{\mu}.$$
(2.15)

In (2.5) we subtract a term proportional to the leading action A_2 from each of the 4derivative interactions. The coefficients $c^{(i)}$ serve to remove the power-like divergence $1/a^p$ from the contribution of the corresponding operator, (note $c^{(4)} = 0$). The subtracted operators then renormalize multiplicatively.

The set of five operators above is redundant ¹. One can use this observation to eliminate, say, the coupling $g_4^{(1)}$ (as in [5]), or alternatively, to check that the final result for physical quantities depends only on the sum of the couplings, $g_4^{(1)} + g_4^{(2)}$.

The total action including only terms to this order is given by

$$\mathcal{A} = Z_4 A_2 + \sum_{i=1}^{5} \frac{g_4^{(i)}}{4} A_4^{(i)}, \qquad (2.18)$$

¹As explained in [5], changing the field variable

$$\mathbf{S}(x) \to [\mathbf{S}(x) + \alpha \Box \mathbf{S}(x)] / |\mathbf{S}(x) + \alpha \Box \mathbf{S}(x)|$$
(2.16)

the leading term of the effective action produces 4-derivative terms:

$$\frac{1}{2}\sum_{x\mu}\partial_{\mu}\mathbf{S}(x)\cdot\partial_{\mu}\mathbf{S}(x)\rightarrow\frac{1}{2}\sum_{x\mu}\partial_{\mu}\mathbf{S}(x)\cdot\partial_{\mu}\mathbf{S}(x)-\alpha\left(A_{4}^{(1)}-A_{4}^{(2)}\right)+\dots$$
(2.17)

up to terms with higher derivatives.

where

$$Z_4 \equiv 1 - \frac{1}{2}g_0^2 \sum_{i=1}^5 g_4^{(i)} c^{(i)} \,. \tag{2.19}$$

2.2 Perturbative expansion

After separating the zero mode as in [12] and changing to $\vec{\pi}$ variables (with $\sum_x \vec{\pi}(x) = 0$) according to $\mathbf{S} = (g_0 \vec{\pi}, \sqrt{1 - g_0^2 \vec{\pi}^2})$ we have

$$A_{2,\text{eff}}[\vec{\pi}] = A_2[\vec{\pi}] + A_{2,\text{measure}}[\vec{\pi}] + A_{2,\text{zero}}[\vec{\pi}], \qquad (2.20)$$

with

$$A_{2,\text{measure}}[\vec{\pi}] = \sum_{x} \ln\left[1 - g_0^2 \vec{\pi}(x)^2\right]^{\frac{1}{2}}, \qquad (2.21)$$

$$A_{2,\text{zero}}[\vec{\pi}] = -n_1 \ln \frac{1}{V} \sum_{x} \left[1 - g_0^2 \vec{\pi}(x)^2 \right]^{\frac{1}{2}}, \qquad (2.22)$$

where

$$n_1 \equiv n - 1 \,. \tag{2.23}$$

 $A_{2,\text{eff}}$ has a perturbative expansion

$$A_{2,\text{eff}} = A_{2,0} + g_0^2 A_{2,1} + g_0^4 A_{2,2} + \dots$$
(2.24)

where (here we will need only $A_{2,0}$ and $A_{2,1}$):

$$A_{2,0} = \frac{1}{2} \sum_{x} \partial_{\mu} \vec{\pi}(x) \cdot \partial_{\mu} \vec{\pi}(x) , \qquad (2.25)$$

$$A_{2,1} = A_{2,1}^{(a)} + A_{2,1}^{(b)}, (2.26)$$

$$A_{2,1}^{(a)} = -\frac{1}{2} \left(1 - \frac{n_1}{V} \right) \sum_x \vec{\pi}(x)^2 , \qquad (2.27)$$

$$A_{2,1}^{(b)} = \frac{1}{8} \sum_{x} \partial_{\mu} \left[\vec{\pi}(x)^2 \right] \partial_{\mu} \left[\vec{\pi}(x)^2 \right] \,. \tag{2.28}$$

We expand the couplings of the 4-derivative terms according to

$$g_4^{(i)} = \sum_{r=0} g_{4,r}^{(i)} g_0^{2r} \,. \tag{2.29}$$

Noting that the coefficients $c^{(i)}$ defined in (2.5) are of order g_0^2 :

$$c^{(i)} = \overline{c}^{(i)}g_0^2 + \dots$$
 (2.30)

the renormalization constant \mathbb{Z}_4 has a perturbative expansion

$$Z_4 = 1 + \sum_{r=2} Z_{4,r} g_0^{2r} , \qquad (Z_{4,1} = 0) , \qquad (2.31)$$

with

$$Z_{4,2} = -\frac{1}{2} \sum_{i=1}^{5} g_{4,0}^{(i)} \overline{c}^{(i)} .$$
(2.32)

The total effective action has a perturbative expansion of the form

$$\mathcal{A} = \sum_{r=0} \mathcal{A}_r g_0^{2r} \,, \tag{2.33}$$

with

$$\mathcal{A}_0 = A_{2,0} \,, \tag{2.34}$$

and

$$\mathcal{A}_1 = A_{2,1} + \sum_{i=1}^5 \frac{g_{4,0}^{(i)}}{4} A_{4,1}^{(i)}, \qquad (2.35)$$

with

$$A_{4,1}^{(1)} = \sum_{x} \Box \vec{\pi}(x) \cdot \Box \vec{\pi}(x) , \qquad (2.36)$$

$$A_{4,1}^{(i)} = 0, \quad i = 2, 3, 4,$$
 (2.37)

$$A_{4,1}^{(5)} = A_{4,1}^{(5a)} - \frac{1}{d+2} \left(2A_{4,1}^{(5b)} + A_{4,1}^{(5c)} \right) , \qquad (2.38)$$

with

$$A_{4,1}^{(5a)} = \sum_{x\mu} \Box_{\mu} \vec{\pi}(x) \cdot \Box_{\mu} \vec{\pi}(x) , \qquad (2.39)$$

$$A_{4,1}^{(5b)} = A_{4,1}^{(1)}, \tag{2.40}$$

$$A_{4,1}^{(5c)} = \sum_{x\mu\nu} \partial_{\mu}\partial_{\mu}\vec{\pi}(x) \cdot \partial_{\nu}\partial_{\nu}\vec{\pi}(x) . \qquad (2.41)$$

The perturbative coefficients of expectation values are sums of expectation values of products of $\vec{\pi}$ fields with respect to the Gaussian free field action \mathcal{A}_0 which are denoted by $\langle \dots \rangle_0$. In particular the 2-point function is given by

$$\langle \pi_a(x)\pi_b(y)\rangle_0 = \delta_{ab}G(x-y)\,,\tag{2.42}$$

with the free propagator

$$G(x) = \frac{1}{V} \sum_{p} {' \frac{\mathrm{e}^{ipx}}{\hat{p}^2}}, \quad \hat{p}_{\mu} = 2\sin\frac{p_{\mu}}{2}, \qquad (2.43)$$

where the sum is over momenta $p_0 = 2\pi n_0/L_t$, $n_0 = 0, \ldots, L_t - 1$ and $p_k = 2\pi n_k/L_s$, $n_k = 0, \ldots, L_s - 1$ and the prime on the sum means that p = 0 is omitted.

2.3 The chemical potential

A chemical potential coupled to the conserved O(n) charge Q_{12} is introduced by replacing terms in the action

$$\mathbf{S}(x) \cdot \mathbf{S}(y) \to [\mathbf{S}(x) \cdot \mathbf{S}(y)]_h, \qquad (2.44)$$

with

$$\begin{aligned} \left[\mathbf{S}(x) \cdot \mathbf{S}(y) \right]_{h} &= e^{(y_{0} - x_{0})h} S_{-}(x) S_{+}(y) + e^{-(y_{0} - x_{0})h} S_{+}(x) S_{-}(y) + \sum_{a=3}^{n} S_{a}(x) S_{a}(y) \\ &= \mathbf{S}(x) \cdot \mathbf{S}(y) + i \sinh\left((y_{0} - x_{0})h\right) \left[S_{1}(x) S_{2}(y) - S_{2}(x) S_{1}(y)\right] \\ &+ \left\{ \cosh\left((y_{0} - x_{0})h\right) - 1 \right\} \left[S_{1}(x) S_{1}(y) + S_{2}(x) S_{2}(y)\right] , \end{aligned}$$

$$(2.45)$$

where $S_{\pm} = \frac{1}{\sqrt{2}}(S_1 \pm iS_2)$. This gives an additional *h*-dependent part \mathcal{A}_h to the total action of the form

$$\mathcal{A}_{h} = Z_{4}A_{2h} + \sum_{i=1}^{5} \frac{g_{4}^{(i)}}{4} A_{4h}^{(i)}. \qquad (2.46)$$

Further writing

$$A_{2h} = ihB_2 + h^2C_2 + \dots , (2.47)$$

$$A_{4h}^{(i)} = ihB_4^{(i)} + h^2C_4^{(i)} + \dots, \qquad (2.48)$$

we have

$$B_2 = -\frac{1}{g_0^2} \sum_x \left[S_1(x) S_2(x+\hat{0}) - S_2(x) S_1(x+\hat{0}) \right] , \qquad (2.49)$$

$$C_2 = -\frac{1}{2g_0^2} \sum_x \left[S_1(x) S_1(x+\hat{0}) + S_2(x) S_2(x+\hat{0}) \right] , \qquad (2.50)$$

and the terms $B_4^{(i)}, C_4^{(i)}$ are given in Appendix A.

The *h*-dependent part of the free energy f_h defined by:

$$e^{-Vf_h} = \langle e^{-\mathcal{A}_h} \rangle_{\mathcal{A}} = 1 - \langle \mathcal{A}_h \rangle_{\mathcal{A}} + \frac{1}{2} \langle \mathcal{A}_h^2 \rangle_{\mathcal{A}} + \dots$$
(2.51)

giving up to the order h^2 :

$$Vf_h = \langle \mathcal{A}_h \rangle_{\mathcal{A}} - \frac{1}{2} \langle \mathcal{A}_h^2 \rangle_{\mathcal{A}} + \frac{1}{2} \langle \mathcal{A}_h \rangle_{\mathcal{A}}^2 + \dots$$
(2.52)

For finite volumes the $\lim_{h\to 0} (f_h/h^2)$ exists; we define the corresponding susceptibility χ by

$$\chi \equiv -2\lim_{h \to 0} \left(f_h / h^2 \right) \,. \tag{2.53}$$

Now

$$\langle B_2 \rangle_{\mathcal{A}} = 0 = \langle B_4^{(i)} \rangle_{\mathcal{A}} \quad \forall i ,$$
 (2.54)

so we have

$$\chi = -2\sum_{s=1}^{5} F_s \,, \tag{2.55}$$

with

$$F_1 = Z_4 \frac{1}{V} \langle C_2 \rangle_{\mathcal{A}} \,, \tag{2.56}$$

$$F_2 = \frac{1}{2} Z_4^2 \frac{1}{V} \langle B_2^2 \rangle_{\mathcal{A}} \,, \tag{2.57}$$

$$F_3 = \sum_{i=1}^5 \frac{g_4^{(i)}}{4} \frac{1}{V} \langle C_4^{(i)} \rangle_{\mathcal{A}}, \qquad (2.58)$$

$$F_4 = Z_4 \sum_{i=1}^5 \frac{g_4^{(i)}}{4} \frac{1}{V} \langle B_2 B_4^{(i)} \rangle_{\mathcal{A}}, \qquad (2.59)$$

$$F_5 = \frac{1}{2} \sum_{ij} \frac{g_4^{(i)}}{4} \frac{g_4^{(j)}}{4} \frac{1}{V} \langle B_4^{(i)} B_4^{(j)} \rangle_{\mathcal{A}} \,.$$
(2.60)

In the following subsections where we compute the contributions F_s we will use the fact that the total action \mathcal{A} is invariant under global O(n) transformations of the spins, so that the expectation value of any observable is equal to the expectation value of its average over O(n) rotations Ω :

$$\langle \mathcal{O}[S] \rangle_{\mathcal{A}} = \langle [\mathcal{O}[S]]_{\Omega} \rangle_{\mathcal{A}}.$$
 (2.61)

For arbitrary spins $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ we will use the following averages

$$[a_1b_1 + a_2b_2]_{\Omega} = \frac{2}{n} (\mathbf{a} \cdot \mathbf{b}), \qquad (2.62)$$

and

$$[(a_1b_2 - a_2b_1)(c_1d_2 - c_2d_1)]_{\Omega} = \frac{2}{n(n-1)} \left[(\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c}) \right] .$$
(2.63)

2.3.1 Computation of F_1 up to O (g_0^2)

Averaging over the rotations (using (2.62)) we have

$$\frac{1}{V} [C_2]_{\Omega} = -\frac{1}{ng_0^2} + \frac{1}{2ng_0^2} U, \qquad (2.64)$$

where

$$U = \frac{1}{V} \sum_{x} \partial_0 \mathbf{S}(x) \cdot \partial_0 \mathbf{S}(x) \,. \tag{2.65}$$

This has the perturbative expansion

$$U = g_0^2 U_1 + g_0^4 U_2 + \dots (2.66)$$

with

$$U_{1} = \frac{1}{V} \sum_{x} \partial_{0} \vec{\pi}(x) \cdot \partial_{0} \vec{\pi}(x) ,$$

$$U_{2} = \frac{1}{4V} \sum_{x} \left[\partial_{0} \vec{\pi}(x)^{2} \right]^{2} .$$
(2.67)

Expanding (2.56) in a perturbative series

$$F_1 = -\frac{1}{ng_0^2} + \sum_{r=0}^{\infty} F_{1,r}g_0^{2r}, \qquad (2.68)$$

we have at leading orders

$$F_{1,0} = \frac{1}{2n} \langle U_1 \rangle_0 \,, \tag{2.69}$$

and

$$F_{1,1} = \frac{1}{2n} \left[-2Z_{4,2} + \langle U_2 \rangle_0 - \langle U_1 A_{2,1} \rangle_0^c - \sum_{i=1}^5 \frac{g_{4,0}^{(i)}}{4} \langle U_1 A_{4,1}^{(i)} \rangle_0^c \right], \tag{2.70}$$

where the superscript c in $\langle \dots \rangle_{0}^{c}$ means the connected part. The correlation functions appearing in (2.69,2.70) are given in Appendix C.1 yielding

$$F_{1,0} = \frac{n_1}{2n} I_{11} , \qquad (2.71)$$

and

$$F_{1,1} = \frac{n_1}{2n} \left[-\frac{2}{n_1} Z_{4,2} + I_{11} \left\{ I_{10} - \frac{1}{4} I_{11} \right\} - \mathcal{F}_1 + \left(1 - \frac{n_1}{V} \right) I_{21} - \frac{g_{4,0}^{(1)}}{2} I_{01} - \frac{g_{4,0}^{(5)}}{2} \left\{ J_{21} - \frac{1}{d+2} \left(2I_{01} + \mathcal{F}_4 \right) \right\} \right].$$

$$(2.72)$$

Here I_{nm} , J_{nm} , \mathcal{F}_1 , \mathcal{F}_4 are momentum sums defined in equations (B.1), (B.2), (B.4), (B.6), (B.9) respectively.

2.3.2 Computation of F_2 up to $O(g_0^2)$

Averaging over the rotations one has, using (2.63),

$$\frac{1}{V} \left[B_2^2 \right]_{\Omega} = \frac{4}{n n_1 g_0^4} W \,, \tag{2.73}$$

where W is given by

$$W = \frac{1}{V} \sum_{xy} \nabla_0 \mathbf{S}(x) \cdot \nabla_0 \mathbf{S}(y) \left[\mathbf{S}(x) \cdot \mathbf{S}(y) - 1 \right], \qquad (2.74)$$

where $\nabla_0 = \frac{1}{2}(\partial_0 + \partial_0^*)$ is the symmetric derivative. W has a perturbative expansion

$$W = g_0^4 W_2 + g_0^6 W_3 + \dots (2.75)$$

with (to the order we need)

$$W_2 = \frac{1}{V} \sum_{xy} \left[\nabla_0 \vec{\pi}(x) \cdot \nabla_0 \vec{\pi}(y) \right] \vec{\pi}(x) \cdot \vec{\pi}(y) , \qquad (2.76)$$

$$W_3 = \frac{1}{2V} \sum_{xy} \left[\nabla_0 \vec{\pi}(x) \cdot \nabla_0 \vec{\pi}(y) \right] \vec{\pi}(x)^2 \vec{\pi}(y)^2 \,. \tag{2.77}$$

Expanding (2.57) in a perturbative series

$$F_2 = \sum_{r=0}^{\infty} F_{2,r} g_0^{2r} , \qquad (2.78)$$

we have at leading order

$$F_{2,0} = \frac{2}{nn_1} \langle W_2 \rangle_0 \,, \tag{2.79}$$

and at next order

$$F_{2,1} = \frac{2}{nn_1} \Big[\langle W_3 \rangle_0 - \langle W_2 A_{2,1} \rangle_0^c - \sum_{i=1}^5 \frac{g_{4,0}^{(i)}}{4} \langle W_2 A_{4,1}^{(i)} \rangle_0^c \Big].$$
(2.80)

The correlation functions appearing in (2.79) and (2.80) are computed in Appendix C.2 yielding

$$F_{2,0} = \frac{2(n_1 - 1)}{n} \left[I_{21} - \frac{1}{4} I_{22} \right] , \qquad (2.81)$$

and

$$F_{2,1} = \frac{1}{n} W_{3c} + \frac{2(n_1 - 1)}{n} \Big[W_{3a} - 2\mathcal{F}_2 + \mathcal{F}_3 + 2\left(1 - \frac{n_1}{V}\right) \left\{ I_{31} - \frac{1}{4} I_{32} \right\} - g_{4,0}^{(1)} \left(I_{11} - \frac{1}{4} I_{12} \right) - g_{4,0}^{(5)} \left(J_{31} - \frac{1}{4} J_{32} - \frac{1}{d+2} \left\{ 2I_{11} - \frac{1}{2} I_{12} + \mathcal{F}_5 \right\} \Big) \Big],$$

$$(2.82)$$

where $\mathcal{F}_2, \mathcal{F}_3 \mathcal{F}_5$ are defined in (B.7, B.8, B.10), and W_{3a}, W_{3c} are defined through

$$W_{3a} = -\sum_{x} G(x)^2 \nabla_0^2 G(x) , \qquad (2.83)$$

$$W_{3c} = \sum_{x} \nabla_0 G(x) \left[(\partial_0 G(x))^2 - (\partial_0^* G(x))^2 \right] = -\frac{1}{6} \sum_{x} \left[\Box_0 G(x) \right]^3 \,. \tag{2.84}$$

2.3.3 Summary

The computation of the leading contributions to F_3 , F_4 , F_5 follows similar steps as in the subsections above and details are presented in Appendices C.3-C.5. Summarizing our results so far, the susceptibility with standard lattice regularization is given by

$$\chi = \frac{2}{ng_0^2} \left(1 + \overline{R}_1 g_0^2 + \overline{R}_2 g_0^4 + \dots \right) \,, \tag{2.85}$$

with

$$\overline{R}_1 = -\frac{n_1}{2}I_{11} - 2(n_1 - 1)\left(I_{21} - \frac{1}{4}I_{22}\right), \qquad (2.86)$$

and

$$\overline{R}_2 = \overline{R}_2^{(a)} + \overline{R}_2^{(b)} , \qquad (2.87)$$

$$\overline{R}_{2}^{(a)} = -\frac{1}{2}n_{1}\left[I_{11}\left\{I_{10} - \frac{1}{4}I_{11}\right\} - \mathcal{F}_{1} + \left(1 - \frac{n_{1}}{V}\right)I_{21}\right] - W_{3c} - 2(n_{1} - 1)\left[W_{3a} - 2\mathcal{F}_{2} + \mathcal{F}_{3} + 2\left(1 - \frac{n_{1}}{V}\right)\left\{I_{31} - \frac{1}{4}I_{32}\right\}\right],$$
(2.88)

and

$$\overline{R}_{2}^{(b)} = \sum_{i=1}^{5} g_{4,0}^{(i)} G^{(i)} , \qquad (2.89)$$

with

$$G^{(1)} = -\frac{1}{2}\overline{c}^{(1)} + 2I_{11} - \frac{1}{2}I_{12} + n_1 \left[I_{00} - \frac{1}{4}I_{01}\right], \qquad (2.90)$$

$$G^{(2)} = -\frac{1}{2}\overline{c}^{(2)} + 2I_{11} + n_1 I_{00}, \qquad (2.91)$$

$$G^{(3)} = -\frac{1}{2}\overline{c}^{(3)} + I_{00} + (n_1 + 1)I_{11}, \qquad (2.92)$$

$$G^{(4)} = -\frac{1}{2}\overline{c}^{(4)} - \frac{(n_1+2)}{(d+2)} \left[I_{00} - dI_{11} \right], \qquad (2.93)$$

$$G^{(5)} = -\frac{1}{2}\overline{c}^{(5)} - \frac{2}{(d+2)} \left\{ 2I_{11} - \frac{1}{2}I_{12} + n_1 \left[I_{00} - \frac{1}{4}I_{01} \right] \right\} - \frac{n_1}{(d+2)} \left[-(d+1) \left\{ 3I_{11} - I_{12} \right\} + \mathcal{F}_6 - \frac{1}{4}(d+2)J_{21} + \frac{1}{4}\mathcal{F}_4 \right] + (n_1 - 1) \left\{ 2J_{31} - \frac{1}{2}J_{32} - \frac{1}{(d+2)} \left[2\mathcal{F}_5 + (d+1) \left(4I_{22} - I_{23} \right) - 2\mathcal{F}_7 \right] \right\}.$$
 (2.94)

A check of (2.88) for the special case of n = 2 is given in Appendix D.

2.4 Renormalization on the lattice

The renormalization procedure depends on the dimension; in the following we will consider the cases d = 2, 3, 4.

2.4.1 Case d = 2

For d = 2 the theory is renormalizable so we can set the 4-derivative couplings $g_4^{(i)}$ to zero. As is well known the theory is asymptotically free.

A renormalized "minimal" lattice coupling $g_{\text{latt}}(\mu)$ is defined through

$$\frac{1}{g_0^2} = \frac{1}{g_{\text{latt}}^2(\mu)} - b_0 \ln(a\mu) - b_1 \ln(a\mu) g_{\text{latt}}^2(\mu) + \dots$$
(2.95)

where b_0, b_1 are the universal 1-, and 2-loop coefficients of the β -function [13, 14]:

$$b_0 = \frac{n-2}{2\pi}, \quad b_1 = \frac{n-2}{4\pi^2}.$$
 (2.96)

In the continuum limit

$$I_{11} = \frac{1}{2} + \mathcal{O}\left(a^2\right) \,, \tag{2.97}$$

$$I_{21} = \frac{1}{4\pi} \ln(L_s/a) + I_{21;0}(\ell) + \mathcal{O}(a^2) , \qquad (2.98)$$

$$I_{22} = \frac{1}{2} - \frac{1}{2\pi} + \mathcal{O}\left(a^2\right) \,. \tag{2.99}$$

The coefficients $I_{nm;r}$ appearing in the large L_s/a expansion of I_{nm} are considered in [8].

So

$$\overline{R}_1 = -b_0 \ln(L_s/a) + \overline{r}_1 + \mathcal{O}\left(a^2\right) , \qquad (2.100)$$

with

$$\overline{r}_1 = -\frac{1}{4} - 2(n-2) \left[I_{21;0}(\ell) + \frac{1}{8\pi} \right] \,. \tag{2.101}$$

Next

$$I_{10} = \frac{1}{2\pi} \ln(L_s/a) + I_{10;0}(\ell) + \mathcal{O}(a^2) , \qquad (2.102)$$

$$I_{32} = \frac{3}{16\pi} \ln(L_s/a) + I_{32;0}(\ell) + O(a^2) , \qquad (2.103)$$

$$\frac{1}{V}I_{31} = I_{31;-1}(\ell) + \mathcal{O}\left(a^2\right), \qquad (2.104)$$

$$\mathcal{F}_{1} = \frac{1}{2\pi} \ln(L_{s}/a) + I_{21;0}(\ell) + \frac{1}{2} I_{10;0}(\ell) - \frac{1}{8} + O(a^{2}) , \qquad (2.105)$$

$$\mathcal{F}_{2} - I_{31} = \frac{1}{8\pi^{2}} \ln^{2}(L_{s}/a) + \frac{1}{2\pi} \left\{ I_{21;0}(\ell) + \frac{1}{2} I_{10;0}(\ell) + \frac{1}{8\pi} - \frac{11}{32} \right\} \ln(L_{s}/a) + \mathcal{F}_{2;0} + \mathcal{O}\left(a^{2}\right), \qquad (2.106)$$

$$\mathcal{F}_{2;0} = \left[I_{10;0}(\ell) - \frac{1}{4}\right] \left\{I_{21;0}(\ell) - \frac{1}{8} + \frac{1}{8\pi}\right\} - I_{31;-1}(\ell) - \frac{1}{4}I_{32;0}(\ell), \qquad (2.107)$$

$$W_{3a} = \frac{1}{8\pi^2} \ln^2(L_s/a) + W_{3a;0x}(\ell) \ln(L_s/a) + W_{3a;0}(\ell) + \mathcal{O}\left(a^2\right) , \qquad (2.108)$$

$$W_{3c} = \frac{1}{48} + \mathcal{O}\left(a^2\right) \,. \tag{2.109}$$

 So

$$\overline{R}_2^{(a)} = -b_1 \ln(L_s/a) + \overline{r}_2 + \mathcal{O}\left(a^2\right) , \qquad (2.110)$$

with

$$\overline{r}_{2} = -\frac{5}{96} + 4(n-2)^{2} I_{31;-1}(\ell) - 2(n-2) \left[W_{3a;0}(\ell) + \frac{1}{64} - 2 \left\{ I_{10;0}(\ell) - I_{21;0}(\ell) - \frac{1}{8} - \frac{1}{8\pi} \right\} \left\{ I_{21;0}(\ell) - \frac{1}{8} + \frac{1}{8\pi} \right\} \right],$$
(2.111)

where we have used the relation

$$W_{3a;0x}(\ell) = \frac{1}{2\pi} \left[I_{10;0}(\ell) - \frac{1}{4} + \frac{1}{4\pi} \right] .$$
 (2.112)

We thus obtain in the continuum limit:

$$\chi = \frac{2}{ng_{\text{latt}}^2(\mu)} \left\{ 1 + \left[-b_0 \ln(\mu L_s) + \overline{r}_1 \right] g_{\text{latt}}^2(\mu) + \left[-b_1 \ln(\mu L_s) + \overline{r}_2 \right] g_{\text{latt}}^4(\mu) + \dots \right\}$$

$$= \frac{2}{ng_{\text{latt}}^2(1/L_s)} \left\{ 1 + \overline{r}_1 g_{\text{latt}}^2(1/L_s) + \overline{r}_2 g_{\text{latt}}^4(1/L_s) + \dots \right\}$$
(2.113)

which is interpreted as an expansion in the running lattice coupling $g_{\text{latt}}(1/L_s)$, the expansion being sensible only for physically small box size L_s .

2.4.2 Case d = 3

For d = 3 we set $g_0^2 = 1/(\rho_0 a)$, where ρ_0 is the bare spin stiffness, and define a renormalized coupling ρ as in [6] through

$$\frac{1}{\rho_0} = \frac{1}{\rho} \left(1 + \frac{b_1}{\rho a} + \frac{b_2}{\rho^2 a^2} + \dots \right) \,. \tag{2.114}$$

Then we have

$$\chi = \frac{2\rho}{n} \left(1 + \frac{1}{\rho a} \hat{R}_1 + \frac{1}{\rho^2 a^2} \hat{R}_2 + \dots \right)$$
(2.115)

with

$$\hat{R}_1 = \overline{R}_1 - b_1 \,, \tag{2.116}$$

$$\hat{R}_2 = \overline{R}_2 - b_2 + b_1^2. \tag{2.117}$$

From [8] for $d = 3 \overline{R}_1$ has a large L_s/a expansion of the form

$$\overline{R}_1 = -\frac{1}{6} - (n-2)I_{10;0} - 2(n-2)I_{21;1}(\ell)\frac{a}{L_s} + \dots$$
(2.118)

with $I_{10:0} = 0.252731009859$, where in d = 3 the large L_s/a expansion of X_A is given by $X_A = \sum_{r=r_0} X_{A;r} (a/L_s)^r$. So for renormalization at leading order we need

$$b_1 = -\frac{1}{6} - (n-2)I_{10;0}. \qquad (2.119)$$

After choosing the $\overline{c}^{(i)}$ appropriately the terms in \hat{R}_2 coming from $\overline{R}_2^{(b)}$ are of order a^3/L_s^{3-2} , so the continuum limit is determined only by $\overline{R}_2^{(a)}$ Further $\overline{R}_2^{(a)}$ has a large L_s/a expansion for d = 3 of the form

$$\overline{R}_{2}^{(a)} = \overline{R}_{2;0}^{(a)} + \overline{R}_{2;1}^{(a)} \frac{a}{L_{s}} + \overline{R}_{2;2}^{(a)} \frac{a^{2}}{L_{s}^{2}} + \dots$$
(2.120)

so renormalization requires

$$b_2 - b_1^2 = \overline{R}_{2;0} , \qquad (2.121)$$

which gives

$$b_2 = b_{20} + b_{21}n_1 + b_{22}n_1^2, (2.122)$$

with coefficients independent of ℓ^{3}

$$b_{20} = 2W_{3a;0} - W_{3c;0} = 0.0102138509611,$$

$$b_{21} = \frac{1}{72} - 2W_{3a;0} - I_{10;0}^2 = -0.0659002864141,$$

$$b_{22} = I_{10;0}^2 = 0.0638729633447.$$
(2.123)

²The couplings of the 4-derivative interactions in d = 3 have dimension in the continuum formulation. ³ Note $4I_{21;0} - I_{22;0} = 2I_{10;0} - 1/d$.

Further we need

$$0 = \overline{R}_{2;1}^{(a)} = 2(n-2) \left[-W_{3a;1} + \left\{ I_{10;0} - \frac{1}{6} \right\} I_{10;1} \right], \qquad (2.124)$$

which we have verified numerically to high precision for $\ell = 1$ and $\ell = 2$ [8].

So finally we have for d = 3 in the continuum limit:

$$\chi = \frac{2\rho}{n} \left(1 - \frac{1}{\rho L_s} 2(n-2) I_{21;1}(\ell) + \frac{1}{\rho^2 L_s^2} \overline{R}_{2;2}^{(a)}(\ell) + \dots \right)$$
(2.125)

with

$$\overline{R}_{2;2}^{(a)} = 2(n-2) \left\{ -W_{3a;2} + 2I_{21;1} \left(I_{10;1} - I_{21;1} \right) + \frac{2}{\ell} (n-2)I_{31;-1} \right\}.$$
(2.126)

This result for the susceptibility agrees with (2.29) of [5]⁴. e.g.:

$$\overline{R}_{2;2}^{(a)}(\ell) = \begin{cases} -0.00920015939 - 0.007071685928(n-2), & \text{for } \ell = 1, \\ 0.01560323409 - 0.01338624986(n-2), & \text{for } \ell = 2. \end{cases}$$
(2.127)

2.4.3 Case d = 4

For d = 4 we set $g_0^2 = 1/(F_0^2 a^2)$ and define a renormalized coupling F (the pion decay constant in chiral PT in the chiral limit) through

$$\frac{1}{F_0^2} = \frac{1}{F^2} \left(1 + \frac{b_1}{F^2 a^2} + \frac{b_2}{F^4 a^4} + \mathcal{O}\left(1/(Fa)^6\right) \right) \,. \tag{2.128}$$

After renormalization we have

$$\chi = \frac{2F^2}{n} \left(1 + \frac{1}{F^2 a^2} \hat{R}_1 + \frac{1}{F^4 a^4} \hat{R}_2 + \dots \right) \,, \tag{2.129}$$

with

$$\hat{R}_1 = \overline{R}_1 - b_1 \,, \tag{2.130}$$

$$\hat{R}_2 = \overline{R}_2 - b_2 + b_1^2.$$
(2.131)

To cancel the $1/a^2$ terms in \hat{R}_1/a^2 one should require

$$b_1 = -\frac{1}{8} - (n-2)I_{10;0}$$

$$= 0.029933390231060214084 - 0.15493339023106021408 n_1.$$
(2.132)

This agrees with the result in [6]. For d = 4 the large L_s/a expansion of quantity X_A appearing here is given by $X_A = \sum_{r=r_0} X_{A;r} (a/L_s)^{2r}$.

⁴with the identification of the notation used there (on the lhs): $\beta_1 = -I_{10;1}, \beta_2 = I_{20;-1}, \tilde{\beta}_1 = -6I_{21;1}, \tilde{\beta}_2 = (12/\ell)I_{31;-1}, \psi = W_{3a;2} - 2I_{10;1}I_{21;1}.$

Next since $I_{11;1} = 0 = I_{22;1}$ after renormalization we obtain

$$\lim_{a \to 0} \left[a^{-2} \hat{R}_1 \right] = -\frac{2(n-2)}{L_s^2} I_{21;1} \,. \tag{2.133}$$

 \hat{R}_2/a^4 has divergent terms proportional to $1/a^4$, $1/a^2$ and $\log(a)$. First we recall that the subtraction coefficients $c^{(i)}$ are used to cancel the leading, $1/a^4$ contributions of the corresponding operators. In leading order $\overline{c}^{(i)}$ (defined in (2.30)) is fixed by requiring

$$\lim_{a/L_s \to 0} G^{(i)} = 0, \qquad (2.134)$$

where $G^{(i)}$ are the coefficients in (2.89), which leads to

$$\overline{c}^{(1)} = n - I_{12;0} = n - 0.7066242375215119838793013966,$$

$$\overline{c}^{(2)} = 2n - 1,$$

$$\overline{c}^{(3)} = \frac{1}{2}n + 2,$$

$$\overline{c}^{(4)} = 0,$$

$$\overline{c}^{(5)} = -0.030936190551839592713n - 0.032327591899970596813.$$
(2.135)

In [6] the overall sign of $\overline{c}^{(i)}$ was wrong and we also disagree here with sign of the constant term in $\overline{c}^{(5)}$.

Demanding the absence of the $1/a^4$ singularity in \hat{R}_2/a^4 determines the second order coefficient

$$b_2 = I_{10;0}^2 \left(n-2\right)^2 + \left(I_{10;0}^2 + \frac{1}{128} - 2W_{3a;0}\right) \left(n-2\right) + \frac{1}{128} - W_{3c;0}$$

$$= 0.024004355408 \left(n-2\right)^2 + 0.028115270716 \left(n-2\right) + 0.005536500909 \,.$$
(2.136)

This agrees with [6].

With the values for $\overline{c}^{(i)}$ above $G^{(i)} = O(a^4/L_s^4) \quad \forall i$. It follows that the $1/a^2$ contribution to \hat{R}_2/a^4 has no more free parameters and should vanish identically. This requires the relation

$$W_{3a;1} = \left(I_{10;0} - \frac{1}{8}\right) I_{10;1}, \qquad (2.137)$$

which indeed holds numerically (see [8]).

As for the renormalization of the 4-derivative couplings one has

$$g_{4,0}^{(i)} = k^{(i)} \log(aM_i), \quad i = 1, 2, 3,$$
 (2.138)

while for i = 4, 5 they are not renormalized to this order.

Moreover it is easy to check that after choosing the $\bar{c}^{(i)}$ as above⁵

$$G^{(1)} = G^{(2)} = \frac{a^4}{L_s^4} \left[2I_{11;2} - \frac{n_1}{\ell} \right] + \mathcal{O}\left(a^6/L_s^6\right) , \qquad (2.139)$$

⁵Note $I_{12;2} = 0$.

so that the part of \hat{R}_2 contributing in the continuum limit depends on $g_{4,0}^{(1)}, g_{4,0}^{(2)}$ only through their sum $g_{4,0}^{(1)} + g_{4,0}^{(2)}$, consistent with our general argument on the redundancy of the 4derivative operators in subsection 2.1. In the following we shall use this redundancy to set $g_4^{(1)} = 0$.

The cancellation of the $\ln(L_s/a)$ terms requires a relation for the coefficient of the $N^{-4} \ln N$ term in W_{3a} ,

$$W_{3a;2x} = \frac{1}{48\pi^2} \left(10I_{11;2} + \frac{1}{\ell} \right) , \qquad (2.140)$$

which is satisfied numerically to high precision. Then the coefficients of the logarithmic terms of $g_{4,0}^{(2)}$ and $g_{4,0}^{(3)}$ are fixed as:

$$-4\pi^2 k^{(2)} = w_1 = \frac{n}{2} - \frac{5}{3}, \qquad (2.141)$$

$$-4\pi^2 k^{(3)} = w_2 = \frac{2}{3}, \qquad (2.142)$$

agreeing with refs. [6] and [2].

Noting the relation

$$W_{3c;2} = -\frac{1}{8} \left(4 I_{10;0} - 1 \right) I_{11;2}, \qquad (2.143)$$

which is satisfied by the numerical values in [8], and inserting eqs. (4.22) and (4.23) one obtains the continuum limit of \hat{R}_2/a^4 :

$$L_s^4 \lim_{a \to 0} \frac{R_2}{a^4} = \hat{H}_0 - H_2 \frac{w_1}{4\pi^2} \ln(M_2 L_s) - H_3 \frac{w_2}{4\pi^2} \ln(M_3 L_s) + H_4 g_{4,0}^{(4)} + H_5 g_{4,0}^{(5)}, \quad (2.144)$$

where

$$H_{2} = -\frac{n-1}{\ell} + 2I_{11;2},$$

$$H_{3} = -\frac{1}{\ell} + n I_{11;2},$$

$$H_{4} = \frac{1}{6}(n+1) \left(\frac{1}{\ell} + 4 I_{11;2}\right),$$

$$H_{5} = \frac{n-1}{2\ell} + (3n-4) I_{11;2} + 2(n-2) (J_{31;2} - 2I_{22;2}),$$
(2.145)

and

$$\widehat{H}_0 = -(n-2)\widehat{w} + \widehat{w}' I_{11;2} + \widehat{w}'' \frac{1}{\ell}, \qquad (2.146)$$

with

$$\widehat{w} = -2\left(I_{10;0} - \frac{1}{8}\right)I_{10;2} + 2W_{3a;2} - 4(I_{10;1} - I_{21;1})I_{21;1}, \qquad (2.147)$$

$$\widehat{w}' = \frac{2}{3}(n-2)(I_{33;0} - 4I_{32;0}) + \frac{2}{3}\left(n - \frac{3}{4}\right)I_{10;0} - \frac{1}{48}(5n-1), \qquad (2.148)$$

$$\widehat{w}'' = \frac{1}{24} (3n^2 + n - 12)I_{10;0} - (n - 2) \left\{ \left(n - \frac{4}{3}\right) I_{32;0} - \frac{1}{6} I_{33;0} + \frac{1}{24} \right\} + 4(n - 2)^2 I_{31;0} \,.$$
(2.149)

Note that the coefficient of $g_{4,0}^{(4)}$ in eq. (2.144) vanishes for the hyper-cubic case, $\ell = 1$.

3 The free energy with dimensional regularization

In this section we work in a continuum volume $V = L_t \times L_s^{d_s}$, $d_s = d - 1$. Again the dynamical variables are spins $S_a(x)$, $a = 1, \ldots, n$ of unit length $\mathbf{S}(x)^2 = 1$ with periodic boundary conditions in all directions. We will dimensionally regularize by adding q extra compact dimensions of size \hat{L} (also with pbc) and analytically continue the resulting loop formulae to $q = -2\epsilon$. We define D = d + q, $V_D = V\hat{L}^q$. We denote aspect ratio of the extra dimensions by $\hat{\ell} \equiv \hat{L}/L_s$.

Many of the formulae are similar to those with lattice regularization and we will duplicate many of the notations hoping that this will not lead to confusions.

3.1 The effective action

The effective action \mathcal{A} is a sum over terms

$$\mathcal{A} = A_2 + A_4 + \dots \,, \tag{3.1}$$

where A_{2r} has 2r derivatives. A_2 is simply given by

$$A_2 = \frac{1}{2g_0^2} \int_x \sum_{\mu} \partial_{\mu} \mathbf{S}(x) \cdot \partial_{\mu} \mathbf{S}(x) \,. \tag{3.2}$$

The four derivative terms are

$$A_4 = \sum_{i=2,3} \frac{g_4^{(i)}}{4} A_4^{(i)}, \qquad (3.3)$$

where (we use redundancy immediately here to set $g_4^{(1)} = 0$),

$$A_4^{(2)} = \int_x \sum_{\mu\nu} \left[\partial_\mu \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) \right] \left[\partial_\nu \mathbf{S}(x) \cdot \partial_\nu \mathbf{S}(x) \right] , \qquad (3.4)$$

$$A_4^{(3)} = \int_x \sum_{\mu\nu} \left[\partial_\mu \mathbf{S}(x) \cdot \partial_\nu \mathbf{S}(x) \right] \left[\partial_\mu \mathbf{S}(x) \cdot \partial_\nu \mathbf{S}(x) \right] \,. \tag{3.5}$$

3.2 Perturbative expansion

After separating the zero mode and changing to $\vec{\pi}$ variables $(\mathbf{S} = (g_0 \vec{\pi}, \sqrt{1 - g_0^2 \vec{\pi}^2}))$

$$A_{2,\text{eff}}[\vec{\pi}] = A_2[\vec{\pi}] + A_{2,\text{zero}}[\vec{\pi}].$$
(3.6)

Note that the measure term is not present with dimensional regularization.

$$A_{2,\text{zero}}[\vec{\pi}] = -n_1 \ln\left(\frac{1}{V_D} \int_x \left(1 - g_0^2 \vec{\pi}(x)^2\right)^{\frac{1}{2}}\right).$$
(3.7)

 $A_{2,\text{eff}}$ has a perturbative expansion

$$A_{2,\text{eff}} = A_{2,0} + g_0^2 A_{2,1} + \mathcal{O}\left(g_0^4\right) , \qquad (3.8)$$

where

$$A_{2,0} = \frac{1}{2} \int_{x} \partial_{\mu} \vec{\pi}(x) \cdot \partial_{\mu} \vec{\pi}(x) , \qquad (3.9)$$

$$A_{2,1} = A_{2,1}^{(a)} + A_{2,1}^{(b)}, (3.10)$$

$$A_{2,1}^{(a)} = \frac{n_1}{2V_D} \int_x \vec{\pi}(x)^2 , \qquad (3.11)$$

$$A_{2,1}^{(b)} = \frac{1}{8} \int_{x} \partial_{\mu} \left[\vec{\pi}(x)^{2} \right] \partial_{\mu} \left[\vec{\pi}(x)^{2} \right] \,. \tag{3.12}$$

The total effective action has a perturbative expansion of the form

$$\mathcal{A} = \sum_{r=0} \mathcal{A}_r g_0^{2r} \,, \tag{3.13}$$

with

$$\mathcal{A}_r = A_{2,r}, \quad r = 0, 1, \qquad (3.14)$$

since

$$A_4^{(i)} = \mathcal{O}\left(g_0^4\right), \ i = 2, 3.$$
 (3.15)

The free 2-point function is given by

$$\langle \pi_a(x)\pi_b(y)\rangle_0 = \delta_{ab}G(x-y), \qquad (3.16)$$

with propagator

$$G(x) = \frac{1}{V_D} \sum_{p} {' \frac{e^{ipx}}{p^2}}, \qquad (3.17)$$

where the sum is over momenta $p_{\mu} = 2\pi n_{\mu}/L_{\mu}$, $n_{\mu} \in \mathbb{Z}$ and the prime on the sum means that p = 0 is omitted.

3.3 The chemical potential

The chemical potential h is introduced by the substitution:

$$\partial_0 \to \partial_0 - hQ$$
, (3.18)

where $(QS)_1 = iS_2$, $(QS)_2 = -iS_1$, and $(QS)_a = 0, a = 3, ..., n$.

This gives an additional *h*-dependent part \mathcal{A}_h to the total action of the form

$$\mathcal{A}_h = A_{2h} + \sum_{i=2,3} \frac{g_4^{(i)}}{4} A_{4h}^{(i)} \,. \tag{3.19}$$

Further writing

$$A_{2h} = ihB_2 + h^2C_2 + \dots , (3.20)$$

$$A_{4h}^{(i)} = ihB_4^{(i)} + h^2C_4^{(i)} + \dots, \qquad (3.21)$$

we have

$$B_2 = -\frac{1}{g_0^2} \int_x j_0(x) \,, \quad j_\mu(x) = S_2(x)\partial_\mu S_1(x) - S_1(x)\partial_\mu S_2(x) \,, \tag{3.22}$$

$$C_2 = \frac{1}{2g_0^2} \int_x [Q\mathbf{S}(x)]^2 \,. \tag{3.23}$$

For the operator 2:

$$B_4^{(2)} = -4 \int_x \partial_\mu \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) \, j_0(x) \,, \qquad (3.24)$$

$$C_4^{(2)} = -2 \int_x \left\{ \partial_\mu \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) \left[S_1(x)^2 + S_2(x)^2 \right] + 2 \left[j_0(x) \right]^2 \right\}, \qquad (3.25)$$

and for the operator 3:

$$B_4^{(3)} = -4 \int_x \partial_0 \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) \, j_\mu(x) \,, \qquad (3.26)$$

$$C_4^{(3)} = -2\int_x \left\{ \partial_0 \mathbf{S}(x) \cdot \partial_0 \mathbf{S}(x) \left[S_1(x)^2 + S_2(x)^2 \right] + 2\left[j_0(x) \right]^2 + \left[j_k(x) \right]^2 \right\}.$$
 (3.27)

The *h*-dependent part of the free energy f_h is defined as in (2.51). Now

$$\langle B_2 \rangle_{\mathcal{A}} = 0 = \langle B_4^{(i)} \rangle_{\mathcal{A}} \quad \forall i ,$$
 (3.28)

so we have

$$\chi = -2\sum_{s=1}^{5} F_s \,, \tag{3.29}$$

with

$$F_1 = \frac{1}{V_D} \langle C_2 \rangle_{\mathcal{A}} \,, \tag{3.30}$$

$$F_2 = \frac{1}{2} \frac{1}{V_D} \langle B_2^2 \rangle_{\mathcal{A}} , \qquad (3.31)$$

$$F_3 = \sum_{i=2,3} \frac{g_4^{(i)}}{4} \frac{1}{V_D} \langle C_4^{(i)} \rangle_{\mathcal{A}}, \qquad (3.32)$$

$$F_4 = \sum_{i=2,3} \frac{g_4^{(i)}}{4} \frac{1}{V_D} \langle B_2 B_4^{(i)} \rangle_{\mathcal{A}}, \qquad (3.33)$$

$$F_5 = \frac{1}{2} \sum_{ij} \frac{g_4^{(i)}}{4} \frac{g_4^{(j)}}{4} \frac{1}{V_D} \langle B_4^{(i)} B_4^{(j)} \rangle_{\mathcal{A}}.$$
(3.34)

Averaging over the rotations we have simply

$$\frac{1}{V_D} [C_2]_{\Omega} = -\frac{1}{ng_0^2} \,, \tag{3.35}$$

and

$$F_1 = -\frac{1}{ng_0^2} \,. \tag{3.36}$$

Next

$$\frac{1}{V_D} \left[B_2^2 \right]_{\Omega} = \frac{4}{n n_1 g_0^4} W, \qquad (3.37)$$

with W given by

$$W = \frac{1}{V_D} \int_{xy} \partial_0 \mathbf{S}(x) \cdot \partial_0 \mathbf{S}(y) \left[\mathbf{S}(x) \cdot \mathbf{S}(y) - 1 \right] \,. \tag{3.38}$$

This has a perturbative expansion

$$W = g_0^4 W_2 + g_0^6 W_3 + \dots (3.39)$$

with

$$W_2 = \frac{1}{V_D} \int_{xy} [\partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y)] \, \vec{\pi}(x) \cdot \vec{\pi}(y) \,, \qquad (3.40)$$

$$W_3 = \frac{1}{2V_D} \int_{xy} \left[\partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y) \right] \vec{\pi}(x)^2 \vec{\pi}(y)^2 \,. \tag{3.41}$$

Expanding (3.31) in a perturbative series

$$F_2 = \sum_{r=0}^{\infty} F_{2,r} g_0^{2r} , \qquad (3.42)$$

we have at leading order

$$F_{2,0} = \frac{2}{nn_1} \langle W_2 \rangle_0$$

= $\frac{2(n-2)}{n} \int_x [\partial_0 G(x)]^2 = \frac{2(n-2)}{n} \overline{I}_{21},$ (3.43)

where dimensionally regularized sums \overline{I}_{nm} are formally defined by

$$\overline{I}_{nm} = \frac{1}{V} \sum_{p}^{\prime} \frac{(p_0^2)^m}{(p^2)^n} \,. \tag{3.44}$$

Sums with m = 0 were treated by Hasenfratz and Leutwyler [15]; we generalize their methods to sums with m = 1 in [8].

At next order

$$F_{2,1} = \frac{2}{nn_1} \left[\langle W_3 \rangle_0 - \langle W_2 A_{2,1} \rangle_0^c \right] \,. \tag{3.45}$$

First

$$\langle W_3 \rangle_0 = \frac{1}{2V_D} \int_{xy} \langle \partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y) \vec{\pi}(x)^2 \vec{\pi}(y)^2 \rangle_0 = n_1 (n-2) \overline{W}, \qquad (3.46)$$

where

$$\overline{W} = -\int_{x} G(x)^2 \partial_0^2 G(x) \,. \tag{3.47}$$

This 2-loop function, the "massless sunset diagram", is calculated in detail in [8].

Next

$$\langle W_2 A_{2,1}^{(a)} \rangle_0^c = \frac{n_1}{2V_D^2} \int_{xyu} \left\langle \partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y) (\vec{\pi}(x) \cdot \vec{\pi}(y)) \vec{\pi}(u)^2 \right\rangle_0^c$$

$$= \frac{2n_1^2(n-2)}{V_D^2} \int_{xyu} \partial_0^x \partial_0^y G(x-y) G(x-u) G(y-u)$$

$$= \frac{2n_1^2(n-2)}{V_D^2} \sum_p' \frac{p_0^2}{(p^2)^3} = \frac{2n_1^2(n-2)}{V_D} \overline{I}_{31} ,$$

$$(3.48)$$

and

$$\langle W_2 A_{2,1}^{(b)} \rangle_0^c = \frac{1}{8V_D} \int_{xyu} \left[\partial_\mu^u \partial_\mu^v \left\langle \partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y) (\vec{\pi}(x) \cdot \vec{\pi}(y)) \vec{\pi}(u)^2 \vec{\pi}(v)^2 \right\rangle_0^c \right]_{v=u}$$

$$= \frac{n_1(n-2)}{V_D} \int_{xyu} \partial_\mu^u \partial_\mu^v \left[2\partial_0^x \partial_0^y G(x-y) G(x-u) G(y-v) G(u-v) \right. \\ \left. -\partial_0^x G(x-u) \partial_0^y G(y-v) G(x-v) G(y-u) \right] \Big|_{v=u}$$

$$= n_1(n-2) \frac{1}{V_D^2} \sum_{pq}' \left[\frac{2p_0^2(p-q)^2}{(p^2)^3 q^2} + \frac{p_0 q_0(p-q)^2}{(p^2)^2 (q^2)^2} \right]$$

$$= 2n_1(n-2) \left[\overline{I}_{21} \overline{I}_{10} + \overline{I}_{31} \overline{I}_{00} - \overline{I}_{21}^2 \right] .$$

$$(3.49)$$

Note that $\overline{I}_{00} = -\Box G(0) = -1/V_D$ since the dimensional regularization sets $\delta(0) = 0$. For the contribution from the 4-derivative terms, averaging over rotations:

$$\left[C_4^{(2)}\right]_{\Omega} = -\frac{4}{nn_1} \int_x \left\{ n_1 \partial_\mu \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) + 2\partial_0 \mathbf{S}(x) \cdot \partial_0 \mathbf{S}(x) \right\} , \qquad (3.50)$$

$$\left[C_4^{(3)}\right]_{\Omega} = -\frac{4}{nn_1} \int_x \left\{ \partial_\mu \mathbf{S}(x) \cdot \partial_\mu \mathbf{S}(x) + n\partial_0 \mathbf{S}(x) \cdot \partial_0 \mathbf{S}(x) \right\} \,. \tag{3.51}$$

So to first order perturbation theory

$$F_{3,1} = \frac{4}{n} \left\{ \frac{g_4^{(2)}}{4} \left[\frac{n_1}{V_D} - 2\overline{I}_{11} \right] + \frac{g_4^{(3)}}{4} \left[\frac{1}{V_D} - n\overline{I}_{11} \right] \right\}.$$
 (3.52)

Finally

$$F_{4,1} = F_{5,1} = 0. (3.53)$$

3.4 Summary

So for the expansion of the susceptibility with DR we have

$$\chi = \frac{2}{ng_0^2} \left(1 + g_0^2 R_1 + g_0^4 R_2 + \dots \right) \,, \tag{3.54}$$

with

$$R_1 = -2(n-2)\overline{I}_{21}, \qquad (3.55)$$

and

$$R_2 = R_2^{(a)} + R_2^{(b)}, (3.56)$$

with

$$R_{2}^{(a)} = 2(n-2) \left\{ -\overline{W} + 2\overline{I}_{21} \left[\overline{I}_{10} - \overline{I}_{21} \right] + \frac{2(n-2)}{V_{D}} \overline{I}_{31} \right\},$$
(3.57)

$$R_2^{(b)} = -4 \left\{ \frac{g_4^{(2)}}{4} \left[\frac{n_1}{V_D} - 2\overline{I}_{11} \right] + \frac{g_4^{(3)}}{4} \left[\frac{1}{V_D} - n\overline{I}_{11} \right] \right\}.$$
 (3.58)

3.5 Case n = 2

Note that $R_1 = 0 = R_2^{(a)}$ for n = 2. This is easily seen since for this special case the 2-derivative action with chemical potential is simply

$$A = \frac{1}{2g_0^2} \int_x \left(\partial_\mu \Phi(x) - ih\delta_{\mu 0}\right)^2 = \frac{1}{2g_0^2} \int_x \left(\partial_\mu \Phi(x)\right)^2 - \frac{h^2}{2g_0^2} V_D.$$
(3.59)

Therefore there are no corrections to the leading term for the susceptibility

$$\chi = \frac{1}{g_0^2} \,. \tag{3.60}$$

3.6 Case d = 2

For d = 2 the theory is renormalizable and as before we set the 4-derivative couplings to zero. Renormalization in the minimal subtraction (MS) scheme is achieved by

$$g_0^2 = \mu^{2\epsilon} g_{\rm MS}^2 Z_1 \,, \tag{3.61}$$

with

$$Z_1^{-1} = 1 + \frac{b_0}{2\epsilon}g^2 + \frac{b_1}{4\epsilon}g^4 + \dots , \qquad (3.62)$$

where b_0, b_1 are as in (2.96).

For $D \sim 2$

$$\overline{I}_{21} \sim -\frac{1}{4\pi} L^{-D+2} \left[\frac{1}{D-2} - \frac{1}{2} \gamma_2 + \kappa_{21} (D-2) + \dots \right], \qquad (3.63)$$

where the functions $\gamma_i(\ell)$ are defined in [8].

Next

$$\overline{I}_{10} = -\frac{1}{2\pi} L^{-D+2} \left[\frac{1}{D-2} - \frac{1}{2} \alpha_1 + \frac{1}{2\mathcal{V}} + \kappa_{10}(D-2) + \dots \right], \qquad (3.64)$$

$$\overline{I}_{31} = \frac{L^2}{64\pi^2} \left[\gamma_3 + 1\right] \,, \tag{3.65}$$

$$\overline{W} = L^{-2D+4} \frac{1}{8\pi^2} \left[\frac{1}{(D-2)^2} + \frac{1}{(D-2)} \left(-\alpha_1 - \frac{1}{2} + \frac{1}{\ell} \right) + \overline{w} + \dots \right] .$$
(3.66)

where $\alpha_i(\ell)$ are defined in [15].

In terms of the renormalized coupling

$$\chi = \frac{2}{ng_{\rm MS}^2} \left\{ 1 - b_0 \left(\ln(\mu L_s) + \frac{1}{2}\gamma_2 \right) g_{\rm MS}^2 - b_1 \left(\ln(\mu L_s) + r_2 \right) g_{\rm MS}^4 + \dots \right\}, \qquad (3.67)$$

with

$$r_2 = \overline{w} - 2\kappa_{10} - \frac{1}{2}\gamma_2 \left(\alpha_1 - \frac{1}{\ell} - \frac{1}{2}\gamma_2\right) - 16\pi^2 \frac{(n-2)}{V_D} \overline{I}_{31}.$$
 (3.68)

For completeness we note that the free energy for large h was computed to NLO with DR at infinite volume in [16, 17] with the result in the $\overline{\text{MS}}$ scheme:

$$f(h) - f(0) = -\frac{h^2}{2} \Big[\frac{1}{g_{\overline{MS}}^2(\mu)} - \frac{(n-2)}{2\pi} \left(\ln(\mu/h) + \frac{1}{2} \right) + O\left(g^2\right) \Big]$$

$$= -\frac{h^2}{2} \Big[\frac{1}{g_{\overline{MS}}^2(h)} - \frac{(n-2)}{4\pi} + O\left(g^2\right) \Big].$$
(3.69)

Noting

$$\frac{1}{g_{\overline{\rm MS}}^2(h)} = \frac{(n-2)}{2\pi} \left[\ln(h/\Lambda_{\overline{\rm MS}}) + \frac{1}{n-2} \ln \ln(h/\Lambda_{\overline{\rm MS}}) + \dots \right],$$
(3.70)

this result can be expressed as

$$f(h) - f(0) = -\frac{(n-2)}{2\pi} \frac{h^2}{2} \left[\ln \frac{h}{\Lambda_{\overline{MS}} \sqrt{e}} + \frac{1}{(n-2)} \ln \ln(h/\Lambda_{\overline{MS}}) + \dots \right].$$
 (3.71)

Eq. (3.71) was compared to the result from a non-perturbative computation invoking the Bethe ansatz [16, 17] thereby obtaining the exact ratio of the mass gap to the Λ -parameter $m/\Lambda_{\overline{\text{MS}}}$. Later the thermodynamic Bethe ansatz equations were extended to study the spectrum at finite volume [18]-[21].

3.7 Case d = 3

For d = 3 the contribution of the 4-derivative terms and are not relevant at $O(L_s^{-2})$ since $R_2^{(b)} = O(L_s^{-3})^{-6}$. We remark however that because the theory is non-renormalizable, it is expected that they are necessary to absorb divergences at higher orders.

For the sums contributing to $R_1, R^{(2a)}$ we have

$$\overline{I}_{10} = -\beta_1 L_s^{-1} \,, \tag{3.72}$$

$$\overline{I}_{21} = \frac{1}{8\pi L_s} \left(\gamma_2 - 2\right) \,, \tag{3.73}$$

$$= -\frac{1}{3L_s}\beta_1 \text{ for } \ell_1 = \ell_2 = \ell_3, \qquad (3.74)$$

$$\overline{I}_{31} = \frac{L_s}{64\pi^2} \left(\gamma_3 + 2\right) \,, \tag{3.75}$$

where the functions $\beta_i(\ell), \gamma_i(\ell)$ are defined in [8]. Also \overline{W} has a finite limit for D = 3, and the results of numerical evaluation for $\ell = 1, \ell = 2$ are given in [8].

The agreement of R_1, R_2 with the lattice results is evident for d = 3 because of the direct relation of the DR sums to the associated coefficients of the lattice sums:

$$\overline{I}_{10} = I_{10;1}/L_s , \quad \overline{I}_{21} = I_{21;1}L_s , \quad \overline{I}_{31} = I_{31;-1}L_s , \quad \overline{W} = W_{3a;2}/L_s^2 .$$
(3.76)

⁶Note that for d = 3 the couplings $g_4^{(i)}$ have dimension, in contrast to d = 4.

3.8 Case d = 4

In d = 4 we set $g_0^2 = 1/F^2$ which is not renormalized with DR.

In ref. [8] we have computed the various functions appearing in R_1, R_2 . First, for d = 4, \overline{I}_{21} has a finite limit as $q \to 0$:

$$\lim_{q \to 0} \overline{I}_{21} = \frac{1}{8\pi L_s^2} \left[\gamma_2(\ell) - 1 \right] \,. \tag{3.77}$$

For $D \sim 4$ we find for the 1-loop functions,

$$\overline{I}_{10} = -\beta_1(\ell)L_s^{-2} + \mathcal{O}(D-4) , \qquad (3.78)$$

$$\overline{I}_{31} = \frac{1}{32\pi^2} \left[\ln L_s - \frac{1}{D-4} + \frac{1}{2}\gamma_3(\ell) \right] + \mathcal{O}(D-4) , \qquad (3.79)$$

and for the 2-loop function

$$\overline{W} = \frac{1}{16\pi^2 L_s^4} \left\{ \left[\frac{1}{D-4} - 2\ln L_s \right] \mathcal{W}_0(\ell) + \frac{1}{3\ell} \ln(\hat{\ell}) - \frac{10}{3} \mathcal{W}_1(\ell, \hat{\ell}) + \overline{\mathcal{W}}(\ell) \right\} + \mathcal{O}\left(D-4\right) ,$$
(3.80)

with

$$\mathcal{W}_0(\ell) = \frac{5}{3} \left[\frac{1}{2} - \gamma_1(\ell) \right] - \frac{1}{3\ell}.$$
 (3.81)

Here we will not need the explicit expression for $W_1(\ell, \hat{\ell})$. Putting the results together for $D \sim 4$

$$R_{2}^{(a)} = 2(n-2)\frac{1}{16\pi^{2}L_{s}^{4}} \left\{ -\left[\frac{1}{D-4} - 2\ln L_{s}\right] \left[\frac{5}{3}\left(\frac{1}{2} - \gamma_{1}(\ell)\right) + \frac{1}{\ell}\left(n - \frac{7}{3}\right)\right] + \frac{1}{\ell}\left(n - \frac{7}{3}\right)\ln(\hat{\ell}) + \frac{10}{3}\mathcal{W}_{1}(\ell,\hat{\ell}) - \frac{1}{2}\left(\gamma_{2}(\ell) - 1\right)^{2} - 4\pi\beta_{1}\left(\gamma_{2}(\ell) - 1\right) + \frac{1}{2\ell}(n-2)\gamma_{3}(\ell) - \overline{\mathcal{W}}(\ell)\right\}.$$
(3.82)

For the 4-derivative terms we should identify

$$\frac{g_4^{(2)}}{4} = -l_1, \quad \frac{g_4^{(3)}}{4} = -l_2, \qquad (3.83)$$

with the bare couplings l_i of Gasser and Leutwyler [2] for the standard $\overline{\text{MS}}$ scheme:

$$l_i = \frac{w_i}{16\pi^2} \left[\frac{1}{D-4} + \ln\left(\overline{c}\Lambda_i\right) \right] \,, \tag{3.84}$$

where $\ln \overline{c} = \overline{C}$ (defined in (4.3)), and

$$w_1 = \frac{n}{2} - \frac{5}{3}, \quad w_2 = \frac{2}{3},$$
 (3.85)

are as given by [2] in (2.141,2.142)⁷. In order to pick up all terms of $R_2^{(b)}$ finite in the limit $D \to 4$ we need also order q = D - 4 terms of \overline{I}_{11} :

$$\overline{I}_{11} = \frac{1}{L_s^4} \left\{ \frac{1}{2} \left(1 - q \ln L_s \right) \left[\gamma_1(\ell) - \frac{1}{2} \right] + q \mathcal{W}_1(\ell, \hat{\ell}) \right\} + \mathcal{O}\left(q^2\right) \,. \tag{3.86}$$

⁷In [2] only the n = 4 result is given. Often the notation γ_i is used for w_i above, but we have already used γ_i in the context of 1-loop integrals.

We then get for $D \sim 4$:

$$R_{2}^{(b)} = \frac{1}{16\pi^{2}L_{s}^{4}} \left\{ 2(n-2) \left[\frac{1}{D-4} - 2\ln L_{s} \right] \left[\frac{5}{3} \left(\frac{1}{2} - \gamma_{1}(\ell) \right) + \frac{1}{\ell} \left(n - \frac{7}{3} \right) \right] - 2(n-2) \left[\frac{1}{\ell} \left(n - \frac{7}{3} \right) \ln(\hat{\ell}) + \frac{10}{3} \mathcal{W}_{1}(\ell, \hat{\ell}) \right] + 4w_{1} \ln\left(\overline{c}\Lambda_{1}L_{s}\right) \left[\frac{(n-1)}{\ell} - \gamma_{1}(\ell) + \frac{1}{2} \right] + 4w_{2} \ln\left(\overline{c}\Lambda_{2}L_{s}\right) \left[\frac{1}{\ell} - \frac{n}{2} \left(\gamma_{1}(\ell) - \frac{1}{2} \right) \right] \right\}.$$
(3.87)

Summing the terms we have for d = 4:

$$R_{2} = \frac{1}{16\pi^{2}L_{s}^{4}} \left\{ -2(n-2) \left[\frac{1}{2} \left(\gamma_{2}(\ell) - 1 \right)^{2} + 4\pi\beta_{1} \left(\gamma_{2}(\ell) - 1 \right) - \frac{1}{2\ell} (n-2)\gamma_{3}(\ell) + \overline{\mathcal{W}}(\ell) \right] + 4w_{1} \ln\left(\overline{c}\Lambda_{1}L_{s}\right) \left[\frac{(n-1)}{\ell} - \gamma_{1}(\ell) + \frac{1}{2} \right] + 4w_{2} \ln\left(\overline{c}\Lambda_{2}L_{s}\right) \left[\frac{1}{\ell} - \frac{n}{2} \left(\gamma_{1}(\ell) - \frac{1}{2} \right) \right] \right\}.$$
(3.88)

Note that not only do the poles at D = 4 cancel, but also $W_1(\ell, \hat{\ell})$, hence the physical amplitude R_2 is independent of $\hat{\ell}$, the aspect ratio of the extra unphysical dimensions, as to be expected.

4 Matching the effective actions for d = 2 and d = 4

4.1 Case d = 2

By matching the results for the susceptibility computed using lattice and dimensional regularizations we should obtain the 2-loop relation between the respective renormalized couplings

$$g_{\text{latt}}^2 = g_{\text{MS}}^2 \left[1 + X_1 g_{\text{MS}}^2 + X_2 g_{\text{MS}}^4 + \dots \right] \,. \tag{4.1}$$

First noting

$$I_{21;0}(\ell) = \frac{1}{8\pi} \left[\gamma_2 + 2\overline{C} + 5\ln 2 \right] , \qquad (4.2)$$

where

$$\overline{C} = -\frac{1}{2} \left[\ln(4\pi) - \gamma_E + 1 \right] = -1.476904292 \,, \tag{4.3}$$

at leading order we reproduce Parisi's result 8 [22]

$$X_1 = \overline{r}_1 + \frac{1}{2}b_0\gamma_2$$

$$= \frac{b_0}{2} \left[\ln\left(\frac{\pi}{8}\right) - \gamma_E \right] - \frac{1}{4}.$$
(4.4)

The ratio of Λ parameters is

$$\frac{\Lambda_{\text{latt}}}{\Lambda_{\text{MS}}} = \exp\left(\frac{X_1}{b_0}\right) \,. \tag{4.5}$$

At next order matching we get

$$X_2 - X_1^2 = \overline{r}_2 + b_1 r_2 \,. \tag{4.6}$$

⁸converted from Pauli Villars regularization to DR

For our purposes it is sufficient to consider the case $\ell = \hat{\ell} = 1$ for which

$$\overline{W} = \frac{1}{D} \left[\overline{I}_{10}^2 - \frac{1}{V_D} \overline{I}_{20} \right], \quad (\ell = \hat{\ell} = 1), \qquad (4.7)$$

so that

$$\overline{w} = 2\kappa_{10} + \frac{1}{4}\alpha_1^2 - \frac{1}{8}[\gamma_3 + 1], \quad (\ell = \hat{\ell} = 1),$$
(4.8)

and from (3.68) (noting $\gamma_s = (2/d)(s-1)\alpha_{s-1}$ for $\ell = 1$)

$$r_{2} = \frac{1}{2}\alpha_{1} - \frac{1}{4}\alpha_{2} - \frac{1}{8} - 16\pi^{2}\frac{(n-2)}{V_{D}}\overline{I}_{31}$$

$$= -0.1022210828989128367197392 - 16\pi^{2}\frac{(n-2)}{V_{D}}\overline{I}_{31}, \qquad \ell = 1$$
(4.9)

On the lattice side we get for $\ell = 1$ from (2.111)

$$\overline{r}_2 = -\frac{5}{96} - (n-2)\left(\frac{1}{2\pi}I_{10;0} - I_{20;-1} - \frac{1}{32} + \frac{1}{16\pi^2} + a_1\right) + 4(n-2)^2I_{31;-1}$$
(4.10)

where we used

$$W_{3a;0} = \frac{1}{2}I_{10;0}^2 - \frac{1}{2}I_{10;0}I_{22;0} - \frac{1}{2}I_{20;-1} + \frac{1}{2}a_1, \qquad \ell = 1$$
(4.11)

and a_1 is the infinite-volume quantity

$$a_{1} = -\frac{1}{4} \int_{k,l} \frac{E_{k+l} - E_{k} - E_{l}}{E_{k} E_{l} E_{k+l}^{2}} \sum_{\mu} \widehat{(k+l)}_{\mu}^{4}$$

$$= -\frac{1}{2} \sum_{x} (G(x) - G(0))^{2} \Box_{0}^{2} G(x) = 0.0461636292439177762(1)$$
(4.12)

(with $E_k = \hat{k}^2$). Inserting the numerical values one gets

$$\overline{r}_2 = -\frac{5}{96} - (n-2) \, 0.02514054820286075900(1) + 4(n-2)^2 I_{31;-1} \,, \quad \ell = 1 \,. \tag{4.13}$$

Noting

$$I_{31;-1}(\ell) = \frac{1}{L_s^2 \ell} \overline{I}_{31} , \qquad (4.14)$$

we obtain

$$X_2 - X_1^2 = -\frac{5}{96} - 1.0947301436539277 \,b_1 \,. \tag{4.15}$$

 X_2 was first computed by Falcioni and Treves [23]:

$$X_2 - X_1^2 = -\frac{5}{96} + b_1 \left[h_1 - \frac{1}{4} + \frac{1}{2} \ln\left(\frac{\pi}{8}\right) - \frac{1}{2}\gamma_E \right] , \qquad (4.16)$$

with the value of h_1 given in [7] ⁹

$$h_1 = -0.088766484(1), \qquad (4.17)$$

 ${}^{9}h_1 = 1/2 - 4\pi^2(a_1 - 1/32)$ with a_1 given in (4.12). The value of h_1 given in [23] was not very precise.

giving

$$X_2 - X_1^2 = -\frac{5}{96} - 1.094730144(1) b_1.$$
(4.18)

The perfect agreement of our result (4.15) with the result obtained above by an independent method gives an additional check on our formulae in subsections 2.3.3, 3.4 which are valid for arbitrary $d \ge 2$.

4.2 Case d = 4

The equality of the lattice and DR results for d = 4 at sub-leading order one requires

$$I_{21;1} = \frac{1}{8\pi} (\gamma_2 - 1), \qquad (4.19)$$

which we have proven in [8].

Comparing (2.87)-(2.89) with (3.88), the coefficients of $\ln(L_s)$ agree due to the relation (see [8]):

$$I_{11;2} = \frac{1}{2} \left(\gamma_1 - \frac{1}{2} \right) \,. \tag{4.20}$$

For general n the matching equation has the form

$$H_2 \overline{g}_{4,0}^{(2)} + H_3 \overline{g}_{4,0}^{(3)} + H_4 g_{4,0}^{(4)} + H_5 g_{4,0}^{(5)} + H_0 = 0, \qquad (4.21)$$

where

$$\overline{g}_{4,0}^{(2)} = g_{4,0}^{(2)} + \frac{1}{4\pi^2} w_1 \ln(a\bar{c}\Lambda_1) = -\frac{1}{4\pi^2} w_1 \ln\left(\frac{M_2}{\bar{c}\Lambda_1}\right) , \qquad (4.22)$$

$$\overline{g}_{4,0}^{(3)} = g_{4,0}^{(3)} + \frac{1}{4\pi^2} w_2 \ln(a\bar{c}\Lambda_2) = -\frac{1}{4\pi^2} w_2 \ln\left(\frac{M_3}{\bar{c}\Lambda_2}\right) , \qquad (4.23)$$

and

$$H_0 = \widehat{H}_0 + 2(n-2) \left[\frac{1}{16\pi^2} \overline{\mathcal{W}} - 2(I_{10;1} - I_{21;1}) I_{21;1} \right] - \frac{(n-2)^2}{16\pi^2 \ell} \gamma_3, \qquad (4.24)$$

where we have used another identity:

$$I_{10;1} = -\beta_1 \,. \tag{4.25}$$

So we have

$$H_0 = -(n-2)w + w'I_{11;2} + w''\frac{1}{\ell}, \qquad (4.26)$$

with

$$w = 2W_{3a;2} - \frac{1}{8\pi^2}\overline{W} - \left(2I_{10;0} - \frac{1}{4}\right)I_{10;2}, \qquad (4.27)$$

$$w' = \widehat{w}'$$

$$w' = w',$$

$$w'' = \frac{1}{24}(3n^2 + n - 12)I_{10;0} - (n - 2)\left\{\left(n - \frac{4}{3}\right)I_{32;0} - \frac{1}{6}I_{33;0} + \frac{1}{24}\right\} + 4(n - 2)^2i_{31;0},$$
(4.28)

$$= \frac{1}{24} (3n^{2} + n - 12) I_{10;0} - (n - 2) \left\{ \left(n - \frac{1}{3} \right) I_{32;0} - \frac{1}{6} I_{33;0} + \frac{1}{24} \right\} + 4(n - 2) I_{31;0},$$

$$(4.29)$$

where \widehat{w}' is given in (2.148) and $i_{31;0}$ is defined by

$$i_{31;0} = I_{31;0}(\ell) - \frac{1}{64\pi^2} \gamma_3(\ell) \,. \tag{4.30}$$

Now we find numerically

$$i_{31;0} = 0.00211856418663447748445$$
, independent of ℓ , (4.31)

so that w'' is independent of ℓ (as is also w').

Now the coefficients H_2 , H_3 , H_4 , H_5 in (4.21) only involve the three linearly independent ℓ -dependent functions $I_{00;2} = -1/\ell$, $I_{11;2}$ and $J_{31;2} - 2I_{22;2}$ so that for consistency a relation for w in (4.27) of the form

$$w = \frac{d_1}{\ell} + d_2 I_{11;2} + d_3 \left(J_{31;2} - 2I_{22;2} \right)$$
(4.32)

should hold with some ℓ -independent constants d_1 , d_2 , d_3 . From numerical data sets with $\ell = 1, 2, 3$ one finds $d_1 = -0.00472740$, $d_2 = 0.00026214$ and $d_3 = 0.00000028$. Inserting these values into the relation with $\ell = 4$ we indeed find consistency within the numerical errors (with the difference in the 6th significant digit). We will assume that actually $d_3 = 0$, and with this one obtains from $\ell = 1, 2$ the values $d_1 = -0.00472752$, $d_2 = 0.00026215$.

Let us define

$$G_1 \equiv -n_1 \overline{g}_{4,0}^{(2)} - \overline{g}_{4,0}^{(3)} + \frac{1}{6} (n_1 + 2) g_{4,0}^{(4)} + \frac{1}{2} n_1 g_{4,0}^{(5)}, \qquad (4.33)$$

$$G_2 \equiv 2\overline{g}_{4,0}^{(2)} + (n_1 + 1)\overline{g}_{4,0}^{(3)} + \frac{2}{3}(n_1 + 2)g_{4,0}^{(4)} + (3n_1 - 1)g_{4,0}^{(5)}.$$
(4.34)

Then matching requires

$$0 = G_1 + q_0^{(1)} + (n-2)q_1^{(1)} + (n-2)^2 q_2^{(1)}, \qquad (4.35)$$

$$0 = G_2 + q_0^{(2)} + (n-2)q_1^{(2)}, \qquad (4.36)$$

$$0 = 2g_{4,0}^{(5)} - d_3, (4.37)$$

with

$$q_0^{(1)} = \frac{1}{12} I_{10;0} , \qquad (4.38)$$

$$q_1^{(1)} = -\frac{1}{24} + \frac{13}{24} I_{10;0} - \frac{2}{3} I_{32;0} + \frac{1}{6} I_{33;0} - d_1, \qquad (4.39)$$

$$q_2^{(1)} = \frac{1}{8} I_{10;0} - I_{32;0} + 4i_{31;0} , \qquad (4.40)$$

$$q_0^{(2)} = -\frac{3}{16} + \frac{5}{6} I_{10;0}, \qquad (4.41)$$

$$q_1^{(2)} = -\frac{5}{48} + \frac{2}{3} I_{10;0} - \frac{8}{3} I_{32;0} + \frac{2}{3} I_{33;0} - d_2.$$
(4.42)

The numerical values are

$$q_0^{(1)} = 0.0129111158,$$
 (4.43)

$$q_1^{(1)} = 0.0434608716,$$
 (4.44)

$$q_2^{(1)} = 0.011640543735, \qquad (4.45)$$

$$q_0^{(2)} = -0.0583888414, \qquad (4.46)$$

$$q_1^{(2)} = -0.0152288420. (4.47)$$

For the special case n = 2 the solution is:

$$g_{4,0}^{(4)} + g_{4,0}^{(5)} = \frac{1}{16} - \frac{1}{3} I_{10;0}, \quad (n=2),$$
 (4.48)

$$\overline{g}_{4,0}^{(2)} + \overline{g}_{4,0}^{(3)} = \frac{1}{32} - \frac{1}{12} I_{10;0}, \quad (n=2).$$
 (4.49)

Note in the continuum limit (e.g. for DR) $A_4^{(2)} = A_4^{(3)}$ for n = 2.

5 The mass gap

The mass of the O(n) vector particle in a periodic spatial volume L_s^{d-1} was computed with lattice regularization for arbitrary d in ref. [6] up to second order in perturbation theory. It takes the form

$$m_1 = \frac{n_1 g_0^2 a^{d-2}}{2L_s^{d-1}} \left\{ 1 + g_0^2 c_2(a/L_s) + g_0^4 \left[c_3(a/L_s) + \sum_{j=2}^5 g_{4,0}^{(j)} d_3^{(j)}(a/L_s) \right] + \mathcal{O}\left(g_0^6\right) \right\}, \quad (5.1)$$

where the coefficients $c_2(a/L_s)$, $c_3(a/L_s)$, $d_3(a/L_s)^{10}$ are given in appendix B of [6]; they depend on d, and for the case d = 2 the coefficients c_2, c_3 agree with those previously computed in [7].

Here we will only discuss the case d = 4. Results are often quoted in terms of the moment of inertia Θ which is simply related to the mass gap through

$$m_1 = \frac{(n-1)}{2\Theta} \,. \tag{5.2}$$

 Θ has a perturbative expansion of the form

$$\frac{\Theta}{F^2 L_s^3} = 1 + \Theta_1 (FL_s)^{-2} + \Theta_2 (FL_s)^{-4} + \dots$$
(5.3)

After renormalization of the couplings as in subsect. 2.4.3, the moment of inertia in the continuum limit is given by (5.3) with coefficients determined from the lattice computation taken from eq. (6.20) of [6]

$$\Theta_1^{\text{latt}} = 0.225784959441 \left(n - 2 \right), \tag{5.4}$$

¹⁰keeping the notation of [6] and not to be confused with previously mentioned quantities with the same letters!

and

$$\Theta_{2}^{\text{latt}} = -\frac{0.8375369106}{12\pi^{2}} \left[(3 n - 10) \ln(M_{2}L_{s}) + 2 n \ln(M_{3}L_{s}) \right] + 0.55835794046(n + 1)g_{4,0}^{(4)} + (1.11639602502 n - 0.55771822866)g_{4,0}^{(5)} - 0.0489028095 + 0.0101978424(n - 2).$$
(5.5)

Using the definitions in (4.22), (4.23) and (4.34) we can rewrite this involving DR scales:

$$\Theta_2^{\text{latt}} = \overline{\theta}_2 - \frac{0.8375369106}{12\pi^2} \left[(3\,n - 10) \ln(\overline{c}\Lambda_1 L_s) + 2\,n \ln(\overline{c}\Lambda_2 L_s) \right] \,, \tag{5.6}$$

with

$$\overline{\theta}_2 = 0.8375369106 \, G_2 - 1.396214707(n-2)g_{4,0}^{(5)} - 0.0489028095 + 0.0101978424(n-2).$$
(5.7)

Finally using eq. (4.36) (with (4.46),(4.47)) which was obtained by matching lattice and DR results for the free energy, and assuming $g_{4,0}^{(5)} = 0$, we obtain

$$\overline{\theta}_2 = 0.0229525597 \left(n - 2 \right). \tag{5.8}$$

Note that the $(n-2)^0$ terms in $\overline{\theta}_2$ cancel to our numerical precision of 10 digits.

The continuum limit of Θ_i should of course be regularization independent. Unfortunately (5.8) does not agree with the result for the moment of inertia previously computed by Hasenfratz [4] using dimensional regularization. For this reason we recomputed the mass gap with DR using free boundary conditions in the time direction in an analogous way to that used for the lattice computation. The computation is rather lengthy and here we only present the final result (for arbitrary d):

$$m_1 = \frac{n_1 g_0^2}{2\overline{V}_D} \left[1 + g_0^2 \triangle^{(2)} + g_0^4 \triangle^{(3)} + \dots \right] , \qquad (5.9)$$

(here $\overline{V}_D = L_s^{d-1} \hat{L}^q = L_s^{D-1} \hat{\ell}^q$), with

$$\Delta^{(2)} = (n-2)R(0), \qquad (5.10)$$

$$\Delta^{(3)} = (n-2) \left[2W + \frac{3}{4\overline{V}_D} \overline{I}_{10:D-1} + (n-3)R(0)^2 \right] - 4 \left(2l_1 + nl_2 \right) \ddot{R}(0) \,. \tag{5.11}$$

Here R(z) is the propagator for an infinitely long strip without the slow modes $\mathbf{p} = 0^{-11}$:

$$R(z) = \frac{1}{2\overline{V}_D} \sum_{\mathbf{p}\neq 0} \frac{\mathrm{e}^{-\omega(\mathbf{p})|z_0| + i\mathbf{p}\mathbf{z}}}{\omega(\mathbf{p})}, \ \omega(\mathbf{p}) = \sqrt{\mathbf{p}^2}.$$
 (5.12)

The singularity of R(z) at z = 0 is regularized with DR. Further $\overline{I}_{10:D-1}$ is the regularized sum \overline{I}_{10} in D-1 dimensions and

$$W = -\int_{-\infty}^{\infty} \mathrm{d}z_0 \, \int_{\mathbf{z}} R(z)^2 \partial_0^2 R(z) \,. \tag{5.13}$$

¹¹Our R(z) is closely related to $\overline{G}^*(z)$ of [4].

The computation of W is the most involved part and we discuss this in detail in [8].

Returning again to the case d = 4, the moment of inertia has an expansion

$$\frac{\Theta}{F^2 L_s^3} = 1 + \Theta_1^{\rm DR} (FL_s)^{-2} + \Theta_2^{\rm DR} (FL_s)^{-4} + \dots$$
 (5.14)

with

$$\Theta_1^{\rm DR} = -(n-2)L_s^2 R(0) \,, \tag{5.15}$$

$$\Theta_2^{\rm DR} = (n-2)L_s^4 \left[-2W + R(0)^2 - \frac{3}{4\overline{V}_D^2} \sum_{\mathbf{p}\neq 0} \frac{1}{\mathbf{p}^2} \right] + 4\left(2l_1 + nl_2\right)\ddot{R}(0).$$
(5.16)

In [8] we find

$$W = \frac{5}{24\pi^2} \ddot{R}(0) \left[\frac{1}{D-4} - \ln L_s \right] + c_w L_s^{-4}, \qquad (5.17)$$

with 12

$$c_w = 0.0986829798. (5.18)$$

Adding the counter-terms using (3.84), the 1/(D-4) singularities cancel (and also the $\hat{\ell}$ -dependent terms coming from O (D-4) contributions in $\ddot{R}(0)$), and we obtain

$$\Theta_2^{\rm DR} = (n-2)\theta_2 + \frac{1}{12\pi^2} L_s^4 \ddot{R}(0) \left[(3n-10)\ln(\bar{c}\Lambda_1 L_s) + 2n\ln(\bar{c}\Lambda_2 L_s) \right] , \qquad (5.19)$$

with 13

$$\theta_2 = -2c_w + L_s^4 R(0)^2 + \frac{3}{4} L_s \beta_1^{(3)} , \qquad (5.20)$$

where in the notation of [15]

$$\beta_1^{(3)} = -\frac{1}{\overline{V}_D} \sum_{\mathbf{p}\neq 0} \frac{1}{\mathbf{p}^2} \,, \tag{5.21}$$

where the sum is over 3 + q dimensional momenta **p**. With dimensional regularization

$$\beta_1^{(3)} = -L_s R(0) \,. \tag{5.22}$$

Putting in the numerical values [8]

$$L_s^2 R(0) = -0.2257849594407580334832664917,$$
(5.23)

$$L_s^4 \ddot{R}(0) = -0.8375369106960818783868948293, \qquad (5.24)$$

we obtain

$$\theta_2 = 0.0229516079\,,\tag{5.25}$$

completely consistent with the lattice result converted to DR in (5.8). Note however that values of $\theta_2, \overline{\theta}_2$ differ in the 6'th decimal place, which indicates that at some stage(s) we have overestimated our numerical precision.

¹²The value $c_w = 0.029492025146$ given in [4] differs from ours.

¹³In ref. [4] the term in (5.20) involving $\beta_1^{(3)}$ is missing.

6 Conclusions

We have established relations between the 4-derivative couplings of effective Lagrangians involving fields in the vector representation of O(n) using both lattice and dimensional regularizations. This allows translation of results obtained on the lattice to those of DR more commonly used in phenomenology. Computations on the lattice are usually algebraically more complicated but conceptually clear.

One application is to the computation of the mass gap of massless 2-flavor QCD in the δ -regime. It is given by

$$\Theta = F^2 L_s^3 \left[1 + 0.4515699182 \frac{1}{F^2 L_s^2} + \frac{1}{F^4 L_s^4} \left(\theta - 0.8375369109 \frac{1}{6\pi^2} \left\{ \ln(\Lambda_1 L_s) + 4\ln(\Lambda_2 L_s) \right\} \right) + \dots \right],$$
(6.1)

with

$$\theta = 2\theta_2 + \frac{5}{6\pi^2} L_s^4 \ddot{R}(0) \overline{C}$$

= 0.1503452489. (6.2)

Note Hasenfratz [4] obtained $\theta = 0.088431628$.

It is convenient to rewrite (6.1) by using the low-energy parameters defined in [2],

$$\overline{l}_i \equiv \ln \frac{\Lambda_i^2}{m_\pi^2} \,, \tag{6.3}$$

where m_{π} is the physical pion mass. We have

$$\Theta = F^2 L_s^3 \left[1 + \frac{0.45157}{F^2 L_s^2} + \frac{1}{F^4 L_s^4} \left(0.1503 - 0.0283 \left[\overline{l}_2 + \frac{1}{4} \overline{l}_1 + \frac{5}{2} \ln \left(L_s m_\pi \right) \right] \right) + \dots \right].$$
(6.4)

The QCDSF collaboration [24-26] compared their data for the mass gap from numerical simulations of lattice QCD to (6.1) using values

$$\bar{l}_1 = -0.4 \pm 0.6, \qquad \bar{l}_2 = 4.3 \pm 0.1.$$
 (6.5)

taken from [27]. They found satisfactory agreement with the analytic result and our new value for θ doesn't change this conclusion.

Although measuring the low lying spectrum is among the simplest and cleanest numerical problems, a difficulty is that the box size needs to reach 3 fm or larger. This is suggested by the NL correction which is 38%, 26% and 15% of the leading order for $L_s = 2.5$, 3, 4 fermi respectively, where for the estimates we have used the value F = 86.2 MeV from Colangelo and Dürr [28]. The NNL correction is unexpectedly small: -0.6%, -0.7% and -0.5% at the same lattice sizes. Note however, that this is due to the cancellation of the two terms in (6.4), and the smallness of the NNL correction does not indicate the smallness of the next, unknown correction. Note that the combination $\overline{l}_2 + \overline{l}_1/4$ enters with a small coefficient, whose value e.g. for $L_s = 3 \text{ fm}$ is -0.0095. As a consequence, the mass gap is not sensitive to these parameters. For the same reason, however, it provides a clean way to obtain the value of F, in particular the constant \overline{l}_4 which controls the ratio F_{π}/F close to the chiral limit. At the physical pion mass the sensitivity of the mass gap in the delta regime to this parameter is roughly $0.2 \overline{l}_4$. Alternatively, knowing F, one can estimate the corresponding lattice artifacts, the goodness of the chiral extrapolation, etc.

Numerical simulations of lattice QCD in the δ -regime potentially still give a good possibility to constrain the LE constants of χPT . The mass gap is unfortunately only sensitive to the decay constant F, and it remains a challenge to find other observables which are sensitive to the \bar{l}_i and also accurately measurable in numerical simulations.

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A The terms $B_4^{(i)}$ and $C_4^{(i)}$

The terms $B_4^{(i)}$ and $C_4^{(i)}$ appearing in (2.48) are given by

$$B_4^{(1)} = B_4^{(5a)} + B_4^{(1a)}, \tag{A.1}$$

$$B_4^{(1a)} = 4 \sum_{xk} (\Box_k S_1 \nabla_0 S_2 - \Box_k S_2 \nabla_0 S_1), \qquad (A.2)$$

$$C_4^{(1)} = C_4^{(5a)} + C_4^{(1a)}, \tag{A.3}$$

$$C_4^{(1a)} = \sum_{xk} \left\{ (2S_1 + \Box_0 S_1) \Box_k S_1 + (2S_2 + \Box_0 S_2) \Box_k S_2 \right\} , \qquad (A.4)$$

where $\nabla_0 = \frac{1}{2}(\partial_0 + \partial_0^*)$ is the symmetric derivative and $\Box_\mu = \partial_\mu \partial_\mu^*$. Here and in the rest of this section we have suppressed the argument of the fields e.g. $S_i = S_i(x)$. Also below we introduce the notation $S'_i = S_i(x + \hat{0})$ and $S''_i = S_i(x + 2\hat{0})$.

$$B_4^{(2)} = -4\sum_x (S_1 S_2' - S_2 S_1') \partial_\mu \mathbf{S} \cdot \partial_\mu \mathbf{S} , \qquad (A.5)$$

$$C_4^{(2)} = -\sum_x \left\{ 4(S_1 S_2' - S_2 S_1')^2 + 2(S_1 S_1' + S_2 S_2') \partial_\mu \mathbf{S} \cdot \partial_\mu \mathbf{S} \right\} .$$
(A.6)

$$B_4^{(3)} = B_4^{(4a)} + B_4^{(3a)} , (A.7)$$

$$B_4^{(3a)} = -4\sum_{xk} (S_1'\partial_k S_2 - S_2'\partial_k S_1)\partial_0 \mathbf{S} \cdot \partial_k \mathbf{S}, \qquad (A.8)$$

$$C_4^{(3)} = C_4^{(4a)} + C_4^{(3a)}, \tag{A.9}$$

$$C_{4}^{(3a)} = 2\sum_{xk} \left[(S_{1}^{\prime}\partial_{k}S_{1} + S_{2}^{\prime}\partial_{k}S_{2})\partial_{0}\mathbf{S} \cdot \partial_{k}\mathbf{S} - (S_{1}^{\prime}\partial_{k}S_{2} - S_{2}^{\prime}\partial_{k}S_{1})^{2} \right].$$
(A.10)

$$B_4^{(4a)} = -4\sum_x (S_1 S_2' - S_2 S_1') \partial_0 \mathbf{S} \cdot \partial_0 \mathbf{S} , \qquad (A.11)$$

$$C_4^{(4a)} = -\sum_x \left\{ 2(S_1S_1' + S_2S_2')\partial_0 \mathbf{S} \cdot \partial_0 \mathbf{S} + 4(S_1S_2' - S_2S_1')^2 \right\} .$$
(A.12)

$$B_4^{(5a)} = -4\sum_x \left(\partial_0^* S_1 \partial_0 S_2 - \partial_0^* S_2 \partial_0 S_1\right) , \qquad (A.13)$$

$$C_4^{(5a)} = -2\sum_x \left\{ -(S_1 \Box_0 S_1 + S_2 \Box_0 S_2) + 2(\partial_0 S_1 \partial_0^* S_1 + \partial_0 S_2 \partial_0^* S_2) \right\},$$
(A.14)

$$B_4^{(5c)} = B_4^{(5a)} + B_4^{(5d)}, \tag{A.15}$$

$$B_4^{(5d)} = -4\sum_x \left\{ [S_1'' - S_1']\partial_k^2 S_2 - [S_2'' - S_2']\partial_k^2 S_1 \right\} , \qquad (A.16)$$

$$C_4^{(5c)} = C_4^{(5a)} + C_4^{(5d)} , \qquad (A.17)$$

$$C_4^{(5d)} = 2\sum_{xk} \left\{ [2S_1'' - S_1'] \partial_k^2 S_1 + [2S_2'' - S_2'] \partial_k^2 S_2 \right\} .$$
(A.18)

B Some lattice momentum sums

We define the following lattice sums:

$$I_{nm} \equiv \frac{1}{V} \sum_{p}' \frac{\left(\hat{p}_{0}^{2}\right)^{m}}{\left(\hat{p}^{2}\right)^{n}},\tag{B.1}$$

$$J_{nm} \equiv \frac{1}{V} \sum_{p}' \frac{(\hat{p}_{0}^{2})^{m} \sum_{\mu} \hat{p}_{\mu}^{4}}{(\hat{p}^{2})^{n}}, \qquad (B.2)$$

$$K_{nm} \equiv \frac{1}{V} \sum_{p}' \frac{(\hat{p}_0^2)^m (\sum_{\mu} \hat{p}_{\mu}^4)^2}{(\hat{p}^2)^n}, \qquad (B.3)$$

$$L_{nm} \equiv \frac{1}{V} \sum_{p}' \frac{(\hat{p}_{0}^{2})^{m}}{(\hat{p}^{2})^{n}} \sum_{\mu\nu} \cos(p_{\mu} - p_{\nu}) \hat{p}_{\mu}^{2} \hat{p}_{\nu}^{2}, \qquad (B.4)$$

$$J_{nmk} \equiv \frac{1}{V} \sum_{p}' \frac{(\hat{p}_0^2)^m \sum_{\mu} \hat{p}_{\mu}^{2k}}{(\hat{p}^2)^n}.$$
 (B.5)

The following momentum sums which appear in our computation are expressed in terms of these:

$$\mathcal{F}_{1} \equiv \frac{1}{V^{2}} \sum_{pq} \left(\frac{\hat{p}_{0}^{2} (\hat{p} + q)^{2}}{(\hat{p}^{2})^{2} \hat{q}^{2}} \right)$$

$$= I_{11}I_{10} + I_{21}I_{00} - \frac{d_{s} + 1}{2d_{s}}I_{22}I_{11} - \frac{1}{2d_{s}}I_{11}I_{00} + \frac{1}{2d_{s}}I_{11}^{2} + \frac{1}{2d_{s}}I_{22}I_{00}.$$
(B.6)

$$\mathcal{F}_{2} \equiv \frac{1}{V^{2}} \sum_{pq}' \frac{\sin^{2} p_{0} \left(\widehat{p+q}\right)^{2}}{\left(\widehat{p}^{2}\right)^{3} \widehat{q}^{2}}$$

= $I_{10} \left(I_{21} - \frac{1}{4}I_{22}\right) + I_{00} \left(I_{31} - \frac{1}{4}I_{32}\right) - \frac{1}{2}I_{11} \left(I_{32} - \frac{1}{4}I_{33}\right)$ (B.7)
+ $\frac{1}{2d_{s}} \left(I_{11} - I_{00}\right) \left(I_{21} - \frac{1}{4}I_{22} - I_{32} + \frac{1}{4}I_{33}\right)$.

The expressions for \mathcal{F}_1 and \mathcal{F}_2 are valid for a spatially symmetric volume, $V = L_s^{d_s} L_t$.

$$\mathcal{F}_{3} \equiv \frac{1}{V^{2}} \sum_{pq}' \frac{\sin p_{0} \sin q_{0} \left(\widehat{p+q}\right)^{2}}{(\widehat{p}^{2})^{2} (\widehat{q}^{2})^{2}} = 2 \left(\frac{1}{V} \sum_{p}' \frac{\sin^{2} p_{0}}{(\widehat{p}^{2})^{2}}\right)^{2} = 2 \left(I_{21} - \frac{1}{4}I_{22}\right)^{2}.$$
(B.8)

$$\mathcal{F}_{4} = L_{21} = \frac{1}{V} \sum_{p}' \frac{\hat{p}_{0}^{2}}{(\hat{p}^{2})^{2}} \sum_{\mu\nu} \cos(p_{\mu} - p_{\nu}) \hat{p}_{\mu}^{2} \hat{p}_{\nu}^{2}$$

$$= I_{01} - J_{11} + \frac{1}{4} K_{21} + J_{213} - \frac{1}{4} J_{214} .$$
(B.9)

$$\mathcal{F}_{5} = \frac{1}{V} \sum_{p}' \frac{\sin^{2} p_{0}}{(\hat{p}^{2})^{3}} \sum_{\mu\nu} \cos(p_{\mu} - p_{\nu}) \hat{p}_{\mu}^{2} \hat{p}_{\nu}^{2} = L_{31} - \frac{1}{4} L_{32}$$

$$= I_{11} - J_{21} + \frac{1}{4} K_{31} + J_{313} - \frac{1}{4} J_{314} - \frac{1}{4} \left[I_{12} - J_{22} + \frac{1}{4} K_{32} + J_{323} - \frac{1}{4} J_{324} \right].$$
(B.10)

$$\mathcal{F}_{6} \equiv \frac{1}{V} \sum_{p}' \frac{1}{\hat{p}^{2}} \sum_{k} \left[2\cos(2p_{0}) - \cos(p_{0}) \right] \cos(p_{k}) \hat{p}_{k}^{2}$$

$$= I_{00} - \frac{7}{2} I_{01} + I_{02} - \frac{1}{2} J_{10} + \frac{7}{4} J_{11} - \frac{1}{2} J_{12} - I_{11} + 4I_{12} - \frac{11}{4} I_{13} + \frac{1}{2} I_{14} .$$
(B.11)

$$\mathcal{F}_{7} \equiv \frac{1}{V} \sum_{p}' \sum_{k} \frac{\left(e^{-ip_{0}} - 1\right) \left(e^{-i2p_{0}} - 1\right) \left(e^{ip_{k}} - 1\right)^{2}}{(\hat{p}^{2})^{2}}$$
$$= -\frac{1}{V} \sum_{p}' \sum_{k} \frac{\hat{p}_{k}^{2} \cos p_{k} \left(\cos 3p_{0} - \cos 2p_{0} - \cos p_{0} + 1\right)}{(\hat{p}^{2})^{2}}$$
$$= 2I_{11} - \frac{5}{2}I_{12} + \frac{1}{2}I_{13} - 2I_{22} + \frac{7}{2}I_{23} - \frac{7}{4}I_{24} + \frac{1}{4}I_{25} - J_{21} + \frac{5}{4}J_{22} - \frac{1}{4}J_{23}.$$
(B.12)

C Correlators appearing in F_r with lattice regularization

C.1 Correlators appearing in $F_{1,0}$ and $F_{1,1}$

First

$$\langle U_1 \rangle_0 = n_1 \frac{1}{V} \sum_p' \frac{\hat{p}_0^2}{\hat{p}^2} = n_1 I_{11} ,$$
 (C.1)

where I_{nm} are defined in (B.1). Next

$$\langle U_2 \rangle_0 = \partial_0^x \partial_0^y \frac{1}{4V} \sum_x \langle \vec{\pi}(x)^2 \vec{\pi}(y)^2 \rangle_0 \bigg|_{y=x} = \frac{n_1}{2} \partial_0^x \partial_0^y \left[\frac{1}{V} \sum_x G(x-y)^2 \right] \bigg|_{y=x}$$

$$= \frac{n_1}{V^2} \sum_{pq} \frac{1 - \cos(p_0 + q_0)}{\hat{p}^2 \hat{q}^2} = n_1 I_{11} \left(I_{10} - \frac{1}{4} I_{11} \right) .$$
(C.2)

$$\langle U_1 A_{2,0} \rangle_0^c = n_1 I_{11} ,$$
 (C.3)

$$\langle U_1 A_{2,1}^{(a)} \rangle_0^c = -n_1 \left(1 - \frac{n_1}{V} \right) I_{21} ,$$
 (C.4)

$$\langle U_1 A_{2,1}^{(b)} \rangle_0^c = \left. \frac{1}{8V} \sum_{xu} \partial_\mu^u \partial_\mu^v \langle \partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(x) \vec{\pi}(u)^2 \vec{\pi}(v)^2 \rangle_0^c \right|_{v=u}$$

$$= \left. \frac{n_1}{V} \sum_{xu} \partial_\mu^u \partial_\mu^v \left\{ \partial_0^x G(x-u) \partial_0^x G(x-v) G(u-v) \right\} \right|_{v=u}$$

$$= n_1 \mathcal{F}_1 ,$$

$$(C.5)$$

where \mathcal{F}_1 is given by (B.6). Also ¹⁴

$$\langle U_1 A_{4,1}^{(1)} \rangle_0^c = 2n_1 I_{01} ,$$
 (C.6)

$$\langle U_1 A_{4,1}^{(i)} \rangle_0^c = 0, \quad i = 2, 3, 4,$$
 (C.7)

$$\langle U_1 A_{4,1}^{(5a)} \rangle_0^c = 2n_1 J_{21} ,$$
 (C.8)

$$\langle U_1 A_{4,1}^{(5b)} \rangle_0^c = 2n_1 I_{01} ,$$
 (C.9)

$$\langle U_1 A_{4,1}^{(5c)} \rangle_0^c = 2n_1 \sum_x \partial_0^* \partial_\mu \partial_\mu G(x) \partial_0^* \partial_\nu \partial_\nu G(x) = 2n_1 \mathcal{F}_4 \,, \tag{C.10}$$

where \mathcal{F}_4 is given by (B.9).

C.2 Correlators appearing in $F_{2,0}$ and $F_{2,1}$

Firstly

$$\langle W_2 \rangle_0 = n_1(n_1 - 1) \left(I_{21} - \frac{1}{4} I_{22} \right) .$$
 (C.11)

¹⁴Note that one can obtain the results of insertions in eqs. (C.3) and (C.6)-(C.10) by observing that $\langle XA_{2,0}\rangle_0^c$ inserts for each propagator appearing in $\langle X\rangle_0$ a factor 1, i.e. simply counts the number of propagators in $\langle X\rangle_0$. Similarly, for the other operators the corresponding insertions are $A_{4,1}^{(1)} \to 2\hat{p}^2$, $A_{4,1}^{(5a)} \to 2\sum_{\mu} \hat{p}_{\mu}^4/\hat{p}^2$, and $A_{4,1}^{(5c)} \to 2\sum_{\mu\nu} \cos(p_{\mu} - p_{\nu})\hat{p}_{\mu}^2\hat{p}_{\nu}^2/\hat{p}^2$.

Next

$$\langle W_3 \rangle_0 = \frac{n_1}{V} \sum_{xy} G(x-y) \left\{ n_1 G(x-y) \nabla_0^x \nabla_0^y G(x-y) + 2 \left[\nabla_0^x G(x-y) \right] \left[\nabla_0^y G(x-y) \right] \right\}$$

= $-n_1^2 \sum_x G(x)^2 \nabla_0^2 G(x) - 2n_1 \sum_x \left[\nabla_0 G(x) \right]^2 G(x)$
= $n_1 (n_1 - 1) W_{3a} + \frac{1}{2} n_1 W_{3c} ,$ (C.12)

where W_{3a}, W_{3c} are defined in (2.83),(2.84) respectively. For the connected correlators we get

$$\langle W_2 A_{2,0} \rangle_0^c = n_1 \sum_{xy\mu} \Big\{ n_1 G(x-y) \partial_{\mu}^* \nabla_0 G(x-z) \partial_{\mu}^* \nabla_0 G(y-z) \\ - n_1 \nabla_0 \nabla_0 G(x-y) \partial_{\mu}^* G(x-z) \partial_{\mu}^* G(y-z) \\ + 2 \nabla_0 G(x-y) \partial_{\mu}^* \nabla_0 G(x-z) \partial_{\mu}^* G(y-z) \Big\}$$
(C.13)
$$= 2n_1(n_1-1) \left[I_{21} - \frac{1}{4} I_{22} \right] .$$

$$\langle W_2 A_{2,1}^{(a)} \rangle_0^c = -2n_1(n_1-1) \left(1 - \frac{n_1}{V} \right) \frac{1}{V} \sum_{xyu} G(x-u) G(y-u) \nabla_0^x \nabla_0^y G(x-y) \\ = -2n_1(n_1-1) \left(1 - \frac{n_1}{V} \right) \frac{1}{V} \sum_p ' \frac{\sin^2 p_0}{(\hat{p}^2)^3}$$
(C.14)
$$= -2n_1(n_1-1) \left(1 - \frac{n_1}{V} \right) \left(I_{31} - \frac{1}{4} I_{32} \right) .$$

$$\langle W_2 A_{2,1}^{(b)} \rangle_0^c = \frac{1}{8V} \sum_{xyu} \partial_{\mu}^u \partial_{\mu}^v \left\langle [\nabla_0 \vec{\pi}(x) \cdot \nabla_0 \vec{\pi}(y)] \vec{\pi}(x) \cdot \vec{\pi}(y) \vec{\pi}(u)^2 \vec{\pi}(v)^2 \right\rangle_0^c \Big|_{v=u}$$

$$= n_1(n_1-1) \frac{1}{V} \sum_{xyu} \partial_{\mu}^u \partial_{\mu}^v \Big[G(x-u) G(y-v) \times$$

$$\{ 2G(u-v) \nabla_0^x \nabla_0^y G(x-y) - \nabla_0^x G(x-v) \nabla_0^y G(y-u) \} \Big]_{v=u}$$

with $\mathcal{F}_2, \mathcal{F}_3$ defined in (B.7),(B.8).

 $= n_1(n_1-1) [2\mathcal{F}_2 - \mathcal{F}_3],$

$$\langle W_2 A_{4,1}^{(1)} \rangle_0^c = 4n_1(n_1 - 1) \left[I_{11} - \frac{1}{4} I_{12} \right],$$
 (C.16)

$$\langle W_2 A_{4,1}^{(i)} \rangle_0^c = 0, \quad i = 2, 3, 4,$$
 (C.17)

$$\langle W_2 A_{4,1}^{(5a)} \rangle_0^c = 4n_1(n_1 - 1) \left[J_{31} - \frac{1}{4} J_{32} \right] ,$$
 (C.18)

$$\langle W_2 A_{4,1}^{(5b)} \rangle_0^c = 4n_1(n_1 - 1) \left[I_{11} - \frac{1}{4} I_{12} \right] ,$$
 (C.19)

$$\langle W_2 A_{4,1}^{(5c)} \rangle_0^c = 4n_1(n_1 - 1)\mathcal{F}_5,$$
 (C.20)

where \mathcal{F}_5 is given by (B.10).

C.3 Computation of F_3 up to O $\left(g_0^2\right)$

We have

$$F_3 = \sum_{i=1}^{5} \frac{g_4^{(i)}}{4} F_3^{(i)}, \quad F_3^{(i)} = \frac{1}{V} \langle C_4^{(i)} \rangle_{\mathcal{A}}.$$
(C.21)

Averaging over the rotations gives the following expressions for the $F_3^{(i)}$:

$$F_3^{(1)} = F_3^{(5a)} + F_3^{(1a)}, (C.22)$$

$$F_3^{(1a)} = \frac{2}{n} \frac{1}{V} \sum_{xk} \langle [2\mathbf{S}(x) + \Box_0 \mathbf{S}(x)] \cdot \Box_k \mathbf{S}(x) \rangle_{\mathcal{A}} \,. \tag{C.23}$$

$$F_{3}^{(2)} = -\frac{4}{nn_{1}} \frac{1}{V} \sum_{x} \langle 2 - 2\{\mathbf{S}(x) \cdot \mathbf{S}'(x)\}^{2} + n_{1}\{\mathbf{S}(x) \cdot \mathbf{S}'(x)\} \partial_{\mu} \mathbf{S}(x) \cdot \partial_{\mu} \mathbf{S}(x) \rangle_{\mathcal{A}}, \quad (C.24)$$

where we have introduced the notation $S'_i(x) = S_i(x + \hat{0})$ and below $S''_i(x) = S_i(x + 2\hat{0})$.

$$F_3^{(3)} = F_3^{(4a)} + F_3^{(3a)}, \tag{C.25}$$

$$F_3^{(3a)} = \frac{4}{nn_1} \frac{1}{V} \sum_{xk} \left\langle \mathbf{S}'(x) \cdot \partial_k \mathbf{S}(x) \left[n_1 \partial_0 \mathbf{S}(x) \cdot \partial_k \mathbf{S}(x) + \mathbf{S}'(x) \cdot \partial_k \mathbf{S}(x) \right]$$
(C.26)

$$-\partial_k \mathbf{S}(x) \cdot \partial_k \mathbf{S}(x) \rangle_{\mathcal{A}}$$
.

$$F_3^{(4)} = F_3^{(4a)} - \frac{1}{d+2} \left(F_3^{(2)} + 2F_3^{(3)} \right) , \qquad (C.27)$$

with

$$F_3^{(4a)} = -\frac{4}{nn_1} \frac{1}{V} \sum_x \left\langle \left\{ n_1 (\mathbf{S}(x) \cdot \mathbf{S}'(x)) \partial_0 \mathbf{S}(x) \cdot \partial_0 \mathbf{S}(x) + 2 - 2(\mathbf{S}(x) \cdot \mathbf{S}'(x))^2 \right\} \right\rangle_{\mathcal{A}}.$$
(C.28)

Next

$$F_3^{(5a)} = -\frac{4}{n} \frac{1}{V} \sum_x \langle -\mathbf{S}(x) \cdot \Box_0 \mathbf{S}(x) + 2\partial_0 \mathbf{S}(x) \cdot \partial_0^* \mathbf{S}(x) \rangle_{\mathcal{A}}.$$
 (C.29)

$$F_3^{(5b)} = F_3^{(1)} \,. \tag{C.30}$$

$$F_3^{(5c)} = F_3^{(5a)} + F_3^{(5d)}, (C.31)$$

$$F_3^{(5d)} = \frac{4}{n} \frac{1}{V} \sum_{xk} \langle \left[2\mathbf{S}''(x) - \mathbf{S}'(x) \right] \cdot \partial_k^2 \mathbf{S}(x) \rangle_{\mathcal{A}} \,. \tag{C.32}$$

 F_3 has a perturbative expansion starting at O ($g_0^2)$:

$$F_3 = \sum_{r=1} F_{3,r} g_0^{2r}, \quad F_3^{(i)} = \sum_{r=1} F_{3,r}^{(i)} g_0^{2r}.$$
(C.33)

C.3.1 Computation of $F_{3,1}^{(i)}$

$$F_{3,1}^{(1)} = F_{3,1}^{(5a)} + F_{3,1}^{(1a)}, \qquad (C.34)$$

$$F_{3,1}^{(1a)} = \frac{2}{n} \frac{1}{V} \sum_{xk} \langle [2\vec{\pi}(x) + \Box_0 \vec{\pi}(x)] \cdot \Box_k \vec{\pi}(x) \rangle_0$$

$$= \frac{2n_1}{n} \sum_k [2 + \Box_0] \Box_k G(0)$$

$$= \frac{2n_1}{n} [-2I_{00} + 2I_{11} + I_{01} - I_{12}]. \qquad (C.35)$$

$$F_{3,1}^{(2)} = -\frac{4}{nn_1} \frac{1}{V} \sum_x \langle 2\partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(x) + n_1 \partial_\mu \vec{\pi}(x) \cdot \partial_\mu \vec{\pi}(x) \rangle_0$$

$$= \frac{4}{n} \{ 2\Box_0 G(0) + n_1 \Box G(0) \}$$

$$= -\frac{4}{n} \{ 2I_{11} + n_1 I_{00} \} .$$
 (C.36)

$$F_{3,1}^{(3)} = F_{3,1}^{(4a)} + F_{3,1}^{(3a)}, \qquad (C.37)$$

$$F_{3,1}^{(3a)} = -\frac{4}{nn_1} \frac{1}{V} \sum \langle \partial_k \vec{\pi}(x) \cdot \partial_k \vec{\pi}(x) \rangle_0$$

$$\begin{aligned} S_{1}^{(a)} &= -\frac{4}{nn_{1}} \frac{1}{V} \sum_{xk} \langle \partial_{k} \vec{\pi}(x) \cdot \partial_{k} \vec{\pi}(x) \rangle_{0} \\ &= -\frac{4}{n} \left[I_{00} - I_{11} \right] \,. \end{aligned}$$
 (C.38)

$$F_{3,1}^{(4a)} = -\frac{4(n_1+2)}{nn_1} \frac{1}{V} \sum_x \langle \partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(x) \rangle_0$$

= $-\frac{4(n_1+2)}{n} I_{11}.$ (C.39)

$$F_{3,1}^{(5a)} = -\frac{4}{n} \frac{1}{V} \sum_{x} \langle -\vec{\pi}(x) \cdot \Box_0 \vec{\pi}(x) + 2\partial_0 \vec{\pi}(x) \cdot \partial_0^* \vec{\pi}(x) \rangle_0$$

$$= \frac{4n_1}{n} \left\{ \Box_0 G(0) + 2\partial_0^2 G(0) \right\}$$

$$= -\frac{4n_1}{n} \left\{ 3I_{11} - I_{12} \right\} .$$
 (C.40)

Finally

$$F_{3,1}^{(5c)} = F_{3,1}^{(5a)} + F_{3,1}^{(5d)}, \qquad (C.41)$$

$$F_{3,1}^{(5d)} = \frac{4}{n} \frac{1}{V} \sum_{xk} \langle \left[2\vec{\pi}''(x) - \vec{\pi}'(x) \right] \cdot \partial_k^2 \vec{\pi}(x) \rangle_0$$

$$= -\frac{4n_1}{n} \mathcal{F}_6, \qquad (C.42)$$

where \mathcal{F}_6 is given by (B.11).

C.4 Computation of F_4 up to O (g_0^2)

 F_4 is given by

$$F_4 = Z_4 \sum_i \frac{g_4^{(i)}}{4} F_4^{(i)}, \quad F_4^{(i)} = \frac{1}{V} \langle BB_4^{(i)} \rangle_{\mathcal{A}}.$$
(C.43)

Again averaging over rotations:

$$F_4^{(1)} = F_4^{(5a)} + F_4^{(1a)}, \qquad (C.44)$$

$$F_4^{(1a)} = -\frac{\partial}{nn_1g_0^2} \frac{1}{V} \sum_{xyk} \langle [\mathbf{S}(x) \cdot \Box_k \mathbf{S}(y)] \, \mathbf{S}'(x) \cdot \nabla_0 \mathbf{S}(y) - [\mathbf{S}(x) \cdot \nabla_0 \mathbf{S}(y)] \, \mathbf{S}'(x) \cdot \Box_k \mathbf{S}(y) \rangle_{\mathcal{A}} \,. \tag{C.45}$$

$$F_4^{(2)} = \frac{8}{nn_1g_0^2} \frac{1}{V} \sum_{xy} \langle \left[\{ \mathbf{S}(x) \cdot \mathbf{S}(y) \} \mathbf{S}'(x) \cdot \mathbf{S}'(y) - \{ \mathbf{S}(x) \cdot \mathbf{S}'(y) \} \mathbf{S}'(x) \cdot \mathbf{S}(y) \right] \partial_\mu \mathbf{S}(y) \cdot \partial_\mu \mathbf{S}(y) \rangle_\mathcal{A} \,.$$
(C.46)

$$F_4^{(3)} = F_4^{(4a)} + F_4^{(3a)}, \qquad (C.47)$$

$$F_4^{(3a)} = \frac{8}{nn_1g_0^2} \frac{1}{V} \sum_{xyk} \langle \left[\{ \mathbf{S}(x) \cdot \mathbf{S}'(y) \} \mathbf{S}'(x) \cdot \partial_k \mathbf{S}(y) - \{ \mathbf{S}'(x) \cdot \mathbf{S}'(y) \} \mathbf{S}(x) \cdot \partial_k \mathbf{S}(y) \right] \partial_0 \mathbf{S}(y) \cdot \partial_k \mathbf{S}(y) \rangle_{\mathcal{A}}. \qquad (C.48)$$

$$F_4^{(4a)} = \frac{8}{nn_1g_0^2} \frac{1}{V} \sum_{xy} \langle \left[\{ \mathbf{S}(x) \cdot \mathbf{S}(y) \} \mathbf{S}'(x) \cdot \mathbf{S}'(y) - \{ \mathbf{S}(x) \cdot \mathbf{S}'(y) \} \mathbf{S}'(x) \cdot \mathbf{S}(y) \right] \partial_0 \mathbf{S}(y) \cdot \partial_0 \mathbf{S}(y) \rangle_{\mathcal{A}} \,.$$
(C.49)

$$F_4^{(5a)} = \frac{8}{nn_1g_0^2} \frac{1}{V} \sum_{xy} \langle \{ \mathbf{S}(x) \cdot \partial_0^* \mathbf{S}(y) \} \mathbf{S}'(x) \cdot \partial_0 \mathbf{S}(y) - \{ \mathbf{S}(x) \cdot \partial_0 \mathbf{S}(y) \} \mathbf{S}'(x) \cdot \partial_0^* \mathbf{S}(y) \rangle_{\mathcal{A}} .$$
(C.50)

$$F_4^{(5b)} = F_4^{(1)} . (C.51)$$

Finally

$$F_{4}^{(5c)} = F_{4}^{(5a)} + F_{4}^{(5d)}, \qquad (C.52)$$

$$F_{4}^{(5d)} = \frac{8}{nn_{1}g_{0}^{2}} \frac{1}{V} \sum_{xyk} \langle \{ \mathbf{S}(x) \cdot [\mathbf{S}''(y) - \mathbf{S}'(y)] \} \mathbf{S}'(x) \cdot \partial_{k}^{2} \mathbf{S}(y) - \{ \mathbf{S}'(x) \cdot [\mathbf{S}''(y) - \mathbf{S}'(y)] \} \mathbf{S}(x) \cdot \partial_{k}^{2} \mathbf{S}(y) \rangle_{\mathcal{A}}. \qquad (C.53)$$

 F_4 has a perturbative expansion starting at O ($g_0^2)$:

$$F_4 = \sum_{r=1} F_{4,r} g_0^{2r} , \quad F_4^{(i)} = \sum_{r=1} F_{4,r}^{(i)} g_0^{2r} .$$
 (C.54)

C.4.1 Computation of $F_{4,1}^{(i)}$

$$F_{4,1}^{(1)} = F_{4,1}^{(5a)} + F_{4,1}^{(1a)}, \qquad (C.55)$$

$$F_{4,1}^{(1a)} = -\frac{4}{nn_1} \frac{1}{V} \sum_{xyk} \langle \Box_k^y \left[(\vec{\pi}(x) - \vec{\pi}(y))^2 \right] \nabla_0^y \left[(\vec{\pi}'(x) - \vec{\pi}(y))^2 \right] \rangle_0$$

$$= -\frac{8}{n} \frac{1}{V} \sum_{xyk} \left[2n_1 \Box_k^y G(x - y) \nabla_0^y G(x + \hat{0} - y) + \left(\Box_k^y \nabla_0^z \left\{ G(\hat{0}) - G(x - z) - G(y - x - \hat{0}) + G(y - z) \right\}^2 \right)_{z=y} \right]$$

$$= \frac{16(n_1 - 1)}{n} \left\{ I_{11} - \frac{1}{4} I_{12} - I_{22} + \frac{1}{4} I_{23} \right\}. \qquad (C.56)$$

$$F_{4,1}^{(2)} = \frac{8}{nn_1} \frac{1}{V} \sum_{xy} \langle \{ \partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y) \} \partial_\mu \vec{\pi}(y) \cdot \partial_\mu \vec{\pi}(y) \rangle_0 = 0.$$
 (C.57)

$$F_{4,1}^{(3)} = F_{4,1}^{(4a)} + F_{4,1}^{(3a)}, \qquad (C.58)$$

$$F_{4,1}^{(3a)} = \frac{8}{nn_1} \frac{1}{V} \sum_{xyk} \langle \{\partial_0 \vec{\pi}(x) \cdot \partial_k \vec{\pi}(y)\} \partial_0 \vec{\pi}(y) \cdot \partial_k \vec{\pi}(y) \rangle_0 = 0.$$
(C.59)

$$F_{4,1}^{(4a)} = \frac{8}{nn_1} \frac{1}{V} \sum_{xy} \langle \{\partial_0 \vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y)\} \partial_0 \vec{\pi}(y) \cdot \partial_0 \vec{\pi}(y) \rangle_0 = 0.$$
(C.60)

$$F_{4,1}^{(5a)} = \frac{8}{nn_1} \frac{1}{V} \sum_{xy} \left\langle \{\vec{\pi}(x) \cdot \partial_0^* \vec{\pi}(y)\} \vec{\pi}'(x) \cdot \partial_0 \vec{\pi}(y) - \{\vec{\pi}(x) \cdot \partial_0 \vec{\pi}(y)\} \vec{\pi}'(x) \cdot \partial_0^* \vec{\pi}(y) \right\rangle_0$$

$$= \frac{8(n_1 - 1)}{n} \frac{1}{V} \sum_{xy} \left\{ \partial_0^{*y} G(x - y) \partial_0^y G(x + \hat{0} - y) - \partial_0^y G(x - y) \partial_0^{*y} G(x + \hat{0} - y) \right\}$$

$$= \frac{16(n_1 - 1)}{n} \left\{ I_{22} - \frac{1}{4} I_{23} \right\},$$

(C.61)

and finally

$$\begin{aligned} F_{4,1}^{(5c)} &= F_{4,1}^{(5a)} + F_{4,1}^{(5d)} , \qquad (C.62) \\ F_{4,1}^{(5d)} &= \frac{8}{nn_1} \frac{1}{V} \sum_{xyk} \langle \{\vec{\pi}(x) \cdot \left[\vec{\pi}''(y) - \vec{\pi}'(y)\right] \} \vec{\pi}'(x) \cdot \partial_k^2 \vec{\pi}(y) \\ &- \{\vec{\pi}'(x) \cdot \left[\vec{\pi}''(y) - \vec{\pi}'(y)\right] \} \vec{\pi}(x) \cdot \partial_k^2 \vec{\pi}(y) \rangle_0 \\ &= \frac{8(n_1 - 1)}{n} \frac{1}{V} \sum_{xyk} \left[\partial_0^y G(x - y - \hat{0}) \partial_k^{y2} G(x + \hat{0} - y) - \partial_0^y G(x - y) \partial_k^{y2} G(x - y) \right] \\ &= \frac{8(n_1 - 1)}{n} \mathcal{F}_7 , \qquad (C.63) \end{aligned}$$

where \mathcal{F}_7 is given by (B.12).

C.5 Computation of F_5 up to O (g_0^2)

$$F_5 = \mathcal{O}\left(g_0^4\right) \,, \tag{C.64}$$

and hence doesn't contribute to the order considered.

D The n = 2 case with lattice regularization

The lattice action with the chemical potential is

$$A = -\frac{1}{g_0^2} \sum_{x\mu} \cos\left(\partial_\mu \Phi(x) - ih\delta_{\mu 0}\right)$$

$$= -\frac{1}{g_0^2} \sum_x \left[\sum_\mu \cos\left(\partial_\mu \Phi(x)\right) + ih\sin\left(\partial_0 \Phi(x)\right) + \frac{1}{2}h^2\cos\left(\partial_0 \Phi(x)\right)\right] + O\left(h^3\right)$$
(D.1)

With $\Phi(x) = g_0 \phi(x)$ we have

$$A|_{h=0} = A_0 + g_0^2 A_1 + g_0^4 A_2 + \dots$$
 (D.2)

where

$$A_0 = \frac{1}{2} \sum_{x\mu} (\partial_\mu \phi(x))^2 , \qquad (D.3)$$

$$A_1 = -\frac{1}{24} \sum_{x\mu} (\partial_\mu \phi(x))^4 \,. \tag{D.4}$$

The h dependent part is given by

$$A_{h} = -\frac{h^{2}}{2g_{0}^{2}}V + ihg_{0}B_{1} + h^{2}\left(B_{20} + g_{0}^{2}B_{21} + \ldots\right)$$
(D.5)

$$B_1 = \frac{1}{6} \sum_{x} (\partial_0 \phi(x))^3 , \qquad (D.6)$$

$$B_{20} = \frac{1}{4} \sum_{x} (\partial_0 \phi(x))^2 , \qquad (D.7)$$

$$B_{21} = -\frac{1}{48} \sum_{x} (\partial_0 \phi(x))^4 \,. \tag{D.8}$$

Note that we need the free energy only up to $h^2 g_0^2$; the omitted terms do not contribute to this order.

$$Vf_{h} = \langle A_{h} \rangle - \frac{1}{2} \langle A_{h}^{2} \rangle + \frac{1}{2} \langle A_{h} \rangle^{2} \dots$$

= $-\frac{h^{2}}{2g_{0}^{2}} V + h^{2} \langle B_{20} \rangle_{0} + h^{2} g_{0}^{2} \left(\langle B_{21} \rangle_{0} - \langle B_{20} A_{1} \rangle_{0}^{c} + \frac{1}{2} \langle B_{1}^{2} \rangle_{0} \right).$ (D.9)

So

$$\chi = \frac{1}{g_0^2} \left(1 + g_0^2 R_1 + g_0^4 R_2 + \dots \right) , \qquad (D.10)$$

with

$$R_{1} = -\frac{2}{V} \langle B_{20} \rangle_{0} = -\frac{1}{2} \left\langle \frac{1}{V} \sum_{x} (\partial_{0} \phi(x))^{2} \right\rangle_{0}$$

$$= \frac{1}{2} \Box_{0} G(0) = -\frac{1}{2V} \sum_{p}' \frac{\hat{p}_{0}^{2}}{\hat{p}^{2}} = -\frac{1}{2} I_{11},$$
 (D.11)

in agreement with (3.55), and

$$R_{2} = -\frac{2}{V} \langle B_{21} \rangle_{0} + \frac{2}{V} \langle B_{20} A_{1} \rangle_{0}^{c} - \frac{1}{V} \langle B_{1}^{2} \rangle_{0}$$

$$= \frac{1}{24} \left\langle \frac{1}{V} \sum_{x} (\partial_{0} \phi(x))^{4} \right\rangle_{0} - \frac{1}{48} \left\langle \frac{1}{V} \sum_{xy\mu} (\partial_{0} \phi(x))^{2} (\partial_{\mu} \phi(y))^{4} \right\rangle_{0}^{c}$$

$$- \frac{1}{36} \left\langle \frac{1}{V} \sum_{xy} (\partial_{0} \phi(x))^{3} (\partial_{0} \phi(y))^{3} \right\rangle_{0}$$

$$= \frac{1}{8} (\Box_{0} G(0))^{2} + \frac{1}{4} \sum_{x\mu} \Box_{0} G(x) \Box_{\mu} G(x) \Box_{\mu} G(0) + \frac{1}{6} \sum_{x} (\Box_{0} G(x))^{3}$$

$$= \frac{1}{8} \left(\frac{1}{V} \sum_{p} \frac{\dot{p}_{0}^{2}}{\dot{p}^{2}} \right)^{2} - \frac{1}{4} \sum_{\mu} \left[\left(\frac{1}{V} \sum_{p} \frac{\dot{p}_{0}^{2} \dot{p}_{\mu}^{2}}{(\dot{p}^{2})^{2}} \right) \left(\frac{1}{V} \sum_{q} \frac{\dot{q}_{\mu}^{2}}{\dot{q}^{2}} \right) \right] - \frac{1}{6} S_{n2}$$

$$= \frac{1}{8} I_{11}^{2} - \frac{1}{4} I_{22} I_{11} - \frac{1}{4d_{s}} (I_{11} - I_{22}) (I_{00} - I_{11}) - W_{3c}.$$
(D.12)

Here

$$S_{n2} = -\sum_{x} \left(\Box_0 G(x) \right)^3 = 6W_{3c} \,. \tag{D.13}$$

The last equation follows from the direct comparison with (2.84). Also

$$-\sum_{x\mu} \Box_0 G(x) \Box_{\mu} G(x) \Box_{\mu} G(0) = I_{22} I_{11} + \frac{1}{d_s} (I_{11} - I_{22}) (I_{00} - I_{11}).$$
(D.14)

The result for R_2 above agrees with the result in (2.88) for $n_1 = 1$.

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