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Finite size and temperature effects in the AF Heisenberg model

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Abstract. The low temperature and large volume effects in the $d=2+1$ antiferomagnetic quantum Heisenberg model are dominated by magnon excitations. The leading and next-to-leading corrections are fully controlled by three physical constants, the spin stiffness, the spin wave velocity and the staggered magnetization. Among others, the free energy, the ground state energy, the low lying excitations, staggered magnetization, staggered and uniform susceptibilities are studied here. The special limits of very low temperature and infinite volume are considered also.

1. Introduction

The low energy properties and the leading finite size and temperature effects of the $d=2+1$ quantum anti-ferromagnetic (AF) Heisenberg model

$$H=J\sum_{n,\mu}\hat{\mathbf{S}}_n\hat{\mathbf{S}}_{n+\mu}, \qquad \hat{\mathbf{S}}_n^2=S(S+1) \tag{1.1}$$

are governed by magnon excitations. The interaction of massless excitations whose existence is due to spontaneous symmetry breaking [1], is strongly constrained by symmetry principles [2]. In particle physics it was the interaction of soft pions where many of the general features of this dynamics were first observed [2–4]. These investigations received new impetus recently [5] by the application of the powerful method of effective Lagrangeans [3, 6] which provides a systematical way to calculate higher order corrections (chiral perturbation theory). Gasser and Leutwyler and their followers treated not only low energy Goldstone boson physics but also finite temperature and finite size effects in QCD [5, 7, 10]. This technique can be immediately generalized to other quantum field theories and critical statistical systems [11] and provides a systematic alternative to other related methods [12–14].

The special, constrained feature of magnon interactions in the AF Heisenberg model has been emphasized and different leading order results were obtained in several recent publications [15–17]. Using current algebra techniques or intuitive reasoning it would be very difficult to go beyond the leading order. On the other hand, this problem becomes a relatively simple book-keeping if the technique of chiral perturbation theory is used. The power of chiral perturbation theory was illustrated in this context in [18] by calculating the first correction to the correlation length at low temperatures. In this paper we present further results beyond leading order. The temperature and size dependence of the free energy density (internal energy density, specific heat), the size dependence of the ground state energy density, the energy of the low lying excitations and its size dependence will be investigated. We calculate the staggered magnetic field dependent part of the free energy density (magnetization and susceptibility) and study the behaviour of the uniform susceptibility. Additionally, we discuss the zero temperature and the infinite volume limits which reveal special physical properties and pose new technical problems.

The results of chiral perturbation theory reflect the symmetries of the underlying model only and depend on free physical parameters whose number is growing with the order of the calculation. As it is well known, the leading order results depend on three physical parameters: the spin stiffness constant ρ_s, the spin wave velocity c and the staggered magnetization $\mathscr{M}_s$. It is less well known, perhaps, that for the quantities we study here the next-to-leading corrections can be expressed in terms of the same constants, no new parameters enter (see [11] and Sect. 4). As we shall discuss, these predictions are free of cut-off effects also.

The three parameters ρ_s, c and $\mathscr{M}_s$ are fixed by the underlying model as the function of the coupling J. An effective way to fix these constants is to compare the results of chiral perturbation theory with the correspond-

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ing numerical results using the Hamilton operator in (1.1). This method has been applied earlier for classical ferromagnetic models and field theories [19].

The hamiltonian in (1.1) is invariant under a global rotation of the spin operators. This O(3) symmetry is broken spontaneously to O(2) producing two massless magnon excitations. Since the dynamics of magnons is essentially determined by the underlying symmetries only, the classical O(3) ferromagnetic Heisenberg model in $d=3$ in the broken phase is described also by the results of this paper. In this case we have to put $c=1$ and interpret $L_t = T^{-1}$ and L_s as giving the size of the euclidean box $L_t \times L_s \times L_s$ on which the model is defined. The classical O(3) Heisenberg model is described by a fixed length vector field with 3 components. This model can be generalized to N-component vectors with $O(N)$ symmetry. Actually, we give all the results for the symmetry group $O(N)$. The quantum AF Heisenberg model in (1.1) corresponds to $N=3$.

The paper is organized as follows. For the readers convenience we summarize the results in Sect. 2. Concerning the notations, results and region of validity, this section is self-contained. Some of the results discussed in Sect. 2 occurred earlier in the literature in the context of classical ferromagnets or field theories. In this case our role is only to insert the proper spin wave velocity dependence and to raise attention to the existence of these results. In Sect. 3 we try to clarify some problematic results which occur in the literature.

Those readers who are interested in the results only, might skip the rest of the paper. Sections 5–8 are sufficiently detailed allowing the reader to reproduce the results. This part is, however not self-contained. It assumes that the reader is familiar with the basic elements of chiral perturbation theory. The summary paper of Gasser and Leutwyler (last reference in [5]) and [11] might serve as an introduction with high energy physics and condensed matter physics background, respectively.

In Sect. 4 we construct the effective Lagrangean which is needed to derive the free energy density $f = f(T, L_s)$ up to next-to-leading order. The effect of a finite cut-off is discussed in some detail there also. In Sect. 5 we calculate $f(T, L_s)$ up to next-to-leading order. Although this calculation is a priori valid for $\hbar c/(TL_s) = O(1)$ only, the $L_s \to \infty$ limit gives correctly the temperature dependence of the infinite volume free energy density at low temperatures. The formal $T \to 0$ limit, however, does not lead to the correct volume dependence of the ground state energy, as we discuss in Sect. 5. The volume dependence of the ground state energy, the lowest lying excitations and their finite volume corrections are considered in Sect. 6. In this section we regularize the effective Lagrangean on a lattice which opens the possibility to discuss the issue of power divergences in chiral perturbation theory. We show that – as expected – all these divergences can be absorbed through the standard renormalization procedure and no mixing between infrared and ultraviolet problems occurs. In Sect. 7 the dependence of the free energy density on a weak staggered magnetic field, the magnetization and susceptibility are considered. Since this problem has been treated before we can keep this part brief. Very low temperatures require special care again as discussed in Sect. 8, where the volume dependence of the staggered susceptibility at $T=0$ is calculated. In Sect. 9 the uniform susceptibility is discussed. In the Appendix A we consider specific lattice momentum sums and integrals. Appendix B contains some asymptotic expressions for the shape coefficients.

Chiral perturbation theory is an exact low energy expansion. It summarizes the symmetry properties of the model in (1.1) in a concised way and it is valid for any spin S. Consequently, if we replace in any quantity considered here the parameters ρ_s, c and $\mathscr{M}_s$ by their spin wave $(1/S)$ expansion, then the spin wave expansion of this quantity is obtained. The relation between these two expansions is discussed further in Sect. 3.

We made an effort to stay close to the notations used earlier in the literature. Since the model in (1.1) gave the motivation for this work, we denoted by ρ_s (rather than by F^2, or Υ) the leading non-magnon scale. We used the index s both to denote staggered quantities and to refer to 'spatial', like spatial volume and size. Certain parts of the calculation are carried out for general dimension d, in which case we kept d as a parameter in the formulas. In the calculations we used the convention "$\hbar = c = 1$" and restored the spin wave velocity dependence only at the end. At some places we introduced more convenient notations with respect to the preprint version of this paper (BUTP-92/46).

2. Results

Let us introduce a staggered external field $\mathbf{B}_s = (B_s, 0, 0)$, and a uniform magnetic field[1] $\mathbf{h}_u = (h_u, 0, 0)$ and generalize (1.1) to

$$H = J \sum_{n,\mu} \hat{\mathbf{S}}_n \hat{\mathbf{S}}_{n+\mu} - \mathbf{B}_s \sum_n (-1)^{\|n\|} \hat{\mathbf{S}}_n - \mathbf{h}_u \sum_n \hat{\mathbf{S}}_n . \tag{2.1}$$

We shall define the field $\mathbf{H}_s$ as

$$\mathbf{H}_s = \frac{\mathbf{B}_s}{a^2}, \tag{2.2}$$

where a is the lattice unit of the square lattice over which (2.1) is defined. We shall consider a system of spatial size $L_s \times L_s$ at temperature T. The spin-stiffness, the spin wave velocity and the staggered magnetization of the infinitely large system at zero temperature and at zero external fields are denoted by ρ_s, c and $\mathscr{M}_s$, respectively. These quantities are fixed by the Hamilton operator in (2.1). On dimensional grounds ρ_s and $\hbar c/a$ are proportional to J. It will be useful to introduce the notation

$$l^3 = \frac{\hbar c}{TL_s}. \tag{2.3}$$

[1] The magnetic moment is included in the definition of h_u

In the path integral formulation we shall work in a euclidean box $L_t \times L_s \times L_s$, where $L_t = \hbar c/T$. We shall refer to the $l = \mathrm{O}(1)$ and $l \gg 1$ cases as "cubic" and "cylinder" geometry, respectively. Concerning dimensions, we have

$$\begin{aligned} &\dim J = \mathrm{erg}, \quad \dim H_s = \frac{\mathrm{erg}}{\mathrm{cm}^2}, \\ &\dim L_s = \mathrm{cm}, \quad \dim T = \mathrm{erg}, \\ &\dim h_u = \mathrm{erg}, \quad \dim \rho_s = \mathrm{erg}, \\ &\dim \mathscr{M}_s = 1, \quad \dim l = 1. \end{aligned} \tag{2.4}$$

The free energy density f is defined as

$$Z = \exp\left(-\frac{L_s^2}{T} f\right), \tag{2.5}$$

where Z is the partition function. As explained in the introduction, the following results apply to classical $\mathrm{O}(N)$ symmetric ferromagnetic systems also, while (2.1) corresponds to $N=3$. In general, magnons dominate the physical properties of the system at low energies, large volumes, low temperatures and weak external fields. More detailed conditions will be given together with the results.

2.1. H_s – dependence of the basic parameters ($L_s = \infty, T=0, H_s \neq 0, h_u = 0$)

In the presence of a nonzero staggered field H_s the magnons (they have a relativistic dispersion relation) pick up a mass M^H. Let us introduce the notation M:

$$(c^2 M)^2 = \frac{(\hbar c)^2 \mathscr{M}_s}{\rho_s} H_s. \tag{2.6}$$

We shall consider weak external staggered fields such that

$$c^2 M \ll \rho_s. \tag{2.7}$$

Denoting the staggered magnetization and the spin stiffness in the presence of the field $H_s \neq 0$ by $\mathscr{M}_s^H$ and ρ_s^H, we have

$$\begin{aligned} \mathscr{M}_s^H &= \mathscr{M}_s \left[1 + \frac{N-1}{8\pi} \cdot \frac{c^2 M}{\rho_s} + \mathrm{O}(H_s)\right], \\ \rho_s^H &= \rho_s \left[1 + 2 \cdot \frac{N-2}{8\pi} \cdot \frac{c^2 M}{\rho_s} + \mathrm{O}(H_s)\right], \\ M^H &= M \left[1 - \frac{1}{2} \cdot \frac{N-3}{8\pi} \cdot \frac{c^2 M}{\rho_s} + \mathrm{O}(H_s)\right]. \end{aligned} \tag{2.8}$$

Actually, these are first order results and – at least in the context of ferromagnetic systems – are well known [12, 5, 11]. We study these relations in Sect. 6 in order to fix the renormalization of the parameters.

2.2. The free energy in "cubic" geometry (L_s = *finite*, $T \neq 0$, $H_s = 0$, $h_u = 0$, $l = \mathrm{O}(1)$)

We consider large volumes and low temperatures relative to typical non-magnon scales:

$$\frac{\hbar c}{L_s} \ll \rho_s, \quad T \ll \rho_s, \tag{2.9}$$

while keeping the ratio l finite, $\mathrm{O}(1)$. The free energy density reads

$$\begin{aligned} &f(T, L_s) \\ &= q_1 + \frac{T}{L_s^2} q_2 - \frac{N-1}{2} \frac{T}{L_s^2} \left\{\frac{1}{3} \ln \frac{L_s^2}{T} + \beta_0(l) \right. \\ &\quad \left. + (N-2) \frac{\hbar c}{\rho_s L_s l} \beta_1(l) + \mathrm{O}\left(\frac{1}{L_s^2}\right)\right]. \end{aligned} \tag{2.10}$$

Here q_1 and q_2 are two non-universal constants which are not fixed by chiral perturbation theory. The constant q_1 is the infinite volume ground state energy density which is studied intensively for the model in (1.1) numerically [20, 22, 30, 32] and otherwise [23–25, 31]. (For a detailed discussion, see [28, 29].) The constant q_2 depends on the precise normalization of the partition function. The internal energy density is already free of q_2. The shape coefficients $\beta_n(l)$ are expressed through $\alpha_n(l)$ by the relations [11]

$$\begin{aligned} \beta_0(l) &= \alpha_0(l) + \ln(4\pi) - \gamma_E - \tfrac{2}{3} \\ &= \alpha_0(l) + 1.287142\ldots, \\ \beta_n(l) &= \left(-\frac{1}{4\pi}\right)^n \left[\alpha_n(l) + \frac{3}{n(2n-3)}\right], \quad n = 1, 2 \ldots. \end{aligned} \tag{2.11}$$

The functions $\alpha_p(l)$ can be calculated easily using the following representation [11]

$$\alpha_p(l) = \hat{\alpha}_{p-3/2}(l) + \hat{\alpha}_{-p}\left(\frac{1}{l}\right), \tag{2.12}$$

where

$$\hat{\alpha}_r(l) = \int_0^1 \mathrm{d}t\, t^{r-1} \left[S\left(\frac{1}{l^2 t}\right)^2 S\left(\frac{l^4}{t}\right) - 1\right], \tag{2.13}$$

with

$$S(x) = \sum_{-\infty}^{\infty} \mathrm{e}^{-\pi n^2 x}. \tag{2.14}$$

For $l=1$ the relevant β_n values are given in Table 1 of [11]. In Appendix B we give approximate analytic forms, which are sufficiently precise for applications.

The internal energy density

$$e(T, L_s) = -T^2 \frac{\partial}{\partial T} (f(T, L_s)/T)$$

can be written in the form

$$e(T,L_s)=q_1-\frac{N-1}{6}\frac{T}{L_s^2}\left\{1+l\frac{\mathrm{d}}{\mathrm{d}l}\beta_0(l)\right.$$
$$\left.-(N-2)\frac{\hbar c}{\rho_s L_s l}\left(\beta_1(l)-l\frac{\mathrm{d}}{\mathrm{d}l}\beta_1(l)\right)+\ldots\right\}. \tag{2.15}$$

In [18] we quoted this result for $N=3$ with a slight error[2], unfortunately: in the T^3 coefficient in the brackets the number "1" was incorrectly given as "2".

2.3. *Thermodynamics at infinite volume* ($L_s=\infty$, $T\neq 0$, $H_s=0$, $h_u=0$)

Although the results in Sect. 2.2 were derived under the condition $l=\mathrm{O}(1)$, the $L_s\to\infty$ ($l\to 0$) limit is smooth[3] and gives correctly the temperature dependence of the free energy and internal energy densities:

$$f(T)=q_1-(N-1)\frac{\zeta(3)}{2\pi(\hbar c)^2}T^3+\mathrm{O}(T^5),$$
$$e(T)=q_1+(N-1)\frac{\zeta(3)}{\pi(\hbar c)^2}T^3+\mathrm{O}(T^5). \tag{2.16}$$

Here $\zeta(3)=1.2020569$. There is no $\sim T^4$ contribution. Equation (2.16) gives for the specific heat

$$C(T)=(N-1)\frac{3\zeta(3)}{\pi(\hbar c)^2}T^2+\mathrm{O}(T^4). \tag{2.17}$$

The $\sim T^3$ term in (2.16) is just the free energy contribution of $N-1$ massless free bosons. This prediction has occured earlier in [17] for the AF Heisenberg model ($N=3$). Although our calculation goes up to order $\sim T^4$, the corresponding coefficient turns out to be zero. There is an amazing mess in the literature on the $\sim T^3$ term in the internal energy density of the AF Heisenberg model. We shall return to this problem in Sect. 3.

2.4. *Volume dependence of the ground state energy density* (L_s=*finite*, $T=0$, $H_s=0$, $h_u=0$)

Equation (2.10) was derived under the condition $l=\mathrm{O}(1)$ and as we shall discuss later, the $T\to 0$ ($l\to\infty$) formal limit of eq. (2.10) does *not* give the correct volume dependence of the ground state energy density. Very low temperatures require special care. We give two different derivations leading to

$$\varepsilon_0(L_s)=q_1-\frac{N-1}{2}\cdot\frac{1.437745(\hbar c)}{L_s^3}$$
$$+\frac{(N-1)(N-2)}{8}\cdot\frac{(\hbar c)^2}{\rho_s L_s^4}+\mathrm{O}\left(\frac{1}{L_s^5}\right). \tag{2.18}$$

The $\sim 1/L_s^3$ correction has been derived earlier for the AF Heisenberg model ($N=3$) using current algebra like techniques [16] and effective Lagrangeans [17]. In some works [20] the $\sim 1/L_s^4$ contribution to the ground state energy density was predicted to be zero, which is incorrect. The problem of the ground state energy has been discussed in the context of QCD in $d=3+1$ with $\mathrm{SU}(n)\times\mathrm{SU}(n)$ symmetry [8]. Since $\mathrm{SU}(2)\times\mathrm{SU}(2)\sim\mathrm{O}(4)$, (2.18) for $N=4$ should agree with the corresponding result for $n=2$ in [8]. After trivial adjustments corresponding to $d=2+1\to d=3+1$ they agree, indeed.

2.5. *The energy of the lowest lying excitations and its volume dependence* (L_s=*finite*, $T=0$, $H_s=0$, $h_u=0$)

It is known since a long time that the tower of lowest excitations in the broken phase is related to the slow precession of the order parameter and, in leading order, it is given by simple quantum mechanics over the symmetry group space [8, 13, 21]. We have calculated the leading finite size correction also and obtained for the energy difference between the excited state with $j=1$, 2,... and the ground state[4]

$$E_j(L_s)-E_0(L_s)=j(j+N-2)\frac{(\hbar c)^2}{2\rho_s L_s^2}$$
$$\times\left[1-(N-2)\frac{\hbar c}{\rho_s L_s}\frac{3.900265}{4\pi}+\mathrm{O}\left(\frac{1}{L_s^2}\right)\right]. \tag{2.19}$$

For the AF Heisenberg model ($N=3$) the leading order result has been discussed in [16].

2.6. *Weak staggered field in "cubic" geometry* (L_s=*finite*, $T\neq 0$, $H_s\neq 0$, $h_u=0$, $l=\mathrm{O}(1)$)

We quote now the H_s-dependent part of the free energy density derived under conditions of (2.9) and[5]

$$u_0\equiv\frac{H_s\mathcal{M}_s L_s^2}{T}\leqq\mathrm{O}(1). \tag{2.20}$$

This result was derived earlier [11], we restored the correct spin wave velocity dependence only:

$$f(T,L_s,H_s)$$
$$=f(T,L_s)-\frac{T}{L_s^2}\left[\ln(Y_N(u))+\gamma_2\cdot\left(\frac{u_0\hbar c}{\rho_s L_s l}\right)^2+\ldots\right], \tag{2.21}$$

where the H_s independent part, $f(T,L_s,H_s=0)\equiv f(T,L_s)$ is given by (2.10). We also introduced the notations[6]

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[2] Neither the text nor the subsequent equations are influenced by this error in [18]

[3] see Appendix B

[4] Equation (2.19) refers to the energy and not to the energy density: $E_0(Ls)=L_s^2\varepsilon_0(L_s)$

[5] With the $\leqq$ sign in (2.20) we want to indicate that H_s can be arbitrarily small

[6] We have changed the notation ρ_1,ρ_2 of [11] to γ_1,γ_2 to avoid confusion with the spin stiffness

$$u = \gamma_1 u_0,$$

$$\gamma_1 = 1 + \frac{N-1}{2} \frac{\hbar c}{\rho_s L_s l} \beta_1(l) - \frac{(N-1)(N-3)}{8} \left(\frac{\hbar c}{\rho_s L_s l}\right)^2 (\beta_1(l)^2 - 2\beta_2(l)), \tag{2.22}$$

$$\gamma_2 = \frac{N-1}{4} \beta_2(l),$$

and $\beta_p(l)$ was defined earlier in (2.11-2.14). The function $Y_N(z)$ can be expressed in terms of the modified Bessel function $I_\nu(z)$,

$$Y_N(z) = \left(\frac{z}{2}\right)^{-\frac{N-2}{2}} I_{\frac{N-2}{2}}(z). \tag{2.23}$$

Some of the properties of the function $Y_N(z)$ are summarized in Appendix F of [11].

Derivatives with respect to the staggered field H_s give the staggered magnetization and susceptibilities,

$$\begin{aligned} \mathcal{M}_s(T, L_s, H_s) &= -\frac{\partial}{\partial H_s} f(T, L_s, H_s) \\ &= \mathcal{M}_s \left\{\gamma_1 \frac{Y_N'(u)}{Y_N(u)} + 2\gamma_2 u_0 \left(\frac{\hbar c}{\rho_s L_s l}\right)^2 + \dots\right\}, \end{aligned} \tag{2.24}$$

$$\begin{aligned} \chi_s^{\parallel}(T, L_s, H_s) &\equiv \frac{\partial \mathcal{M}_s(T, L_s, H_s)}{\partial H_s} = a^2 \frac{\partial \mathcal{M}_s(T, L_s, H_s)}{\partial B_s} \\ &= \mathcal{M}_s^2 \frac{L_s^2}{T} \left\{\gamma_1^2 \left[\frac{Y_N''(u)}{Y_N(u)} - \left(\frac{Y_N'(u)}{Y_N(u)}\right)^2\right] + 2\gamma_2 \left(\frac{\hbar c}{\rho_s L_s l}\right)^2 + \dots\right\}, \end{aligned} \tag{2.25}$$

$$\chi_s^{\perp}(T, L, H_s) = \frac{\mathcal{M}_s(T, L_s, H_s)}{H_s}.$$

In the $H_s \to 0$ limit $\mathcal{M}_s(T, L_s, H_s) \to 0$ as it should, and

$$\chi_s^{\parallel}(T, L_s, 0) = \chi_s^{\perp}(T, L_s, 0) = \frac{1}{N} \mathcal{M}_s^2 \frac{L_s^2}{T} \times \left\{1 + (N-1)\left(\frac{\hbar c}{\rho_s L_s l}\right) \cdot \beta_1(l) + \frac{N-1}{2}\left(\frac{\hbar c}{\rho_s L_s l}\right)^2 (\beta_1(l)^2 + (2N-3)\beta_2(l)) + \dots\right\}. \tag{2.26}$$

2.7. *Volume dependence of the staggered susceptibility at small temperature* ($T \ll \hbar c/L_s$, $H_s = 0$, $h_u = 0$)

As we mentioned before, low temperatures require special treatment. For $T \ll \hbar c/L_s$ the coefficients multiplying the expansion parameter $\hbar c/\rho_s L_s$ in (2.26) become large. The dynamics is dominated by the low lying modes of the effective O(N) rotator. The corresponding susceptibility is calculated in Sect. 8. We note here only that for temperatures

$$\frac{T L_s^2 \rho_s}{(\hbar c)^2} \ll 1, \tag{2.27}$$

the susceptibility becomes independent of the temperature and it is proportional to the square of the spatial volume:

$$\chi_s(T, L_s) = \frac{4}{N(N-1)} \frac{\mathcal{M}_s^2 \rho_s}{(\hbar c)^2} L_s^4 \times \left[1 + (2N-3)\frac{\hbar c}{\rho_s L_s} \frac{3.900265}{4\pi} + O\left(\frac{1}{L_s^2}\right)\right]. \tag{2.28}$$

The basic reason of this strong volume dependence lies in the smallness of the excitation energies which are proportional to the inverse spatial volume, (2.19).

2.8. *Uniform susceptibility* ($H_s = 0$, $h_u = 0$)

For cubic geometry, $T = O(\hbar c/L_s)$ and under the conditions in (2.9) we obtain for the uniform susceptibility at $h_u = 0$

$$\begin{aligned} \chi_u(T, L_s) &= \frac{2}{N} \frac{\rho_s}{(\hbar c)^2} \left\{1 + \frac{N-2}{3} \frac{\hbar c}{\rho_s L_s l} \tilde{\beta}_1(l) + \frac{N-2}{3}\left(\frac{\hbar c}{\rho_s L_s l}\right)^2 \right. \\ &\left. \times [(N-2)\tilde{\beta}_2(l) - \tfrac{1}{3}\tilde{\beta}_1(l)^2 - 6\psi(l)]\right\}. \end{aligned} \tag{2.29}$$

Here we introduced the shorthand notations

$$\tilde{\beta}_1(l) = \frac{1}{l} \frac{d}{dl}(l^2 \beta_1(l)), \quad \tilde{\beta}_2(l) = \frac{1}{l^3} \frac{d}{dl}(l^4 \beta_2(l)). \tag{2.30}$$

In the next-to-leading order a new shape coefficient $\psi(l)$ enters, whose definition is given in Sect. 9. For $l = 1$ it can be expressed through β_n,

$$\psi(1) = -\tfrac{1}{3}\beta_1(1)^2 - \tfrac{1}{3}\beta_2(1) = -0.020529, \tag{2.31}$$

for other values of l it requires a less trivial numerical evaluation. In Appendix B we give approximate analytic expressions for $\psi(l)$.

In the infinite volume limit (2.29) gives

$$\chi_u(T) = \frac{2}{N} \frac{\rho_s}{(\hbar c)^2} \left[1 + (N-2)\frac{T}{2\pi\rho_s}\right.$$

$$+(N-2)\left(\frac{T}{2\pi\rho_s}\right)^2+\ldots\Bigg]. \quad (2.32)$$

Here $\chi_u(T)$ is the angular average of the transversal and longitudinal susceptibilities. This is reflected in the result $\chi_u(T\to 0)=(2/N)\,\rho_s/(\hbar c)^2=(2/N)\chi_u^{\perp}$.

For $T\ll\hbar c/L_s$ the result is again given by the effective $O(N)$ rotator. In particular for very small temperatures $TL_s^2\rho_s/(\hbar c)^2\ll 1$ the susceptibility becomes exponentially small

$$\chi_u(T,L_s)=\frac{2}{N}\,\frac{1}{L_s^2 T}\exp\left\{-\frac{N-1}{2}\,\frac{(\hbar c)^2}{\rho_s L_s^2 T}\right\}. \quad (2.33)$$

3. Chiral perturbation theory vs. spin wave expansion. Discussion on some problematic results in the literature

Chiral perturbation theory is an exact low energy expansion. The basic condition for the validity of this expansion is that the scales where the magnon physics is probed (like T or $\hbar c/L_s$) should be much smaller than the typical non-magnon scales (like ρ_s). In (2.10, 2.18), for example, $\hbar c/\rho_s L_s$ enters as an expansion parameter. For large spin S[7], $\rho_s\sim JS^2$, while $\hbar c\sim JS$, therefore the expansion parameter is $\hbar c/\rho_s L_s\sim 1/S$. Since the spin wave expansion is an $1/S$ expansion, for certain quantities the two expansions show analogies. The differences are more important, however. Consider (2.16), for example. This result says that the internal energy of the AF Heisenberg model satisfies

$$\lim_{T\to 0}\frac{e(T)-e(0)}{T^3}=\frac{2\,\zeta(3)}{\pi\,(\hbar c)^2}, \quad (3.1)$$

which is an *exact* statement. There are no corrections to this result from higher order chiral perturbation theory or from other sources. Spin wave expansion gives only a $1/S$ expansion for the $\sim T^3$ coefficient. On the other hand, as it is discussed in the introduction, (3.1) is a symmetry relation only, it is satisfied for any S. Consequently, replacing the left and right hand sides of (3.1) by the corresponding spin wave expansion one obtains an identity. This might serve as a good check on the results.

As a further example consider the temperature dependence of the uniform susceptibility in the large volume limit, (2.32). By replacing ρ_s and $\hbar c$ in it by their spin wave expansion form, which is available up to $O(1/S^2)$ [33], one obtains the spin wave expansion for the uniform susceptibility. This result is consistent with a direct spin wave expansion for $\chi_u(T)$ up to the known order [24].

In the following we would like to discuss some problematic results in the AF Heisenberg model.

3.1. The leading temperature dependence of the internal energy

The exact result, as we discussed before, is given by (3.1). Leading spin wave expansion predicts $\hbar c=\sqrt{2}\,Ja$ which gives on the right hand side of (3.1) $0.3826/(Ja)^2$. This is in agreement with the leading spin wave result for the left hand side [23]. Including next-to-leading corrections one obtains [24] $\hbar c=\sqrt{2}\,Ja\cdot 1.158$. Inserting this number in (3.1), the $\sim T^3$ coefficient is predicted to be $0.2853/(Ja)^2$. This is in agreement with Takahashi's modified[8] spin wave theory, (26) in [24].

These results are consistent. Schwinger boson mean field theory [25] leads to the same equations as the modified spin wave theory in [24]. These equations were studied numerically in [25] and $(0.77\pm 0.03)/(Ja)^2$ was predicted for the right hand side of (3.1). This is almost a factor 3 larger than the correct result and is due, presumably, to some numerical problems in solving the equations [26]. In [27] this incorrect result was confirmed in a Monte Carlo calculation. The reason might be that the simulation did not reach sufficiently low temperatures to be compared with a $C(T)\sim T^2$ behaviour. In [28], the modified spin wave result for $e(T)$ was incorrectly quoted as $2\cdot 0.2853/(Ja)^2\cdot T^3$. This factor of 2 influenced some related conclusions in [28].

3.2. The $O(1/L_s^4)$ correction to the ground state energy density

As we discussed in Sect. 2.5, the lowest excitations are described by a quantum mechanical rotator giving a $\sim j(j+1)\cdot 1/L_s^4$ contribution to the energy density. Although this term is zero for $j=0$ (ground state), there are non-zero $\sim 1/L_s^4$ corrections to the ground state energy density from other fluctuations (see (2.18)). This term is missing in earlier discussions and analyses [20, 28, 32]. For $N=3$ we can write

$$\varepsilon_0(L_s)=q_1-\frac{1.4377\,(\hbar c)}{L_s^3}\times\left[1-\frac{\hbar c}{5.7508\,\rho_s}\cdot\frac{1}{L_s}\right]+O\left(\frac{1}{L_s^5}\right). \quad (3.2)$$

If we take $\rho_s/J\approx 0.2$, $\hbar c/Ja\approx 1.6$ [28, 29], the correction is significant for $L_s/a\in(4,\ldots,12)$ where the best numerical results are available. A $1/L_s^3$ fit might lead to a significantly distorted spin wave velocity.

3.3. Uniform magnetic field at infinite volume and at low temperatures

The uniform external field is coupled to a conserved quantity in the AF Heisenberg model. It enters the Hamilton operator like a chemical potential. In the effective Lagrangean this chemical potential shows up like

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[7] We consider $N=3$ and discuss the AF Heisenberg model in this section

[8] Takahashi's result corresponds to inserting $\hbar c$ at $S=1/2$ into the denominator in (3.1) rather than expanding the expression in $1/S$

the t-component of a constant imaginary non-Abelian gauge field. Here t is the third ("temperature") direction in the $L_s \times L_s \times (\hbar/T)$ euclidean box.

Switch off now the magnetic field and take $L_s = \infty$, $T \ll \rho_s$. As it is observed before, new non-perturbative effects occur in this limit, which can be related to the $d=2$ classical non-linear sigma model [15, 18]. The $\infty \times \infty \times (\hbar/T)$ slab is reduced to an $\infty \times \infty$ two dimensional model. The intuitive reason is that the correlation length along the spatial dimensions is exponentially large in $1/T$, so the width of the slab $(\hbar/T)$ becomes very small compared to the correlation length. In the $d=2$ non-linear sigma model it is an excellent technical tool to probe the system under a chemical potential corresponding to a constant gauge field along one of the two spatial directions [18, 36]. Among others, exact results can be obtained for the chemical potential dependence of the free energy. This chemical potential has, however, no direct relation to the uniform magnetic field in the AF Heisenberg model, which corresponds to a constant gauge field along the "temperature" direction. This fact modifies the conclusions of a recent paper [37] significantly.

4. The effective Lagrangean. Discussion on the cut-off effects

In this section we construct the effective Lagrangean which serves to derive the free energy density up to next-to-leading order. Since for quantum field theories or critical statistical systems this problem has been discussed in detail before [5, 7, 9, 11], we can be brief on those points.

The AF quantum Heisenberg model in (1.1) has two parameters: the coupling J which sets the scale and the value of the spin S which takes discrete values. The smaller is S, the closer is the system to the boundary between the broken and symmetric phases. It is rigorously established that the ground state is ordered for $S \geqq 1$ [38]. Approximate analytic and numerical results suggest that $S = 1/2$ is in the broken phase also [39]. For every S we have two massless excitations (magnons) with a relativistic dispersion relation. This is similar to the case of a continuum quantum field theory, or a classical ferromagnet in the critical region with a broken O(3) symmetry. On the other hand, in the later cases the non-Goldstone boson scales (e.g. ρ_s) are also much smaller than the cut-off. This is not so in the model in (1.1). Take, for example the length scale corresponding to the spin stiffness, $\xi_\rho = \hbar c/\rho_s$. For an order of magnitude estimate we can take $\hbar c = 1.6 \cdot Ja$, $\rho_s = 0.2 \cdot J$ [28, 29] giving $\xi_\rho / a = 8$, as opposed to a critical system where this ratio goes to infinity. In general, this cut-off dependence modifies the effective prescription.

In the method of effective Lagrangeans one writes down the most general local Lagrangean L_{eff} (in terms of the smooth field corresponding to the order parameter) which respects the symmetries of the underlying model. The natural – although strictly unproved – expectation is that the predictions from L_{eff} reflect the symmetries only and correspond to any underlying model having the same kind of Goldstone bosons (magnons) and symmetries. This method becomes practically interesting through the observation that Goldstone bosons (magnons) interact weakly at low energies and a systematic perturbative expansion can be advised. In any given order only a finite number of unknown low energy constants enter.

Forget about the cut-off effects first and consider the problem of the free energy density $f(T, L_s)$ for small T and L_s^{-1} under the condition $l = \mathrm{O}(1)$ where l is defined in (2.3). Let us take "$\hbar c = 1$" in the following discussion, the missing $\hbar c$ factors can be inserted at the end using dimensional analysis. The effective Lagrangean is constructed as a general non-linear σ-model in terms of the field variables $\mathbf{S}$, $\mathbf{S}^2 = 1$:

$$\begin{aligned} &\mathbf{S}(x) = ((1-\boldsymbol{\pi}^2(x))^{1/2}, \boldsymbol{\pi}(x)), \\ &\boldsymbol{\pi}(x) = (\pi^1(x), \pi^2(x)), \qquad x_\mu = (x_0 = t, x_1, x_2). \end{aligned} \tag{4.1}$$

The low energy excitations carry momenta $p \sim L_s^{-1} \sim T$. Then, in the effective Lagrangean, every derivative ∂_μ is counted as $\sim p$. The terms in the effective model should comply with the symmetries (most notably with the O(3) symmetry) of the underlying theory in (1.1). The different terms in the effective Lagrangean are multiplied with unknown couplings. The leading term in the effective action contains the least number of derivatives[9],

$$\begin{aligned} \mathscr{A} &= \int_0^{1/T} \mathrm{d}t \int_0^{L_s} \mathrm{d}^2 x \tfrac{1}{2} \rho_s \, \partial_\mu \mathbf{S}(x) \, \partial_\mu \mathbf{S}(x) \\ &= \int_0^{1/T} \mathrm{d}t \int_0^{L_s} \mathrm{d}^2 x \tfrac{1}{2} \rho_s \left\{ \partial_\mu \boldsymbol{\pi} \, \partial_\mu \boldsymbol{\pi} + \frac{(\boldsymbol{\pi}\,\partial_\mu \boldsymbol{\pi})(\boldsymbol{\pi}\,\partial_\mu \boldsymbol{\pi})}{1-\boldsymbol{\pi}^2} \right\}, \\ &\mu = 0, 1, 2. \end{aligned} \tag{4.2}$$

In (4.2), we denoted the coupling by ρ_s using the well known result that for $T=0$, $L_s = \infty$ this coupling is the spin stiffness (helicity modulus, square of the Goldstone boson decay constant) and the fact that the couplings of the effective Lagrangean are independent of T and L_s [9][10]. The field $\boldsymbol{\pi}$ should be counted as $\sim p^{1/2}$, since fluctuations of this size have a Boltzmann factor of O(1). Indeed, the leading term in the Lagrange density in (4.2) is

$$\tfrac{1}{2} \rho_s \, \partial_\mu \boldsymbol{\pi} \, \partial_\mu \boldsymbol{\pi} \sim p^3, \tag{4.3}$$

which is integrated over a region $L_s^2/T \sim 1/p^3$. The leading term in (4.3) gives an $\mathrm{O}(p^3)$ contribution to the free energy density. The terms obtained by expanding the denominator in the second term in (4.2) give contributions of $\mathrm{O}(p^4)$, $\mathrm{O}(p^5)$...Of course, there are other terms in the general effective Lagrangean which can also contribute in higher order. The terms with four derivatives have the form

$$\begin{aligned} &\tfrac{1}{2} g_4^{(1)} (\partial_\mu \partial_\mu \mathbf{S} \, \partial_\nu \partial_\nu \mathbf{S}) + \tfrac{1}{4} g_4^{(2)} (\partial_\mu \mathbf{S} \, \partial_\mu \mathbf{S})^2 \\ &\quad + \tfrac{1}{4} g_4^{(3)} (\partial_\mu \mathbf{S} \, \partial_\nu \mathbf{S})(\partial_\mu \mathbf{S} \, \partial_\nu \mathbf{S}). \end{aligned} \tag{4.4}$$

[9] repeated indices are summed

[10] This is true if periodic boundary conditions are used which we shall assume in the following

By a change of integration variable in the path integral the first term in (4.4) can be transformed away [11], so we can take $g_4^{(1)}=0$. As it is easy to see, the other terms in (4.4) are at least $O(p^6)$. Terms in the effective Lagrangean containing more than four derivatives are even more suppressed. We can conclude therefore that if the cut-off- effects can be neglected, the effective action in (4.2) determines the $O(p^3)$, $O(p^4)$ and $O(p^5)$ parts in the free energy density. Only two unknown parameters, ρ_s and – after restoring dimensions – c, enter up to this order.

Let us now discuss the cut-off effects. The effective prescription is influenced by a finite cut-off in two ways. First, the finite cut-off might break some of the symmetries (for example, space rotation symmetry) which the underlying model would have in the continuum limit. This results in new terms in the effective Lagrangean which at infinite cut-off would be excluded. Second, the Fourier integrals (sums) of the chiral perturbation theory will depend on a finite cut-off. The divergent cut-off dependence is absorbed by the couplings through the usual renormalization procedure. There remain contributions, however, which contain inverse cut-off powers and depend on T and L_s.

We want to argue now that the cut-off effects enter the free energy density on the $O(p^5)$ level first. At finite cut-off spatial rotation symmetry is lost, only the 90° discrete symmetry of the square lattice remains. We need at least four derivatives to observe the difference. Since every term contains at least two $\boldsymbol{\pi}$ fields, the new term is $O(p^5)$ or higher. Actually, there is a new contribution at $O(p^5)$ already. The reduced symmetry allows the new four-derivative term

$$\tfrac{1}{2}g_4^{(4)}\sum_{i=1,2}(\partial_i\partial_i\mathbf{S}\,\partial_i\partial_i\mathbf{S}),\tag{4.5}$$

which is invariant under 90° spatial rotation but not rotation symmetric. The corresponding leading term

$$\tfrac{1}{2}g_4^{(4)}\sum_{i=1,2}(\partial_i\partial_i\boldsymbol{\pi}\,\partial_i\partial_i\boldsymbol{\pi}),\tag{4.6}$$

is $O(p^5)$. The leading contribution to the free energy density coming from this term is

$$\sim\frac{T}{L_s^2}\sum_p\frac{p_1^4+p_2^4}{p_0^2/c^2+p_1^2+p_2^2},\tag{4.7}$$

where the denominator is the magnon propagator in leading order. It is easy to show that (4.7) has a non-zero, $O(p^5)$ temperature and volume dependence. Consider now the second source of cut-off dependence generated by the momentum sums in chiral perturbation theory. The leading $O(p^3)$ contribution is a 1-loop graph corresponding to a momentum sum[11]. The leading cut-off effect in bosonic sums and integrals is $\sim(1/\Lambda^{\text{cut}})^2$. We expect therefore $p^3\cdot p^2/(\Lambda^{\text{cut}})^2=O(p^5)$ cut-off dependent corrections.

These considerations show that the effective action in (4.2), which after restoring the dimensions has the form

$$\int_0^{\hbar/T}\mathrm{d}t\int_0^{L_s}\mathrm{d}^2x\,\tfrac{1}{2}\rho_s\times\left[\frac{1}{c^2}\,\partial_t\mathbf{S}\,\partial_t\mathbf{S}+\sum_{i=1,2}\partial_i\mathbf{S}\,\partial_i\mathbf{S}\right],\tag{4.8}$$

is sufficient to derive the leading ($O(p^3)$) and next-to-leading ($O(p^4)$) contributions to the free energy density. These contributions depend therefore on two parameters ρ_s and c only and are cut-off independent. Equation (4.8) can be generalized trivially to $O(N)$ symmetry by defining $\mathbf{S}$ as an N-vector and $\boldsymbol{\pi}$ as an $(N-1)$-vector. In [40], the cut-off dependence has been investigated in the large-N limit of the classical $O(N)$ ferromagnetic Heisenberg model. The exact solution showed a cut-off dependence which is consistent with our discussion above.

5. The free energy density $f(T, L_s)$ up to next-to-leading order ("cubic" geometry)

We take "$\hbar=c=1$" and restore the dimensions at the end. It is useful to introduce the notations

$$L_t=\frac{1}{T},\qquad V=L_s^2\cdot L_t,\qquad L=V^{1/3},\qquad x=(x_0=t,x_1,x_2).\tag{5.1}$$

In the effective prescription the partition function is given by

$$Z=\prod_x\int\mathrm{d}\mathbf{S}(x)\,\delta(\mathbf{S}^2(x)-1)\cdot\mathrm{e}^{-\mathscr{A}(\mathbf{S})},\tag{5.2}$$

where the action $\mathscr{A}$ is given in (4.2). As we discussed before, the field $\boldsymbol{\pi}(x)$ is small, $O(p^{1/2})$ which is the basis of the perturbative expansion in (5.2). The euclidean box $L_t\times L_s\times L_s$ is large compared to the scale of non-magnon excitations and we shall assume that its shape is essentially cubic

$$L_s\gg\frac{1}{\rho_s},\qquad L_t\gg\frac{1}{\rho_s},\qquad l^3=\frac{L_t}{L_s}=O(1).\tag{5.3}$$

Perturbation theory in a box of this kind has a technical problem due to the existence of zero modes. The physical reason is that the dominant $\mathbf{S}$-configurations have a net (staggered) magnetization, i.e. a non-zero value for

$$\frac{1}{V}\int\mathrm{d}^3x\,\mathbf{S}(x),\tag{5.4}$$

which freely rotates around in the $O(N)$ group space. One has to separate these modes before starting a perturbative expansion. Since the technique is standard we quote the result only [41, 11]. Equation (5.2) can be written in the form

[11] The summand is essentially the logarithm of the leading magnon propagator. See Sect. 5

$$Z=\prod_x \left(\int \mathrm{d}\boldsymbol{\pi}(x)\frac{1}{(1-\boldsymbol{\pi}^2(x))^{1/2}}\right)$$
$$\times\prod_{i=1}^{N-1}\delta\left(\frac{1}{V}\int \mathrm{d}^3x\pi^i(x)\right)$$
$$\times\exp\left\{-\mathscr{A}(\mathbf{S})+(N-1)\right.$$
$$\left.\times\ln\left[\frac{1}{V}\int \mathrm{d}^3x(1-\boldsymbol{\pi}^2(x))^{1/2}\right]\right\}. \quad (5.5)$$

Going over to Fourier-space, we have

$$\prod_x\left(\int \mathrm{d}\boldsymbol{\pi}(x)\right)\cdot\prod_{i=1}^{N-1}\delta\left(\frac{1}{V}\int \mathrm{d}^3x\pi^i(x)\right)$$
$$\to\prod_k\left(\int \mathrm{d}\tilde{\boldsymbol{\pi}}_k\right)\prod_{i=1}^{N-1}\delta(\tilde{\pi}^i_{k=0})\cdot \mathrm{e}^{\frac{N-1}{2}\ln V}. \quad (5.6)$$

Eliminating the zero modes therefore has the following consequences: in the Fourier sums the $k=(0,0,0)$ mode should be left out, the action receives an additional, field-dependent contribution (the second term in the exponent in (5.5)) and a field independent, but size dependent constant $\frac{1}{2}(N-1)\ln V$ occurs in the exponent.

One follows the rules of standard perturbation theory except that in calculating Feynman graphs in the momentum sums the zero mode does not enter. According to (5.5., 5.6) in leading and next-to-leading order the Lagrangean has the form

$$\mathscr{L}=\mathscr{L}_0+\mathscr{L}_1,$$
$$\mathscr{L}_0=\tfrac{1}{2}\rho_s\,\partial_\mu\boldsymbol{\pi}\,\partial_\mu\boldsymbol{\pi}-\frac{N-1}{2V}\ln V, \quad (5.7)$$
$$\mathscr{L}_1=\tfrac{1}{2}\rho_s(\boldsymbol{\pi}\,\partial_\mu\boldsymbol{\pi})(\boldsymbol{\pi}\,\partial_\mu\boldsymbol{\pi})+\frac{N-1}{2V}\boldsymbol{\pi}^2.$$

Here $\mathscr{L}_1$ is $\mathrm{O}(p^4)$ and can be treated as a perturbation. As discussed in Sect. 4, there are no T- and L_s-dependent cut-off effects up to the order of our calculation, $\mathrm{O}(p^4)$. Therefore, the results are universal, independent of the regularization used in the effective theory. A conventional possibility is dimensional regularization [42]. In this case the factor $(1-\boldsymbol{\pi}^2(x))^{-1/2}$ in the measure in (5.5) can be suppressed [43][12]. One obtains for the free energy density

$$f=f_0+f_1$$
$$f_0=\frac{N-1}{2V}\sum_k{}'\ln k^2-\frac{N-1}{2V}\ln V, \quad (5.8)$$
$$f_1=\langle\mathscr{L}_1\rangle_0,$$

where $\sum'$ denotes a summation over the discrete momenta $k_\mu=(k_0,k_1,k_2)$ of the periodic box $L_t\times L_s\times L_s$ with the $k_\mu=(0,0,0)$ mode left out, while $k^2=k_0^2+k_1^2+k_2^2$. The notation $\langle\,\rangle_0$ refers to the expectation value with the leading $\mathscr{L}_0$ in the exponent:

$$\langle\mathscr{L}_1\rangle_0=\frac{1}{2\rho_s}(N-1)\bar{G}(0)\,\partial^x_\mu\,\partial^y_\mu\,\bar{G}(x-y)|_{x=y}$$
$$+\frac{1}{2\rho_s V}(N-1)^2\bar{G}(0), \quad (5.9)$$

where

$$\bar{G}(x)=\frac{1}{V}\sum_k{}'\frac{\mathrm{e}^{ikx}}{k^2}. \quad (5.10)$$

In calculating the momentum sums in (5.8, 5.9) one separates first the $V=\infty$ part, which is in general divergent. This part is absorbed through the renormalization of the parameters of the effective Lagrangean. In dimensional regularization this renormalization is trivial, since the corresponding integrals are defined to be zero.[13] The remaining finite, T- and L_s-dependent part can be written in a form which allows an easy numerical evaluation for any value of the shape parameter $l^3=L_t/L_s$. Since these steps were repeatedly discussed in the literature [7, 8, 11], we quote the final result only. Equations (5.8, 5.9) can be written as

$$f_0=q_1+\frac{q_2}{V}-\frac{N-1}{2V}\left[\tfrac{1}{3}\ln V+\beta_0(l)\right],$$
$$f_1=-\frac{(N-1)(N-2)}{2V}\cdot\frac{1}{\rho_s L_s l}\beta_1(l), \quad (5.11)$$

where q_1 and q_2 are two non-universal constants, l and the functions $\beta_n(l)$ were defined in (2.3) and (2.11–2.14), respectively. By restoring the dimensions, (5.11) leads to the result quoted in (2.10).

These results have been derived under the assumption that $l=(\hbar c/TL_s)^{1/3}$ is $\mathrm{O}(1)$. What happens if we take the $T\to0$, or $L_s\to\infty$ limit?

The $T\to0$ ($L_t\to\infty$, or $l\to\infty$) limit corresponds to an infinitely elongated cylinder geometry. As it is well known [8, 13, 21] in this geometry there are additional quasi-zero modes corresponding to the slow rotation of the (staggered) magnetization of the $L_s\times L_s$ planes as we move along the t-direction. These quasi-zero modes should be treated separately. The expansion used to derive (5.11) breaks down in the $l\to\infty$ limit and does *not* give the correct ground state energy. For later reference we quote the result of this limit, nevertheless:

$$(5.11)|_{l\to\infty}:\quad f_0-\frac{N-1}{2}\frac{\hbar c}{L_s^3}\cdot1.437745,$$
$$f_1\to\frac{(N-1)(N-2)}{24}\frac{\hbar c}{\rho_s L_s^4}. \quad (5.12)$$

There is an other way to see the problem with the $T\to0$ limit. In this limit we have effectively a $d=1$ non-linear

[12] Dimensional regularization is very convenient, but certain aspects of it are rather formal. We have checked that the final results of this section remain unchanged if lattice regularization is used

[13] In Sects. 6 and 8, where lattice regularization will be used, we carry through this renormalization process explicitly

σ-model. In $d=1$, the $L_t \to \infty$ limit can not be interchanged with the weak coupling expansion [41]. Since this problem is specific to $d=1$, we do not expect similar problems in the $L_s \to \infty$ ($l \to 0$) limit, where we obtain a two-dimensional slab. Although there are new non-perturbative effects in this limit which generate a finite mass m to the magnons [15, 18], this mass is exponentially small in $1/T$. The effect of such a small mass is negligible in the free energy density assuming that there are no infrared divergences in the $m \to 0$ limit, i.e. assuming that the perturbative expansion for f in $d=2$ is infrared finite. This is actually the case [44]. Equation (5.11) gives then

$$f(T)=q_1-(N-1)\frac{\zeta(3)}{2\pi}T^3+\mathrm{O}(T^5). \tag{5.13}$$

There is no $\sim T^4$ contribution, since $f_1|_{l\to 0}=0$. This is the result (after restoring dimensions) announced in (2.16).

6. Volume dependence of the ground state energy and of the lowest lying excitations

The special properties of the cylinder geometry corresponding to this problem have been observed and discussed before [8, 13, 21]. The next-to-leading volume correction to the ground state energy has been calculated in $d=4$ for the symmetry group $\mathrm{SU}(n)\times\mathrm{SU}(n)$ relevant for the strong interactions [8]. The next-to-leading ground state energy for $\mathrm{O}(N)$ and the volume correction to the lowest excitation energies to be discussed here are new results.

Since this problem is a somewhat non-trivial application of chiral perturbation theory, we use this occasion to discuss some technical issues: we consider a "physical" regularization (lattice, as opposed to dimensional regularization of Sect. 5) and discuss the renormalization process explicitly, especially the problem of power divergences. We give also some details on the way collective coordinates are introduced in treating the zero and quasi-zero modes.

We shall consider a d-dimensional euclidean cylinder $L_s^{d-1}\times L_t$ in the $L_t\to\infty$ limit. The AF Heisenberg model corresponds to $d=3$, $N=3$ in the following expressions. We shall use a (hyper)cubic lattice to regularize the effective theory. We put the lattice unit equal to 1 ($a=1$) and denote the lattice points by $x=(t,x)$, where $t=1,2,\dots,L_t$, etc. The Fourier transform is defined as

$$\pi(x)=\frac{1}{\sqrt{V}}\sum_k \mathrm{e}^{ikx}\tilde{\pi}(k), \qquad V=L_s^{d-1}\cdot L_t, \tag{6.1}$$

and we introduce the notation Δ_μ:

$$\Delta_\mu g(x)=g(x+\hat{\mu})-g(x), \tag{6.2}$$

where $\hat{\mu}$ is the unit vector in the μ-th direction.

6.1. Introducing collective coordinates

Until $L_t=\mathrm{O}(L_s)$, it is sufficient to take special care of the freely moving total magnetization. For large L_t/L_s, however, the magnetization of distant time slices in the cylinder can differ significantly. We have to treat these slowly moving variables (they are the $k=(k_0,\mathbf{k}=\mathbf{0})$ modes) non-perturbatively.

The action in (5.2) has the regularized form

$$\mathscr{A}(\mathbf{S})=\tfrac{1}{2}\rho_s^0\sum_{x,\mu}\Delta_\mu\mathbf{S}(x)\Delta_\mu\mathbf{S}(x), \tag{6.3}$$

where we denoted the coupling by ρ_s^0 anticipating a non-trivial renormalization. A possibility to introduce appropriate collective coordinates is to insert into the path integral

$$1=\prod_t\left[\int \mathrm{d}\mathbf{m}(t)\prod_{n=0}^{N-1}\delta\left(m^n(t)-\frac{1}{V_s}\sum_{\mathbf{x}}S^n(t,\mathbf{x})\right)\right], \tag{6.4}$$

where $V_s=L_s^{d-1}$. We write

$$\begin{aligned}&\mathbf{m}(t)=m(t)\mathbf{e}(t), \quad \mathbf{e}(t)^2=1,\\ &\mathrm{d}\mathbf{m}(t)=m(t)^{N-1}\mathrm{d}m(t)\,\mathrm{d}\mathbf{e}(t),\\ &\int \mathrm{d}\mathbf{e}\equiv\kappa=\frac{2\pi^{N/2}}{\Gamma(N/2)}.\end{aligned} \tag{6.5}$$

Introduce the $\mathrm{O}(N)$ rotation $\Omega(t)$

$$\begin{aligned}&\mathbf{e}(t)=\Omega(t)\mathbf{n}, \quad \mathbf{n}=(1,0,\dots,0),\\ &\Omega\in\mathrm{O}(N), \quad \int\mathrm{d}\Omega=1.\end{aligned} \tag{6.6}$$

Clearly, the vector $\mathbf{e}$ does not completely fix the matrix Ω. On the other hand, integrating over Ω rather than $\mathbf{e}$ gives an $\mathbf{e}$-independent constant factor only. The partition function has the form

$$\begin{aligned}Z=&\prod_x\int\mathrm{d}\mathbf{S}(x)\,\delta(\mathbf{S}^2(x)-1)\\ &\times\prod_t\int\mathrm{d}m(t)\,m(t)^{N-1}\\ &\times\kappa\int\mathrm{d}\Omega(t)\,\delta^{(N)}\left(m(t)\Omega(t)\mathbf{n}-\frac{1}{V_s}\sum_{\mathbf{x}}\mathbf{S}(t,\mathbf{x})\right)\\ &\times\exp\{-\mathscr{A}(\mathbf{S})\}.\end{aligned} \tag{6.7}$$

Replace $\mathbf{S}$ by the new integration variable $\mathbf{R}$:

$$\mathbf{S}(t,\mathbf{x})=\Omega(t)\mathbf{R}(t,\mathbf{x}). \tag{6.8}$$

Since the measure is $\mathrm{O}(N)$ invariant, we get

$$\begin{aligned}Z=&\prod_x\int\mathrm{d}\mathbf{R}(x)\,\delta(\mathbf{R}^2(x)-1)\\ &\times\prod_t\int\mathrm{d}m(t)\,m(t)^{N-1}\\ &\times\kappa\int\mathrm{d}\Omega(t)\,\delta^{(N)}\left(m(t)\mathbf{n}-\frac{1}{V_s}\sum_{\mathbf{x}}\mathbf{R}(t,\mathbf{x})\right)\\ &\times\exp\{-\mathscr{A}(\Omega\mathbf{R})\}.\end{aligned} \tag{6.9}$$

Write

$$R^i = \pi^i, \quad i=1,\dots,N-1, \quad R^0 = (1-\boldsymbol{\pi}^2)^{1/2}, \tag{6.10}$$

and integrate over the δ-functions

$$Z = \prod_x \int \mathrm{d}\boldsymbol{\pi}(x) \prod_t \int \mathrm{d}\Omega(t) \prod_{i=1}^{N-1} \delta\left(\frac{1}{V_s}\sum_{\mathbf{x}} \pi^i(t,\mathbf{x})\right) \times \exp\{-\mathscr{A}_1(\Omega,\boldsymbol{\pi})\},$$
$$\mathscr{A}_1(\Omega,\boldsymbol{\pi}) = \mathscr{A}(\Omega\mathbf{R}) + \tfrac{1}{2}\sum_x \ln(1-\boldsymbol{\pi}^2(x)) - (N-1)\sum_t \ln\left(\frac{1}{V_s}\sum_{\mathbf{x}} R^0(t,\mathbf{x})\right) - L_t \ln\kappa. \tag{6.11}$$

Going over to Fourier variables, (6.11) leads to

$$Z = \left(\prod_k \prod_{i=1}^{N-1} \int \mathrm{d}\tilde{\pi}^i(k)\right)\left(\prod_t \int \mathrm{d}\Omega(t)\right) \times \left(\prod_{k^0}\prod_{i=1}^{N-1} \delta(\tilde{\pi}^i(k^0,\mathbf{k}=\mathbf{0}))\right) \times \exp\left\{-\mathscr{A}_1(\Omega,\boldsymbol{\pi}) - L_t\frac{N-1}{2}\ln V_s\right\}. \tag{6.12}$$

6.2. *Integrating over the collective variables*

The action $\mathscr{A}(\mathbf{R})$ can be written as

$$\mathscr{A}(\mathbf{R}) = \tfrac{1}{2}\rho_s^0 \sum_{x,\mu} (\mathbf{R}(x+\hat{\mu}) - \mathbf{R}(x))^2 = \mathrm{d}V\rho_s^0 - \rho_s^0 \sum_{x,\mu} \mathbf{R}(x+\hat{\mu})\cdot\mathbf{R}(x). \tag{6.13}$$

Since Ω is independent of $\mathbf{x}$, we have

$$\mathscr{A}(\Omega\mathbf{R}) = \mathrm{d}V\rho_s^0 - \rho_s^0 \sum_x \sum_{i=1}^{d-1} \mathbf{R}(x+\hat{\imath})\mathbf{R}(x) - \rho_s^0 \sum_{t,\mathbf{x}} \Omega(t+1)\mathbf{R}(t+1,\mathbf{x})\cdot\Omega(t)\mathbf{R}(t,\mathbf{x}). \tag{6.14}$$

Consider the sum in the last term of (6.14)

$$\sum_{\mathbf{x}} [\Omega(1)^T\Omega(2)\mathbf{R}(2,\mathbf{x})\cdot\mathbf{R}(1,\mathbf{x}) + \Omega(2)^T\Omega(3)\mathbf{R}(3,\mathbf{x})\cdot\mathbf{R}(2,\mathbf{x}) + \dots]. \tag{6.15}$$

As (6.6) shows, the direction $\mathbf{e}(t)$ of the magnetization of a time slice is not influenced by the part of $\Omega(t)$ which leaves the vector $\mathbf{n}$ invariant. These are superious degrees of freedom in the $\mathrm{O}(N)$ matrix Ω. We shall get rid of these superious variables by changing integration variables in (6.12) appropriately. Replace the integration variable $\Omega(2)$ in (6.12) by

$$V(2) = \Omega(1)^T\Omega(2), \tag{6.16}$$

and introduce the rotated vectors

$$\hat{\mathbf{R}}(2,\mathbf{x}) = \hat{V}(2)\mathbf{R}(2,\mathbf{x}). \tag{6.17}$$

Here $\hat{V}(2)$ is an $\mathrm{O}(N)$ element with the structure

$$\hat{V}(2) = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & \ddots & & \\ \vdots & & \hat{V}_{ik}(2) & \\ 0 & & & \ddots \end{pmatrix}, \quad i,k = 1,2,\dots,N-1. \tag{6.18}$$

The $\mathrm{O}(N-1)$ rotation $\hat{V}_{ik}(2)$ serves to exclude the spurious degrees of freedom in $V(2)$ and will be specified further later. Equation (6.17) is an $\mathrm{O}(N-1)$ rotation on the integration variables $\pi^i(2,\mathbf{x})$

$$\hat{\pi}^i(2,\mathbf{x}) = \hat{V}_{ik}(2)\pi^k(2,\mathbf{x}). \tag{6.19}$$

We can introduce $\hat{\pi}^i(2,\mathbf{x})$ as new integration variables in the $t=2$ plane in (6.12). The measure is invariant and the $\delta(\tilde{\pi}^i(k_0,\mathbf{k}=\mathbf{0}))$ constraint is as well since the rotation is independent of $\mathbf{x}$. The terms in the exponent in (6.12) are also invariant, except that (6.15) goes over to

$$\sum_{\mathbf{x}} [V(2)\hat{V}(2)^T\hat{\mathbf{R}}(2,\mathbf{x})\cdot\mathbf{R}(1,\mathbf{x}) + (\Omega(1)V(2)\hat{V}(2)^T)^T\Omega(3)\mathbf{R}(3,\mathbf{x}) \cdot\hat{\mathbf{R}}(2,\mathbf{x})\dots\}. \tag{6.20}$$

Now we can repeat this procedure with the second term in (6.20). We replace the integration variable $\Omega(3)$ by

$$V(3) = (\Omega(1)V(2)\hat{V}(2)^T)^T\Omega(3), \tag{6.21}$$

and transform the variables in the $t=3$ plane by the $\mathbf{x}$-independent rotation

$$\hat{\mathbf{R}}(3,\mathbf{x}) = \hat{V}(3)\mathbf{R}(3,\mathbf{x}), \tag{6.22}$$

where $\hat{V}(3)$ has the structure of (6.18). Repeating these steps in the $t=4,\dots$ planes, (6.20) goes over

$$\sum_{\mathbf{x}} [V(2)\hat{V}(2)^T\hat{\mathbf{R}}(2,\mathbf{x})\cdot\mathbf{R}(1,\mathbf{x}) + V(3)\hat{V}(3)^T\hat{\mathbf{R}}(3,\mathbf{x})\cdot\hat{\mathbf{R}}(2,\mathbf{x}) + \dots]. \tag{6.23}$$

Boundary effects can be neglected for $L_t \to \infty$. Introducing the notation

$$\tilde{V}(t-1) = V(t)\hat{V}(t)^T \tag{6.24}$$

and suppressing the "hat" on $\hat{\mathbf{R}}$, we get

$$Z = \left(\prod_k \int \mathrm{d}\tilde{\pi}^i(k)\right)\left(\prod_t \int \mathrm{d}V(t)\right) \times \left(\prod_{k^0}\prod_{i=1}^{N-1} \delta(\tilde{\pi}^i(k^0,\mathbf{k}=\mathbf{0}))\right)$$

$$\times \exp - \Big\{ \mathscr{A}(V,\mathbf{R}) + \tfrac{1}{2} \sum_x \ln(1-\boldsymbol{\pi}^2(x))$$

$$-(N-1)\sum_t \ln\left(\frac{1}{V_s}\sum_{\mathbf{x}} R^0(t,\mathbf{x})\right)$$

$$-L_t \ln\kappa - L_t \frac{N-1}{2}\ln V_s\Big\}, \qquad (6.25)$$

where

$$\mathscr{A}(V,\mathbf{R}) = \mathrm{d}V\rho_s^0 - \rho_s^0 \sum_x \sum_{i=1}^{d-1} \mathbf{R}(x+\hat{\imath})\cdot\mathbf{R}(x)$$

$$-\rho_s^0 \sum_{t,\mathbf{x}} \tilde{V}(t)\mathbf{R}(t+1,\mathbf{x})\cdot\mathbf{R}(t,\mathbf{x})$$

$$= \tfrac{1}{2}\rho_s^0 \sum_{x,\mu} \Delta_\mu \mathbf{R}\Delta_\mu \mathbf{R}$$

$$-\rho_s^0 \sum_{t,\mathbf{x}} Q(t)\mathbf{R}(t+1,\mathbf{x})\cdot\mathbf{R}(t,\mathbf{x}), \qquad (6.26)$$

with the notation

$$Q(t) = \tilde{V}(t) - 1. \qquad (6.27)$$

We write the exponent in (6.25) as

$$\{\ldots\} = \mathscr{A}^{(\pi)} + \mathscr{A}^{(\pi,V)}$$

$$-L_t\ln\kappa - L_t\frac{N-1}{2}\ln V_s, \qquad (6.28)$$

where $\mathscr{A}^{(\pi)}$ is the π-dependent part, while $\mathscr{A}^{(\pi,V)}$ is the V-dependent part including the $\pi - V$ interactions. Since we have replaced the dangerous components $\tilde{\pi}^i(k_0,\mathbf{k}=\mathbf{0})$ by collective variables, we can consider the remaining $\tilde{\pi}$ variables as small, and expand. Equations (6.25, 6.26) give for the π-dependent part

$$\mathscr{A}^{(\pi)} = \mathscr{A}_0^{(\pi)} + \mathscr{A}_1^{(\pi)} + \ldots,$$

$$\mathscr{A}_0^{(\pi)} = \tfrac{1}{2}\rho_s^0 \sum_{x,\mu} \Delta_\mu\boldsymbol{\pi}\Delta_\mu\boldsymbol{\pi},$$

$$\mathscr{A}_1^{(\pi)} = \tfrac{1}{2}\rho_s^0 \sum_{x,\mu} [(\boldsymbol{\pi}\Delta_\mu\boldsymbol{\pi})(\boldsymbol{\pi}\Delta_\mu\boldsymbol{\pi}) \qquad (6.29)$$

$$+(\boldsymbol{\pi}\Delta_\mu\boldsymbol{\pi})(\Delta_\mu\boldsymbol{\pi}\Delta_\mu\boldsymbol{\pi})$$

$$+\tfrac{1}{4}(\Delta_\mu\boldsymbol{\pi}\Delta_\mu\boldsymbol{\pi})(\Delta_\mu\boldsymbol{\pi}\Delta_\mu\boldsymbol{\pi})]$$

$$+\frac{N-1}{2V_s}\sum_x \boldsymbol{\pi}^2 - \tfrac{1}{2}\sum_x \boldsymbol{\pi}^2(x).$$

The last term in $\mathscr{A}_1^{(\pi)}$ comes from the measure, it plays the role of a counterterm in the renormalization as we shall see. In deriving (6.29) we used the identity

$$\Delta_\mu(f(x)g(x)) = \Delta_\mu f(x)\cdot g(x) + f(x)$$

$$\cdot\Delta_\mu g(x) + \Delta_\mu f(x)\cdot\Delta_\mu g(x), \qquad (6.30)$$

(no summation over μ). The V-dependent part is generated by the last term in (6.26). Expanding in π, we get for this term

$$-\sum_t \{Q_{00}(t)\rho_s^0 V_s - Q_{00}(t)A(t) + Q_{ik}(t)B_{ik}(t)$$

$$+Q_{ik}(t)C_{ik}(t) + \mathrm{O}(\pi\pi\pi)\}, \qquad (6.31)$$

where

$$A(t) = \rho_s^0 \sum_{\mathbf{x}} [\boldsymbol{\pi}^2(t,\mathbf{x}) + \tfrac{1}{2}\Delta_0(\boldsymbol{\pi}^2(t,\mathbf{x}))],$$

$$B_{ik}(t) = \rho_s^0 \sum_{\mathbf{x}} [\pi_i(t,\mathbf{x})\pi_k(t,\mathbf{x})$$

$$+\tfrac{1}{2}\Delta_0\pi_i(t,\mathbf{x})\pi_k(t,\mathbf{x}) \qquad (6.32)$$

$$+\tfrac{1}{2}\pi_i(t,\mathbf{x})\Delta_0\pi_k(t,\mathbf{x})],$$

$$C_{ik}(t) = \tfrac{1}{2}\rho_s^0 \sum_{\mathbf{x}} [\Delta_0\pi_i(t,\mathbf{x})\pi_k(t,\mathbf{x})$$

$$-\pi_i(t,\mathbf{x})\Delta_0\pi_k(t,\mathbf{x})].$$

As (6.25, 6.31) show, in every time slice t we have to perform the group integral

$$\int \mathrm{d}V \exp\{\rho_s^0 L_s^{d-1}(\tilde{V}_{00}-1)$$

$$-Q_{00}A + Q_{ik}B_{ik} + Q_{ik}C_{ik}\}, \qquad (6.33)$$

where $\tilde{V}$ and Q are related to V through (6.24, 6.27). Due to the form of $\hat{V}$, (6.18), we have

$$\tilde{V}_{00} = V_{00}, \quad Q_{00} = V_{00} - 1. \qquad (6.34)$$

For $\rho_s^0 L_s^{d-1}$ large, the typical V matrices contributing to the integral in (6.33) are

$$\tilde{V}_{00} = V_{00} = 1-\varepsilon^2, \quad \varepsilon^2 = \mathrm{O}\left(\frac{1}{\rho_s^0 L_s^{d-1}}\right), \qquad (6.35)$$

where ε is small. Then $V_{i0} = \mathrm{O}(\varepsilon)$. We shall now specify the matrix $\hat{V}$ in (6.18) in terms of the matrix elements V_{ik} in such a way that the integrand in (6.33) becomes free of the spurious degrees of freedom discussed before. We shall take $\hat{V}_{ik}$ essentially equal to V_{ik}, plus corrections needed to make $\hat{V}_{ik}$ an element of $\mathrm{O}(N-1)$:

$$\hat{V}_{ik} = \alpha_i V_{ik} + \sum_j \beta_{ij} V_{jk}, \quad \text{no sum over } i,$$

$$\beta_{ij} = \beta_{ji}, \quad \beta_{ii} = 0. \qquad (6.36)$$

For small ε we have

$$\alpha_i = 1 + \tfrac{1}{2}(V_{i0})^2 + \mathrm{O}(\varepsilon^3),$$

$$\beta_{ij} = \tfrac{1}{2}V_{i0}V_{j0} + \mathrm{O}(\varepsilon^3), \quad i \neq j. \qquad (6.37)$$

Then $\tilde{V}$ in (6.24) has the form

$$\tilde{V} = V\hat{V}^T = \begin{pmatrix} V_{00} & -V_{00}V_{i0} & \ldots \\ \ddots & & \\ V_{i0} & 1-\tfrac{1}{2}V_{i0}^2 - \tfrac{1}{2}V_{i0}V_{k0} & \\ & -\tfrac{1}{2}V_{i0}V_{k0} & \\ \vdots & & \ddots \end{pmatrix} + \mathrm{O}(\varepsilon^3). \qquad (6.38)$$

Only V_{00} and V_{i0}, with $V_{00}^2+\sum_i V_{i0}^2=1$ enter in (6.38), representing the motion of $\mathbf{e}$ in (6.6) without additional spurious degrees of freedom. Equation (6.38) shows that $Q_{00}\sim Q_{ik}\sim O(1/\rho_s^0 L_s^{d-1})$. This is just the order we want to go. Expanding (6.33) in terms of Q_{00} and Q_{ik}, we get

$$\int \mathrm{d}V \exp\{\rho_s^0 L_s^{d-1} Q_{00}\}\left[1-Q_{00}A+\sum_{i,k} Q_{ik}B_{i,k}\right], \tag{6.39}$$

where

$$Q_{00}=V_{00}-1, \quad Q_{ik}=-\tfrac{1}{2}V_{i0}V_{k0}. \tag{6.40}$$

In (6.39) we can replace A and B_{ik} by their expectation value calculated with the leading part of $\mathscr{A}^{(\pi)}$ (the first term in (6.29)):

$$\begin{aligned} &A\to\langle A\rangle=(N-1)V_s D^*(0),\\ &B_{ik}\to\delta_{ik}\langle B\rangle=\delta_{ik}V_s(D^*(0)+\Delta_0 D^*(0)), \end{aligned} \tag{6.41}$$

where

$$D^*(0)=\frac{1}{V}\sum_k{}^{*}\frac{1}{\sum_\mu 4\sin^2(k_\mu/2)}. \tag{6.42}$$

In (6.42) a constrained summation over the momenta occurs,

$$\sum_k{}^{*}\equiv\sum_{k\neq(k^0,\mathbf{k}=0)}. \tag{6.43}$$

Using

$$\begin{aligned}\sum_{i=1}^{N-1}Q_{ii}&=-\tfrac{1}{2}\sum_{i=1}^{N-1}V_{i0}^2\\ &=-\tfrac{1}{2}(1-V_{00}^2)=Q_{00}+O(\varepsilon^3),\end{aligned} \tag{6.44}$$

we can write (6.39) in the form

$$\begin{aligned} &\int \mathrm{d}V(t)\exp\{\Theta_{\mathrm{eff}}Q_{00}\},\\ &\Theta_{\mathrm{eff}}=\rho_s^0 L_s^{d-1}-\langle A\rangle+\langle B\rangle. \end{aligned} \tag{6.45}$$

At this stage it is clear that (6.45) represents the motion of an $O(N)$ rotator with inertia Θ_{eff}. Indeed, we have

$$\begin{aligned} Q_{00}(t)&=V_{00}(t)-1=(\Omega(t-1)^T\Omega(t))_{00}-1\\ &=\Omega(t-1)\mathbf{n}\cdot\Omega(t)\mathbf{n}-1\\ &=-\tfrac{1}{2}(\mathbf{e}(t)-\mathbf{e}(t-1))^2, \end{aligned} \tag{6.46}$$

and the integral in (6.45) can be written as

$$\frac{1}{\kappa}\int \mathrm{d}\mathbf{e}(t)\exp\{-\tfrac{1}{2}\Theta_{\mathrm{eff}}(\mathbf{e}(t)-\mathbf{e}(t-1))^2\}. \tag{6.47}$$

Here we used that $\mathrm{d}V(t)=\mathrm{d}\Omega(t)=\mathrm{d}\mathbf{e}(t)/\kappa$.

The group integral in (6.45) can be easily performed. For large $\rho_s^0 V_s$ we get

$$\omega\exp\left\{-\frac{N-1}{2}\ln(\rho_s^0 V_s)-\frac{(N-1)(N-3)}{8\rho_s^0 V_s}+\frac{N-1}{2\rho_s^0 V_s}(\langle A\rangle-\langle B\rangle)\right\}, \tag{6.48}$$

where

$$\omega=\Gamma\left(\frac{N}{2}\right)\frac{1}{2\sqrt{\pi}}2^{\frac{N-1}{2}}. \tag{6.49}$$

The corresponding part of the free energy density reads

$$\begin{aligned} f^{(\pi,V)}&=\frac{N-1}{2V_s}\ln(\rho_s^0 V_s)+\frac{(N-1)(N-3)}{8\rho_s^0 V_s^2}\\ &-\frac{N-1}{2\rho_s^0 V_s}[(N-2)D^*(0)-\Delta_0 D^*(0)]\\ &-\frac{1}{V_s}\ln\omega. \end{aligned} \tag{6.50}$$

6.3. *Contribution from the perturbative fast modes*

The leading contribution is given by the first term in (6.29) which leads to

$$f_0^{(\pi)}=\frac{N-1}{2V}\sum_k{}^{*}\ln\left(\frac{1}{2\pi}\rho_s^0\mathrm{d}(k)\right), \tag{6.51}$$

where

$$\mathrm{d}(k)=4\sum_\mu\sin^2\frac{k_\mu}{2} \tag{6.52}$$

and $\sum^*$ is defined in (6.43). We can write

$$\begin{aligned}\sum_k{}^{*}\ln(\mathrm{d}(k))&=\sum_{k\neq(0,\ldots,0)}\ln(\mathrm{d}(k))\\ &-\sum_{k^0\neq 0}\ln(\mathrm{d}(k^0,\mathbf{k}=0)).\end{aligned} \tag{6.53}$$

The sums on the right hand side of (6.53) are standard in chiral perturbation theory and can be evaluated easily. In the $L_t\to\infty$ limit one obtains[14]

$$\begin{aligned} f_0^{(\pi)}&=-\frac{N-1}{2L_s^d}\left[\alpha_{-1/2}^{(d-1)}(1)+2-\frac{2}{d}\right]\\ &-\frac{N-1}{2L_s^{d-1}}\ln\frac{\rho_s^0}{2\pi}, \end{aligned} \tag{6.54}$$

where $\alpha_p^{(d)}$ are the "shape coefficients" defined earlier for $d=3$ (2.12–2.14). In (6.54) we need the shape coefficients of a $(d-1)$ dimensional cube only which are listed in

[14] We suppress the non-universal terms $\sim$const. or $\sim$const.$/V$ in f

Table 1 in [11]. The next-to-leading correction is given by the expectation value of $\mathscr{A}_1^{(\pi)}$ in (6.29). Using the relations (Appendix A)

$$\Delta_\mu^x \Delta_\mu^y D^*(x-y)|_{x=y} = -2\Delta_\mu D^*(0)$$

(no sum over μ),

$$2\sum_\mu \Delta_\mu D^*(0) = \frac{1}{V_s} - 1, \tag{6.55}$$

one obtains

$$f_1^{(\pi)} = \frac{1}{\rho_s^0}\left[-\frac{N-1}{2}\Delta_\mu D^*(0)\Delta_\mu D^*(0) + \frac{(N-1)(N-2)}{2V_s} D^*(0)\right]. \tag{6.56}$$

6.4. The ground state energy

Collecting the size dependent constants (the last two terms in (6.28)), the contributions from the collective coordinates (6.50) and from the fast modes (6.56) we get a surprisingly simple result for the ground state density

$$\begin{aligned}\varepsilon_0(L_s) &= \lim_{T\to 0} f(T, L_s) \\ &= -\frac{N-1}{2L_s^d}\left[\alpha_{-1/2}^{(d-1)}(1) + 2 - \frac{2}{d}\right] \\ &\quad -\frac{N-1}{2\rho_s^0}\left[\Delta_\mu D^*(0)\Delta_\mu D^*(0) - \frac{1}{V_s}\Delta_0 D^*(0)\right] \\ &\quad + \frac{(N-1)(N-3)}{8\rho_s^0 V_s^2}.\end{aligned} \tag{6.57}$$

In obtaining (6.57) we used the definitions of κ and ω in (6.5) and (6.49), respectively. In order to proceed further we need the explicit form of the lattice Green functions in (6.57). As it is discussed in Appendix A, all the dangerous cut-off dependence cancels in (6.57), and up to a non-universal volume independent constant we can write

$$\Delta_\mu D^*(0)\Delta_\mu D^*(0) - \frac{1}{V_s}\Delta_0 D^*(0) \to -\frac{1}{4V_s^2}. \tag{6.58}$$

The spin-stiffness occurs in (6.57) first in the correction only, we can therefore replace ρ_s^0 by the renormalized, physical ρ_s. (The renormalization properties will be discussed in Sect. 6.7). We get then ($V_s = L_s^{d-1}$)

$$\begin{aligned}&\varepsilon_0(L_s) - \varepsilon_0(\infty) \\ &= -\frac{N-1}{2L_s^d}\left[\alpha_{-1/2}^{(d-1)}(1) + 2 - \frac{2}{d}\right] \\ &\quad + \frac{(N-1)(N-2)}{8\rho_s V_s^2}.\end{aligned} \tag{6.59}$$

The shape coefficients $\alpha_{-1/2}^{(d-1)}(1)$ are listed in Table 1 in [11]. The result quoted in (2.18) is obtained after restoring the dimensions and setting $d=3$. For $N=4$, $d=4$ (6.59) agrees with the result in [8] obtained for $SU(2)\times SU(2)$.

6.5. An alternative, intuitive method

Since the previous calculation is rather involved, it is reassuring that the result in (6.59) can be reproduced in a simple intuitive way. The following considerations offer additional insight into the physics of the problem also.

In Sect. 5 we studied the free energy density $f(T, L_s)$ under conditions $T \ll \rho_s$, $1/L_s \ll \rho_s$, $TL_s =$ fixed constant. Very low temperature corresponds chosing this fixed constant very small, but even in this limit the temperature T remains $\sim 1/L_s$. Standard Goldstone boson (magnon) excitations carry momenta $\sim 1/L_s$ and they freeze out at these low temperatures. The rotator excitations, however, carry energies $\sim 1/L_s^2$ and for those excitations the temperature is high even in this limit. They are fully excited and included in the free energy. This is the reason why (5.12) disagrees with the correct ground state energy density (2.18). Rather, (5.12) should agree with the free energy density coming from the $O(N)$ rotator

$$\hat{H} = \frac{1}{2\Theta_{\text{eff}}}\hat{\mathbf{L}}^2 + E_0(L_s) \tag{6.60}$$

in the *high* temperature limit, where $\Theta_{\text{eff}} \approx \rho_s L_s^2$ and $E_0(L_s)$ is the ground state energy we are looking for. The operator $\hat{\mathbf{L}}^2$ is, in coordinate representation, the Laplace operator on the $N-1$ dimensional unit sphere. This matching condition can be used to calculate the ground state energy $E_0(L_s)$. We need the high temperature expansion of the partition function

$$Z^{\text{rot}} = \operatorname{Tr}\exp\left(-\frac{\hat{H}}{T}\right) = \exp\left(-\frac{L_s^2\varepsilon_0(L_s)}{T}\right) \times \operatorname{Tr}\exp\left(-\frac{\hat{\mathbf{L}}^2}{2\Theta_{\text{eff}}T}\right). \tag{6.61}$$

An elegant way to obtain the result is to use Seeley's expansion giving [45]

$$\begin{aligned}&\operatorname{Tr}\exp(-\hat{\mathbf{L}}^2 t)|_{t\to 0} \\ &= A t^{-(N-1)/2}\left[1 + \frac{(N-1)(N-2)}{6}t + \frac{(N-1)(N-2)(5N^2-17N+18)}{360}t^2 \dots\right],\end{aligned} \tag{6.62}$$

with the renormalization factor $A = \pi^{1/2} 2^{-N+2}/\Gamma(N/2)$, which will not be important for us. The free energy density predicted by the rotator problem has the form

$$f^{\text{rot}} = \varepsilon_0(L_s) - \frac{N-1}{2}\frac{T}{V_s}\ln(TV_s) - \frac{(N-1)(N-2)}{12\rho_s V_s^2} + \dots. \tag{6.63}$$

Matching (6.63) with (5.12) we find the next-to-leading correction to $\varepsilon_0(L_s)$

$$\frac{(N-1)(N-2)}{12\rho_s V_s^2}+\frac{(N-1)(N-2)}{24\rho_s V_s^2}=\frac{(N-1)(N-2)}{8\rho_s V_s^2}, \quad (6.64)$$

which is the result obtained before, (6.59).

6.6. The lowest lying excitations and their volume dependence

The collective slow modes correspond to an O(N) rotator with inertia $\Theta \sim L_s^{d-1}$. The corresponding excitations are $\sim 1/L_s^{d-1}$, lying much below the exctiations of the fast π-modes which are $\sim 1/L_s$. Using (6.40, 6.41, 6.44) we can write (6.39) in the form

$$\int \mathrm{d}V \exp\{(\rho_s^0 L_s^{d-1}-\langle A\rangle+\langle B\rangle)(V_{00}-1)\}. \quad (6.65)$$

Equation (6.65) shows that the π-modes modify the inertia of the O(N) rotator to

$$\rho_s^0 L_s^{d-1} \to \rho_s^0 L_s^{d-1}-\langle A\rangle+\langle B\rangle = V_s[\rho_s^0-(N-2)D^*(0)+\Delta_0 D^*(0)]. \quad (6.66)$$

As we shall discuss in Sect. 6.7, (6.82), the relation between the bare and renormalized spin stiffness in our order reads

$$\rho_s^0=\rho_s+(N-2)D_\infty(0)+\frac{1}{2d}, \quad (6.67)$$

where $D_\infty(x)$ is the infinite volume lattice propagator. Using the explicit form of the Green functions (Appendix A) we get

$$\Theta_{\mathrm{eff}}=\rho_s L_s^{d-1}\left[1+\frac{N-2}{4\pi\rho_s L_s^{d-2}} \times\left(-\alpha_{1/2}^{(d-1)}(1)+2\,\frac{d-1}{d-2}\right)\right]. \quad (6.68)$$

The excitations of the O(N) rotator are given by

$$E_j-E_0=\frac{j(j+N-2)}{2\Theta_{\mathrm{eff}}}, \quad (6.69)$$

which, at $d=3$, leads to the result quoted in (2.19).

6.7. Renormalizations. Relations at infinite volume and zero temperature

The physical parameters ρ_s, c and $\mathcal{M}_s$ are defined at infinite spatial volume and zero temperature. In the following we study briefly their renormalization with lattice regularization in $d=3$ and, as a side product, we rederive the results quoted in (2.8).

Switch on an external symmetry breaking staggered field $\mathbf{H}_s=(H_s,0,\ldots,0)$. The corresponding leading term in the effective action reads [11]

$$-\sum_x \mathcal{M}_s^0 \mathbf{H}_s \mathbf{S}(x), \quad (6.70)$$

where $\mathcal{M}_s^0$ is the bare staggered magnetization. We consider a $d(=3)$ dimensional infinitely large hypercubic lattice. There are no special zero modes in this case. Expanding the action ((6.3) and (6.70)) and the measure in the π fields one obtains

$$Z=\prod_x \int \mathrm{d}\pi(x)\exp\left\{-\sum_x(\mathscr{L}_0+\mathscr{L}_1+\ldots)\right\}, \quad (6.71)$$

where

$$\mathscr{L}_0=\tfrac{1}{2}\rho_s^0\left(\sum_\mu \Delta_\mu\pi\Delta_\mu\pi+M_0^2\pi^2\right)-\mathcal{M}_s^0 H_s,$$

$$\mathscr{L}_1=\tfrac{1}{2}\rho_s^0\left\{\sum_\mu[(\pi\Delta_\mu\pi)(\pi\Delta_\mu\pi) +(\pi\Delta_\mu\pi)(\Delta_\mu\pi\Delta_\mu\pi) +\tfrac{1}{4}(\Delta_\mu\pi\Delta_\mu\pi)(\Delta_\mu\pi\Delta_\mu\pi)] +\tfrac{1}{4}M_0^2(\pi^2)^2\right\}-\tfrac{1}{2}\pi^2, \quad (6.72)$$

with the notation

$$M_0^2=\frac{\mathcal{M}_s^0 H_s}{\rho_s^0}. \quad (6.73)$$

Let us calculate first the (staggered) magnetization:

$$\mathcal{M}_s^H=\frac{1}{V}\,\frac{1}{Z}\,\frac{\partial}{\partial H_s}Z=\mathcal{M}_s^0\langle(1-\pi^2(0))^{1/2}\rangle =\mathcal{M}_s^0\left(1-\frac{N-1}{2\rho_s^0}D_\infty^{(M_0)}(0)\right). \quad (6.74)$$

Equation (6.74) and the subsequent equations of this section are understood as relations in the first non-trivial order. In (6.74) $D_\infty^{(M_0)}(x)$ is the infinite volume massive lattice propagator

$$D_\infty^{(M_0)}(x)=\int_{-\pi}^{\pi}\frac{\mathrm{d}^d k}{(2\pi)^d}\,\frac{\mathrm{e}^{ikx}}{\mathrm{d}(k)+M_0^2}, \quad (6.75)$$

where $\mathrm{d}(k)$ is defined in (6.52). At $H_s=0$, $\mathcal{M}_s^H$ goes over to the spontaneous magnetization $\mathcal{M}_s$ which determines the relation between the bare and renormalized magnetizations

$$\mathcal{M}_s=\mathcal{M}_s^0\left(1-\frac{N-1}{2\rho_s}D_\infty^{(0)}(0)\right), \quad (6.76)$$

where we replaced ρ_s^0 by ρ_s since the difference is of higher order. Equations (6.74, 6.76) and the relation

$$D_\infty^{(M_0)}(0) = D_\infty^{(0)}(0) - \frac{M_0}{4\pi}, \quad (d=3) \tag{6.77}$$

lead to the result

$$\mathscr{M}_s^H = \mathscr{M}_s \left(1 + \frac{N-1}{8\pi} \cdot \frac{M}{\rho_s}\right), \tag{6.78}$$

where we replaced M_0 by $M = \mathscr{M}_s H_s / \rho_s$. After restoring the dimensions, (6.78) gives the result quoted in (2.8). In (6.76) $D_\infty^{(0)}(0)$ is linear in the cut-off in $d=3$. This power divergence is absorbed in the bare parameter $\mathscr{M}_s^0$ leading to a cut-off independent, universal relation (6.78).

The procedure is very similar in case of the spin stiffness. A possibility to study the spin stiffness is to calculate the two-point function of Goldstone bosons. This Green-function should have a pole at $k^2=0$ (for $H_s=0$) which fixes the wave function renormalization factor z. For the two-point function one obtains

$$\sum_x e^{-ikx} \frac{1}{Z} \frac{\delta}{\delta H_s^i(x)} \frac{\delta}{\delta H_s^j(0)} Z \bigg|_{\substack{H_s \to 0 \\ k \to 0}}$$

$$= \frac{\delta_{ij}}{k^2} \frac{(\mathscr{M}_s^0)^2}{\rho_s^0} \left[1 - \frac{1}{\rho_s^0}\left(D_\infty^{(0)}(0) - \frac{1}{2d}\right)\right]. \tag{6.79}$$

The residue of the pole gives z:

$$z = \frac{(\mathscr{M}_s^0)^2}{\rho_s^0} \left[1 - \frac{1}{\rho_s^0}\left(D_\infty^{(0)}(0) - \frac{1}{2d}\right)\right]. \tag{6.80}$$

Using the Ward identity [46, 11]

$$\rho_s = \frac{\mathscr{M}_s}{z^{1/2}}, \tag{6.81}$$

(6.76, 6.80) determine the relation between ρ_s and ρ_s^0:

$$\rho_s = \rho_s^0 \left[1 - \frac{1}{\rho_s}\left((N-2) D_\infty^{(0)}(0) + \frac{1}{2d}\right)\right], \quad d=3. \tag{6.82}$$

Repeating the calculation for the two-point function in (6.79) with $H_s \neq 0$, the pole position is shifted from $k^2=0$ which determines the Goldstone boson mass. One obtains

$$(M^H)^2 = M_0^2 \left[1 + \frac{1}{2\rho_s^0}\left((N-3) D_\infty^{(M_0)}(0) + \frac{1}{\mathrm{d}}\right)\right]. \tag{6.83}$$

In the limit $H_s \to 0$, (6.76, 6.82, 6.83) are consistent with the Ward identity [11]

$$(M^H)^2|_{H_s \to 0} = \frac{\mathscr{M}_s}{\rho_s} H_s. \tag{6.84}$$

The residue of the pole $(k^2 + (M^H)^2)^{-1}$ in the two-point function gives the wave-function renormalization z_H, and the Ward identity [11]

$$\rho_s^H = \frac{z_H}{(M^H)^4} H_s^2 \tag{6.85}$$

gives then ρ_s^H. The wave-function renormalization z_H has the form of z in (6.80) replacing $D_\infty^{(0)}$ by $D_\infty^{(M_0)}$. Equation (6.85) leads to the result

$$\rho_s^H = \rho_s \left[1 + 2\frac{N-2}{8\pi\rho_s} M\right]. \tag{6.86}$$

Expressing (6.83) in terms of the renormalized parameters we get finally

$$(M^H)^2 = M^2 \left[1 - \frac{N-3}{8\pi} \cdot \frac{M}{\rho_s}\right]. \tag{6.87}$$

After restoring dimensions, (6.86) and (6.87) give the result quoted in (2.8).

The procedure above shows that the power divergences can be consistently absorbed in the bare parameters, the physical predictions are free of divergences as $a \to 0$, and they satisfy the Ward identities.

7. The effect of a weak staggered field

Consider an euclidean box $L_s^{d-1} \times L_t$ with "cubic" geometry, i.e. $L_t/L_s = \mathrm{O}(1)$. If the staggered field is zero, the total (staggered) magnetization moves freely in the $\mathrm{O}(N)$ group space. Switching on an external field $\mathbf{H}_s = (H_s, 0, \ldots, 0)$, the distribution of the total staggered magnetization will be concentrated around the 0-th direction. For weak fields

$$0 \leq H_s = \mathrm{O}\left(\frac{1}{\mathscr{M}_s L_s^2 L_t}\right) \tag{7.1}$$

this distribution remains broad and there is a need to treat the corresponding motion non-perturbatively. The external field dependence of the free energy, staggered magnetization and susceptibilities with $\mathrm{O}(N)$ symmetry have been worked out in [11] up to next-to-leading order. After restoring the spin wave velocity dependence we enumerated the results in (2.21–2.26).

Increasing the box size L_s at fixed temperature, the staggered susceptibility has the form

$$\chi_s(T, L_s) = \frac{1}{N} \mathscr{M}_s^2 \frac{L_s^2}{T} \left\{1 + (N-1)\frac{T}{2\pi\rho_s} \times (-\ln(L_s T) + \tfrac{1}{2} 2.852929) + \ldots\right\}. \tag{7.2}$$

This behaviour remains valid until $L_s \ll \xi(T)$, where $\xi(T) \propto \exp(b/T)$, with $b = 2\pi\rho_s/(N-2)$ is the nonperturbatively generated correlation length [15, 18]. For infinite volume ($L_s \gg \xi(T)$) the spatial size is expected to be replaced by the correlation length.

These results were derived under the condition $T = \mathrm{O}(1/L_s)$ and, in general, the $T \to 0$, L_t = fixed limit does not lead to the correct zero temperature behaviour. The physical reason was discussed in detail in Sect. 6.5. As we argued there, the result of (2.26) in this limit should agree with that given by the high temperature limit of an $\mathrm{O}(N)$ rotator. We shall discuss this problem in the next section.

8. Low temperature limit of the finite volume staggered susceptibility

As we discussed in Sect. 6, if the temperature is very low ($T \ll 1/L_s$), the excitations of an $\mathrm{O}(N)$ rotator dominate the partition function. Let us check first, how the rotator problem in (6.47) is modified in the presence of a small staggered field $\mathbf{H}_s = (H_s, 0, \ldots, 0)$. In the effective action a new term enters

$$-\mathcal{M}_s^0 \mathbf{H}_s \cdot \sum_x \mathbf{S}_x, \tag{8.1}$$

where $\mathcal{M}_s^0$ is the bare staggered magnetization. Using (6.5–6.12) this term can be written as

$$-\mathcal{M}_s^0 V_s \sum_t \mathbf{H}_s \mathbf{e}(t) \frac{1}{V_s} \sum_{\mathbf{x}} (1-\boldsymbol{\pi}^2(x))^{1/2}. \tag{8.2}$$

Considering the first correction we can replace $\boldsymbol{\pi}^2(x)$ by $(1/\rho_s^0)(N-1) D^*(0)$, and (8.2) leads to a new term in the exponent of (6.47):

$$\frac{1}{\kappa} \int \mathrm{d}\mathbf{e}(t) \exp\left\{-\tfrac{1}{2}\Theta_{\mathrm{eff}}(\mathbf{e}(t)-\mathbf{e}(t-1))^2 + \mathbf{h}_s \mathbf{e}(t)\right\}, \tag{8.3}$$

where

$$\mathbf{h}_s = (h_s, 0, \ldots, 0), \quad h_s = H_s \mathcal{M}_s^{\mathrm{eff}} V_s,$$
$$\mathcal{M}_s^{\mathrm{eff}} = \mathcal{M}_s^0 \left(1 - \frac{N-1}{2\rho_s^0} D^*(0)\right). \tag{8.4}$$

The corresponding Hamilton operator reads

$$\hat{H} = \frac{1}{2\Theta_{\mathrm{eff}}} \hat{\mathbf{L}}^2 - \mathbf{h}_s \hat{\mathbf{X}} = \hat{H}_0 - \mathbf{h}_s \hat{\mathbf{X}}, \quad \hat{\mathbf{X}}^2 = 1, \tag{8.5}$$

where we suppressed the h_s-independent constant $E_0(L_s)$ of (6.60). Notice that this effective rotator picture is valid only in first order, i.e. including $\mathrm{O}(1/\rho_s L_s)$ corrections. This is the order considered in this section. The staggered susceptibility is given by

$$\chi_s(T, L_s) = \frac{T}{V_s} \frac{\partial^2}{\partial H_s^2} \ln Z \Big|_{H_s=0}$$
$$= (\mathcal{M}_s^{\mathrm{eff}})^2 V_s T \frac{\partial^2}{\partial h_s^2} \ln Z \Big|_{h_s=0}, \tag{8.6}$$

where

$$Z = \mathrm{Tr}(\mathrm{e}^{-\hat{H}/T}). \tag{8.7}$$

In taking the derivatives in (8.6) we have to be careful since $\hat{X}$ does not commute with $\hat{H}_0$. One obtains

$$\chi_s = (\mathcal{M}_s^{\mathrm{eff}})^2 V_s \frac{1}{Z_0} \mathrm{Tr} \int_0^{1/T} \mathrm{d}\lambda\, \mathrm{e}^{-\lambda \hat{H}_0} \hat{X}_0 \mathrm{e}^{-(1/T-\lambda)\hat{H}_0} \hat{X}_0, \tag{8.8}$$

where Z_0 is the partition function with $\hat{H}_0$, and $\hat{X}_0$ is the 0-th component of $\hat{\mathbf{X}}$.

The excitations of $\hat{H}_0$ are described by the quantum number $j = 0, 1, \ldots$

$$E_j = \frac{1}{2\Theta_{\mathrm{eff}}} j(j+N-2), \tag{8.9}$$

while the corresponding multiplicity is given by

$$g_j = \frac{(j+N-3)!}{j!(N-2)!}(2j+N-2). \tag{8.10}$$

We shall denote the set of quantum numbers which characterize the subspace with a given j by m. Inserting a complete set of states in (8.8) we get

$$\chi_s = (\mathcal{M}_s^{\mathrm{eff}})^2 V_s \frac{2}{Z_0} \sum_{j=0}^{\infty} \frac{\mathrm{e}^{-E_j/T} - \mathrm{e}^{-E_{j+1}/T}}{E_{j+1}-E_j} a_j, \tag{8.11}$$

where

$$a_j = \sum_m |\langle j+1, m | \hat{X}_0 | j, m\rangle|^2. \tag{8.12}$$

In deriving (8.11) we used that $\hat{X}_0$ connects the state $|j, m\rangle$ with $|j \pm 1, m\rangle$ only. Using the relation

$$\sum_m \sum_{j', m'} |\langle j', m' | \hat{X}_0 | j, m\rangle|^2$$
$$= \sum_m \langle j, m | \hat{X}_0^2 | j, m\rangle = \frac{1}{N} g_j \tag{8.13}$$

and observing that the left hand side of (8.13) is just $a_j + a_{j+1}$, we obtain

$$a_j = \frac{1}{N} \frac{(j+N-2)!}{j!(N-2)!}. \tag{8.14}$$

Writing (8.14) into (8.11), after some algebra we get

$$\chi_s = \frac{4}{N(N-1)} (\mathcal{M}_s^{\mathrm{eff}})^2 \Theta_{\mathrm{eff}} V_s \frac{1}{Z_0} \sum_{j=0}^{\infty} g_j \mathrm{e}^{-E_j/T}$$
$$\times \frac{(N-1)(N-3)}{8\Theta_{\mathrm{eff}} E_j + (N-1)(N-3)}$$
$$= \frac{4}{N(N-1)} (\mathcal{M}_s^{\mathrm{eff}})^2 \Theta_{\mathrm{eff}} V_s \frac{1}{Z_0} U(t), \tag{8.15}$$

where $t = 1/(2\Theta_{\mathrm{eff}} T)$ and $U(t)$ satisfies the differential equation

$$\frac{\partial U}{\partial t} = \frac{(N-1)(N-3)}{4} [U(t) - Z_0(t)]. \tag{8.16}$$

For $N=3$ (8.15) simplifies since in this case $U(t) \equiv 1$.

Let us consider the effective parameters $\mathcal{M}_s^{\mathrm{eff}}$ and Θ_{eff} of the $\mathrm{O}(N)$ rotator. Using the definitions, (6.41, 6.45, 8.4) and replacing the bare spin stiffness and magnetization by their renormalized values, (6.76, 6.82) we have

$$\mathcal{M}_s^{\mathrm{eff}} = \mathcal{M}_s \left[1 + \frac{N-1}{2\rho_s}(D(0) - D^*(0))\right],$$

$$\Theta_{\rm eff}=\rho_s V_s \left[1+\frac{N-2}{\rho_s}(D(0)-D^*(0)) + \frac{a}{\rho_s}\left(\frac{a^{1-d}}{2d}+\Delta_0 D^*(0)\right)\right], \tag{8.17}$$

where $D(0)$ is the lattice propagator at infinite volume and zero temperature. In (8.17) we restored the lattice unit dependence to see clearly how the ultraviolet divergences cancel. As (A7, A14) in Appendix A show, $D(0)$, $D^*(0)$ and $\Delta_0 D^*(0)$ are ultraviolet divergent. On the other hand, the combinations

$$D(0)-D^*(0) = \frac{1}{4\pi L_s^{d-2}}\left(-\alpha_{1/2}^{(d-1)}(1)+2\frac{d-1}{d-2}\right) \tag{8.18}$$

$$\frac{a^{1-d}}{2d}+\Delta_0 D^*(0)=\frac{1}{2V_s}$$

entering the effective parameters are finite.

Equations (8.15–8.16) allows us to calculate χ_s both for $t \ll 1$ and $t \gg 1$ analytically. (Numerically, of course, it is not difficult to perform the calculation for arbitrary t.) At very low temperatures, the $j=0$ term contributes only in (8.15) and in $Z_0(t)$, giving

$$\chi_s(T,L_s)=\frac{4}{N(N-1)}(\mathcal{M}_s^{\rm eff})^2 \times \Theta_{\rm eff} V_s[1+\mathrm{O}(\mathrm{e}^{-1/T\Theta_{\rm eff}})], \quad TV_s\rho_s \ll 1. \tag{8.19}$$

or

$$\chi_s(T,L_s)=\frac{4}{N(N-1)}\mathcal{M}_s^2 \rho_s V_s^2 \times\left[1+\frac{2N-3}{4\pi\rho_s L_s^{d-2}}\left(-\alpha_{1/2}^{(d-1)}(1)+2\frac{d-1}{d-2}\right)\right], \quad TV_s\rho_s \ll 1. \tag{8.20}$$

For the relevant case, $d=3$ we get

$$\chi_s(T,L_s)=\frac{4}{N(N-1)}\mathcal{M}_s^2 \rho_s L_s^4 \times\left[1+\frac{2N-3}{4\pi\rho_s L_s}3.900265\right], \quad TL_s^2\rho_s \ll 1, \quad d=3. \tag{8.21}$$

At large temperatures $TV_s\rho_s \gg 1$ (but $TL_s \ll 1$) we can use Seeley's expansion (6.62) and integrate the differential equation in (8.16). We obtain

$$U(t)=A\frac{N-1}{2}t^{-(N-3)/2} \times\left[1+\frac{(N-1)(N-3)}{6}t + \frac{(N-1)(N-3)(5N^2-22N+18)}{360}t^2+\ldots\right], \tag{8.22}$$

$$\frac{U(t)}{Z_0(t)}=\frac{2}{N-1}t\left[1-\frac{N-1}{6}t + \frac{(N-1)(N+1)}{180}t^2+\ldots\right].$$

Up to leading order corrections this leads to

$$\chi_s(T,L_s)=\frac{1}{N}(\mathcal{M}_s^{\rm eff})^2\frac{V_s}{T}\left[1-\frac{N-1}{12T\Theta_{\rm eff}}\right]. \tag{8.23}$$

For $d=3$ we get

$$\chi_s(T,L_s)=\frac{1}{N}\mathcal{M}_s^2\frac{L_s^2}{T}\left[1-\frac{N-1}{\rho_s L_s} \times\left(-\frac{1}{12}\frac{1}{L_sT}+\frac{1}{4\pi}3.900265\right)+\ldots\right]. \tag{8.24}$$

According to (8.21), in the limit $T\to 0$, V_s = fixed, the staggered susceptibility becomes independent of T and is proportional to the square of the spatial volume. As the temperature is increased to $T \gg \Theta=\rho_s V_s$, but $T \ll 1/L_s$, the rotator becomes highly excited, while the fast Goldstone modes (whose typical energy is $\sim 1/L_s$) remain frozen. In this region the susceptibility in (8.24) should match the *low* temperature limit of (2.26). Indeed, using the asymptotic expressions for $L_t \gg L_s$ given in Appendix B, one finds that, in the order considered in this section, the two expressions coincide up to $\mathrm{O}(\exp(-\pi/L_sT))$ corrections, coming from the fast modes which are included in the cubic geometry. It is interesting to note that the susceptibility given by the effective rotator, (8.24) reproduces the leading correction in (2.26) surprisingly well even at temperatures as high as $T\sim 1/L_s$. (See the discussion in Appendix B.)

9. Uniform susceptibility

The uniform magnetic field h_u in (2.1) is coupled to the generator of the O(3) rotation around the direction of $\mathbf{h}_u$. For general N, h_u will be coupled to an O(N) generator Q, say Q_{12} generating a rotation in the 1-2 plane. We have $(Q\mathbf{S})_1=iS_2$, $(Q\mathbf{S})_2=-iS_1$, the other components of $Q\mathbf{S}$ being zero. In the effective Lagrangean formulation, (4.2), the uniform field h_u enters as the time component of a constant imaginary gauge potential:

$$\partial_0 \to D_0=\partial_0-h_u Q. \tag{9.1}$$

The effective Lagrangean in (4.2) receives an extra contribution

$$\delta\mathcal{L}_u=-h_u\rho_s(\partial_0\mathbf{S}(x)Q\mathbf{S}(x))+\tfrac{1}{2}h_u^2\rho_s^2(Q\mathbf{S}(x))^2. \tag{9.2}$$

For small h_u it is again important to treat properly the zero modes. Let us consider first the "cubic" geometry. Introducing the global rotation $\Omega: \mathbf{S}(x) = \Omega \mathbf{R}(x)$ one has to average $\exp(-\int \delta \mathscr{L}_u)$ over the O(N) rotations Ω. This gives a contribution to the free energy

$$\delta f_u = -\frac{1}{N} h_u^2 \rho_s - \frac{2}{N(N-1)} h_u^2 \rho_s^2 \left\langle \frac{1}{V} \int_x \int_y (\partial_0 \mathbf{R}(x) \mathbf{R}(y)) \times (\partial_0 \mathbf{R}(y) \mathbf{R}(x)) \right\rangle_{h_u=0} + \mathrm{O}(h_u^3). \tag{9.3}$$

Here we have used the following relations for averaging over the group space:

$$\langle a_1' b_1' \rangle_\Omega = \frac{1}{N} (\mathbf{ab}),$$
$$\langle (a_1' b_2' - a_2' b_1')(c_1' d_2' - c_2' d_1') \rangle_\Omega = \frac{2}{N(N-1)} [(\mathbf{ac})(\mathbf{bd}) - (\mathbf{ad})(\mathbf{bc})], \tag{9.4}$$

where $\mathbf{a}' = \Omega \mathbf{a}$, $\mathbf{b}' = \Omega \mathbf{b}, \ldots$ are rotated O(N) vectors. The expectation value in (9.3) can be evaluated using standard steps of chiral perturbation theory. One obtains for the uniform susceptibility at $h_u = 0$ the result quoted in (2.29).

In (2.29) a new shape coefficient appears defined as

$$\frac{1}{L^2} \psi(l) = -\int_V \mathrm{d}^3 x \, \partial_0^2 \tilde{G}(x) \tilde{G}^2(x). \tag{9.5}$$

Here $\tilde{G}(x) = \bar{G}(x) + \beta_1(l)/L = 1/(4\pi |x|) + \mathrm{O}(x^2)$, where $\bar{G}(x)$ is defined in (5.10). For $l=1$ $\psi(l)$ is related to $\beta_n(1)$ (2.31), while for small l its asymptotic form is given by

$$\psi(l) = -\frac{1}{4\pi^2 l^4} + \mathrm{O}(\mathrm{e}^{-2\pi/l^3}), \quad l \ll 1. \tag{9.6}$$

For generic values of l it should be evaluated numerically using methods discussed in detail in [34, 35]. In Appendix B we give approximate analytic expressions for $\psi(l)$.

A small staggered field H_s will fix the direction of the staggered magnetization provided $H_s \mathscr{M}_s L_s^2 \gg T$. Relative to this direction we can define the transversal and longitudinal uniform susceptibilities, $\chi_u^\perp(T, L_s)$ and $\chi_u^\parallel(T, L_s)$, respectively.[15] The susceptibility $\chi_u(T, L_s)$ given in (2.29) corresponds to $H_s = 0$, and is given by the "angular" average over the O(N) group space

$$\chi_u(T, L_s) = \frac{2}{N(N-1)} \left[(N-1) \chi_u^\perp(T, L_s) + \frac{(N-1)(N-2)}{2} \chi_u^\parallel(T, L_s) \right]. \tag{9.7}$$

[15] For the general O(N) case "parallel" is defined by the O(N) generators under which the staggered magnetization is invariant

In the infinite volume limit $\chi_u^\perp(T)$ and $\chi_u^\parallel(T)$ are infrared divergent in chiral perturbation theory. On the other hand, the O(N) invariant average $\chi_u(T)$ remains finite and it is given by (2.32).

Small temperatures $T \ll 1/L_s$ should be considered again separately. The Hamiltonian for the effective O(N) rotator in this case is

$$\hat{H} = \frac{1}{2\Theta_{\mathrm{eff}}} \hat{\mathbf{L}}^2 - h_u \hat{\mathbf{L}}_z, \tag{9.8}$$

where we denoted for simplicity by $\hat{\mathbf{L}}_z$ the O(N) generator coupled to h_u. With the notation of Sect. 8 we obtain

$$\chi_u(T, L_s) = -\frac{2}{N(N-1)} \frac{1}{V_s T} \frac{1}{Z_0(t)} \frac{\partial}{\partial t} Z_0(t). \tag{9.9}$$

For $T V_s \rho_s \gg 1$ (but $T \ll 1/L_s$) Seeley's expansion gives

$$\chi_u(T, L_s) = \frac{2}{N} \rho_s \left\{ 1 + \frac{N-2}{\rho_s L_s^{d-2}} \left[-\frac{1}{6 L_s T} + \frac{1}{4\pi} \left(-\alpha_{1/2}^{(d-1)}(l) + 2 \frac{d-1}{d-2} \right) \right] \right\}, \tag{9.10}$$

in agreement with the low temperature behaviour obtained from (2.29).

For very low temperatures, $T V_s \rho_s \ll 1$, only the lowest lying rotator states contribute, leading to an exponentially small susceptibility given by (2.33).

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A. Momentum sums and integrals on the lattice

It is useful to introduce the notations

$$\hat{k}_\mu = \mathrm{e}^{\mathrm{i}k_\mu} - 1, \quad \hat{k}_\mu^* = \mathrm{e}^{-\mathrm{i}k_\mu} - 1,$$
$$\mathrm{d}(k) = 4 \sum_{\mu=1}^{4} \sin^2 \frac{k_\mu}{2},$$
$$\int_k = \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{\mathrm{d}^d k}{(2\pi)^d},$$
$$\sum_k^* = \sum_{\substack{k \\ k^0 \neq 0}}, \quad \sum_k' = \sum_{\substack{k \\ k \neq (0,\ldots,0)}}, \tag{A.1}$$

$$D^*(x) = \frac{1}{V} \sum_k^* \frac{\mathrm{e}^{\mathrm{i}kx}}{\mathrm{d}(k)} \tag{A.2}$$

With the help of the identities

$$-(\hat{k}_\mu + \hat{k}_\mu^*) = \hat{k}_\mu \hat{k}_\mu^* = 4 \sin^2 \frac{k_\mu}{2}, \quad (\text{no sum over } \mu), \tag{A.3}$$

one obtains

$$\Delta_\mu^x \Delta_\mu^y D^*(x-y)|_{x=y} = \frac{1}{V} \sum_k{}^* \frac{\not{k}_\mu \not{k}_\mu^*}{\mathrm{d}(k)} \tag{A.4}$$

$$= -\frac{1}{V} \sum_k{}^* \frac{\not{k}_\mu + \not{k}_\mu^*}{\mathrm{d}(k)} = -2\Delta_\mu D^*(0).$$

$$\text{(no sum over } \mu) \tag{A.5}$$

In the following we shall discuss the volume dependence of $D^*(0)$ and $\Delta_\mu D^*(0)$ in a euclidean box $L_s^{d-1} \times L_t$ in the $L_t \to \infty$ limit.

The sum in $D^*(0)$ can be written as

$$D^*(0) = \frac{1}{V} \sum_k{}^* \frac{1}{\mathrm{d}(k)}$$

$$= \lim_{M^2 \to 0} \left\{ \frac{1}{V} \sum_k \frac{1}{\mathrm{d}(k) + M^2} - \frac{1}{V} \sum_{k^0} \frac{1}{\mathrm{d}(k^0, \mathbf{k}=0) + M^2} \right\}. \tag{A.6}$$

We divide the sums in (A.6) into the infinite volume contribution and the rest, which is volume dependent and remains finite as the lattice unit $a \to 0$:

$$D^*(0) = \lim_{M^2 \to 0} \left\{ \int_k \frac{1}{\mathrm{d}(k) + M^2} + g_1^{(d)} - \frac{1}{V_s} \left[\int_{k^0} \frac{1}{4\sin^2 \frac{k_0}{2} + M^2} + g_1^{(d=1)} \right] \right\}. \tag{A.7}$$

Since we are not interested in cut-off effects which go to zero as the cut-off goes to infinity, we can evaluate $g_1^{(d)}$ in the $a \to 0$ continuum limit. This problem is discussed in detail in the Appendix B of [11] and we quote the result only:

$$g_1^{(d)}|_{\substack{M \to 0 \\ L_t \to \infty}} = \frac{1}{4\pi L_s^{d-2}} \times \left[\alpha_{1/2}^{(d-1)}(1) + \frac{4\pi}{2ML_s} - 2\frac{d-1}{d-2} \right], \tag{A.8}$$

$$g_1^{(1)}|_{L_t \to \infty} = 0.$$

In the $M \to 0$ limit the first integral in (A.7) is finite while the second one gives $1/2M$. We obtain

$$D^*(0)|_{L_t \to \infty} = \int_k \frac{1}{\mathrm{d}(k)} + \frac{1}{4\pi L_s^{d-2}} \left[\alpha_{1/2}^{(d-1)}(1) - 2\frac{d-1}{d-2} \right]. \tag{A.9}$$

The first term is a volume independent but cut-off dependent constant, while the number $\alpha_{1/2}^{(d-1)}(1)$ can be found in Table 1 in [11].

The steps are similar for $\Delta_\mu D^*(0)$:

$$\Delta_\mu D^*(0) = \frac{1}{V} \sum_k{}^* \frac{\not{k}_\mu}{\mathrm{d}(k)}$$

$$= \lim_{M^2 \to 0} \left\{ \frac{1}{V} \sum_k \frac{\not{k}_\mu}{\mathrm{d}(k) + M^2} - \delta_{\mu 0} \frac{1}{V_s} \frac{1}{L_t} \sum_{k^0} \frac{1}{\mathrm{d}(k^0, \mathbf{k}=0) + M^2} \right\}. \tag{A.10}$$

The second term in (A.10) gives $+\delta_{\mu 0}/2V_s$. In the first term we separate the infinite volume contribution:

$$\lim_{M^2 \to 0} \frac{1}{V} \sum_k \frac{\not{k}_\mu}{\mathrm{d}(k) + M^2} = \frac{1}{2} \int_k \frac{\not{k}_\mu + \not{k}_\mu^*}{\mathrm{d}(k)} + Q_\mu, \tag{A.11}$$

where

$$Q_\mu = \lim_{M^2 \to 0} \frac{1}{2} \left[\frac{1}{V} \sum_k \frac{\not{k}_\mu + \not{k}_\mu^*}{\mathrm{d}(k) + M^2} - \int_k \frac{\not{k}_\mu + \not{k}_\mu^*}{\mathrm{d}(k) + M^2} \right]. \tag{A.12}$$

It is easy to show that

$$Q_i = -\frac{1}{d-1} Q_0, \quad i = 1, \ldots, d-1. \tag{A.13}$$

Indeed, for $L_t \to \infty$ we can write

$$Q_0 = \frac{1}{2} \left(\frac{1}{V_s} \sum_{\mathbf{k}} - \int_{\mathbf{k}} \right) \int_{-\pi}^{\pi} \frac{dk_0}{2\pi} \frac{-4\sin^2 \frac{k_0}{2}}{\mathrm{d}(k)}$$

$$= \frac{1}{2} \left(\frac{1}{V_s} \sum_{\mathbf{k}} - \int_{\mathbf{k}} \right) \int_{-\pi}^{\pi} \frac{dk_0}{2\pi} \frac{\sum_i 4\sin^2 \frac{k_i}{2}}{\mathrm{d}(k)}$$

$$= -\sum_i Q_i. \tag{A.14}$$

since we have a box $L_s^{d-1} \times L_t$, Q_i is independent of i and (A.13) follows. The first term in (A.11) gives

$$\frac{1}{2} \int_k \frac{\not{k}_\mu + \not{k}_\mu^*}{\mathrm{d}(k)} = -\frac{1}{2d} \frac{1}{a^{d-1}}, \tag{A.15}$$

where on the right hand side we restored the cut-off dependence explicitly. We have, therefore

$$\Delta_0 D^*(0) = -\frac{1}{2d} \frac{1}{a^{d-1}} + \frac{1}{2V_s} + Q_0,$$
$$\Delta_i D^*(0) = -\frac{1}{2d} \frac{1}{a^{d-1}} - \frac{1}{d-1} Q_0. \tag{A.16}$$

In the expression for the ground state energy (6.57) the combination

$$\Delta_\mu D^*(0)\Delta_\mu D^*(0)-\frac{1}{V_s}\Delta_0 D^*(0)$$
$$=\left(-\frac{1}{2d}\frac{1}{a^{d-1}}+\frac{1}{2V_s}+Q_0\right)^2$$
$$+(d-1)\left(-\frac{1}{2d}\frac{1}{a^{d-1}}-\frac{1}{d-1}Q_0\right)^2$$
$$-\frac{1}{V_s}\left(-\frac{1}{2d}\frac{1}{a^{d-1}}+\frac{1}{2V_s}+Q_0\right) \tag{A.17}$$

enters. Equation (A.17) leads to the result

$$\Delta_\mu D^*(0)\Delta_\mu D^*(0)-\frac{1}{V_s}\Delta_0 D^*(0)$$
$$=\frac{1}{4d}\frac{1}{a^{2d-2}}+\frac{d}{d-1}Q_0^2-\frac{1}{4V_s^2}. \tag{A.18}$$

As expected, there is no mixing between divergent cut-off powers and volume dependence in (A.18). Since Q_0 is finite in the $a\to 0$ limit, we can write

$$Q_0=\lim_{M^2\to 0}\left(-\tfrac{1}{2}\right)\left[\frac{1}{V_s}\sum_{\mathbf{k}}-\int_{\mathbf{k}}\right]\int_{-\infty}^{\infty}\frac{dk_0}{2\pi}\frac{k_0^2}{k_0^2+\mathbf{k}^2}$$
$$=\tfrac{1}{2}\left[\frac{1}{V_s}\sum_{\mathbf{k}}(\mathbf{k}^2)^{1/2}-\int_{\mathbf{k}}(\mathbf{k}^2)^{1/2}\right]$$
$$=-\frac{1}{4\sqrt{\pi}}g_{-1/2}^{(d-1)}|_{M^2\to 0}, \tag{A.19}$$

where, in the last step, we used the notation of [11]. Since $g_{-1/2}^{(d-1)}\sim L_s^{-d}$, after restoring the dimensions we get

$$Q_0=\mathrm{O}\left(\frac{a}{L_s^d}\right), \tag{A.20}$$

and Q_0^2 can be neglected in (A.18) in our order. We can write therefore

$$\Delta_\mu D^*(0)\Delta_\mu(0)-\frac{1}{V_s}\Delta_0 D^*(0)|_{\substack{L_t\to\infty\\ a\to 0}}$$
$$=\frac{1}{4d}\frac{1}{a^{2d-2}}-\frac{1}{4V_s^2}. \tag{A.21}$$

The divergent first term contributes to the non-universal constant of the ground state energy density only.

B. Asymptotic expressions

For the "slab geometry", $l\ll 1$ (or $L_t\ll L_s$) and for the "cylinder geometry", $l\gg 1$ ($L_t\gg L_s$) one can derive simple asymptotic expressions for the functions $\alpha_r(l)\equiv\alpha_r^{(3)}(l)$, which are related by (2.11) to the functions $\beta_n(l)$, $n=0$, 1, 2 appearing in the finite size corrections. One can show that for $l\leqq 1$

$$\alpha_r^{(3)}(l)=l^{4r-6}\left[\alpha_{-r+3/2}^{(1)}(1)+\frac{1}{(r-1)(2r-3)}\right]$$
$$+l^{-2r}\left[\alpha_r^{(2)}(1)+\frac{1}{r(r-1)}\right]$$
$$-\frac{3}{r(2r-3)}+\mathrm{O}(\mathrm{e}^{-\pi/l^2}),\quad l\leqq 1. \tag{B.1}$$

For $l\geqq 1$ one has the approximation:

$$\alpha_r^{(3)}(l)=l^{4r}\left[\alpha_r^{(1)}(1)+\frac{1}{r(2r-1)}\right]$$
$$+l^{3-2r}\left[\alpha_{-r+3/2}^{(2)}(1)+\frac{4}{(2r-1)(2r-3)}\right]$$
$$-\frac{3}{r(2r-3)}+\mathrm{O}(\mathrm{e}^{-\pi l^2}),\quad l\geqq 1. \tag{B.2}$$

Using these expressions and the equality $\alpha_p^{(d)}(1)=\alpha_{d/2-p}^{(d)}(1)$ one can relate the shape coefficients to those corresponding to a symmetric box in d dimensions, listed in Table 1 of [11].

In particular we have for $l\leqq 1$

$$\begin{aligned}\beta_0(l)&=l^{-6}\cdot 0.382626+2\ln l+1.054689+\delta\beta_0^-(l),\\ \frac{1}{l}\beta_1(l)&=\frac{1}{4\pi l^3}[2.852929+6\ln l]+\frac{1}{l}\delta\beta_1^-(l),\\ \frac{1}{l^2}\beta_2(l)&=\frac{1}{(4\pi)^2}\left[\frac{0.610644}{l^6}+1.047198\right]\\ &\quad+\frac{1}{l^2}\delta\beta_2^-(l).\end{aligned} \tag{B.3}$$

For $l\geqq 1$ we get

$$\begin{aligned}\beta_0(l)&=l^3\cdot 1.437745-4\ln l+\delta\beta_0^+(l),\\ \frac{1}{l}\beta_1(l)&=-\frac{1}{12}l^3+\frac{3.900265}{4\pi}+\frac{1}{l}\delta\beta_1^+(l),\\ \frac{1}{l^2}\beta_2(l)&=\frac{1}{720}l^6+\frac{1.437745}{(4\pi)^2l^3}+\frac{1}{l^2}\delta\beta_2^+(l).\end{aligned} \tag{B.4}$$

The correction terms $\delta\beta_n^{\mp}(l)$ are exponentially small for $l\ll 1$ and $l\gg 1$, respectively. They can be parametrized in a simple form

$$\begin{aligned}\delta\beta_n^-(l)&=a_n^-\,l^{b_n^-}\,\mathrm{e}^{-2\pi/l^3},\quad l\leqq 1,\\ \delta\beta_n^+(l)&=a_n^+\,l^{b_n^+}\,\mathrm{e}^{-2\pi l^3},\quad l\geqq 1.\end{aligned} \tag{B.5}$$

The exponential factors are expected on physical grounds, while the parameters $a_n^{\pm}$, $b_n^{\pm}$ can be determined from the known values of $\beta_n(1)$ and the fact that $\beta_n'(1)=0$. They are summarized in Table 1. It is remarkable that this simple parametrization gives a relative error smaller than 10^{-5} in the whole range of l values.

For the shape coefficients $\psi(l)$ defined in (9.5) one can also give approximate analytic expressions

$$\psi(l) = -\frac{1}{4\pi^2 l^4} + 2.57\,\mathrm{e}^{-2\pi/l^3}, \qquad l \leqq 1,$$

$$\psi(l) = -\frac{1}{120} l^8 + \frac{3.900265}{24\pi} l^5 - 0.055\, l^2 - 4.78\,\mathrm{e}^{-2\pi l^3}, \qquad l \geqq 1. \tag{B.6}$$

Table 1. Values of the parameters in (B.5)

n	a_n^-	b_n^-	a_n^+	b_n^+
0	8.85264	−0.959427	8.62200	−0.608985
1	−0.66610	−0.321512	−0.671988	0.553185
2	0.058438	1.35468	0.061051	1.25040

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