Technical notes on a 2-d lattice O(N) model problem

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This paper provides a technical companion to M. Aguado and E. Seiler, [4], in which the fate of perturbation theory in the thermodynamic limit is discussed for the O(N) model on a 2d lattice and different boundary conditions. The techniques used to compute perturbative coefficients are explained, and results for all boundary conditions considered reviewed in detail.

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1 Introduction

Perturbation theory is the standard method to study quantum field theories in the small coupling regime. However, the interplay of the perturbative expansion and the thermodynamic limit remains controversial. In particular, arguments were put forward that the infinite volume limit of perturbative coefficients does not give the correct infinite volume asymptotic perturbation expansion of asymptotically free theories [1]. In addition to the standard free (FBC), periodic (PBC), and Dirichlet (DBC) boundary conditions for the spin model considered, a novel boundary condition was introduced in [1], namely superinstanton boundary conditions (SIBC). The latter consist of Dirichlet conditions on the boundary of the system, and the additional freezing of one spin in the center of the sample. Perturbative coefficients were shown to have different thermodynamic limits for standard boundary conditions and SIBC.

It was argued in [2] (see also [3]) that SIBC do not possess a well defined perturbation expansion, the third order coefficient being predicted to diverge in the infrared. Thus, perturbation theory was assumed to be consistent as the $V \to \infty$ limit for standard boundary conditions is taken.

This is a companion paper to [4] (so far the last contribution to the controversy, see citations therein), in which the volume dependence of perturbation theory coefficients for the O(N) vector model with different boundary conditions was investigated up to third order, confirming the points of [2] regarding independence of the infinite volume perturbative coefficients for ‘standard’ b.c.

The aim of this paper is to describe in detail the method used to compute the perturbative coefficients in [4], and give a broader view of the results, including the IR divergence of SIBC correlators at third order.
2 O(N) model: Perturbation theory

The partition function for the O(\(N\)) spin model on a 2-dimensional lattice \(\Lambda\) is

\[
Z = \int \prod_x d^N\vec{S}_x\, \delta(\vec{S}_x^2 - 1) \exp \left( \beta \sum_{(x,y)} \vec{S}_x \cdot \vec{S}_y \right), \tag{1}
\]

where \(\sum_{(x,y)}\) stands for a sum over nearest neighbour pairs. The delta functions constrain spins to have unit norm, i.e. \(\vec{S} \in S^{N-1} \subset \mathbb{R}^N\, \forall x \in \Lambda\).

The perturbative expansion of this model around the classical vacuum configuration \(\vec{S}_x = \vec{S}_x^{(0)} = (1, \vec{0})\, \forall x \in \Lambda\) is constructed by writing

\[
\vec{S}_x = (\sigma_x, \vec{\pi}_x), \quad \sigma_x = +\sqrt{1 - \vec{\pi}_x^2}, \tag{2}
\]

and Taylor expanding in powers of \(\vec{\pi}_x\).

Assume for simplicity that the problem has no zero modes, i.e. the boundary conditions are such that the only vacuum configuration is \(\{\vec{S}_x^{(0)}\}\). The case with zero modes will be treated in next section.

The measure of the functional integral, in terms of \(\vec{\pi}_x\), is written as

\[
\prod_x d^N\vec{S}_x\, \delta(\vec{S}_x^2 - 1) = \prod_x d^{N-1}\vec{\pi}_x / \sqrt{1 - \vec{\pi}_x^2}, \tag{3}
\]

with unconstrained \(\vec{\pi}_x\).

The square roots can be exponentiated and added to the action terms in the exponent of (1). This yields

\[
Z \sim \int \left[ \prod_x d^{N-1}\vec{\pi}_x \right] \times \exp \left\{ \beta \sum_{(x,y)} \left( \vec{\pi}_x \cdot \vec{\pi}_y + \sqrt{1 - \vec{\pi}_x^2} \sqrt{1 - \vec{\pi}_y^2} \right) - \frac{1}{2} \sum_x \ln (1 - \vec{\pi}_x^2) \right\}. \tag{4}
\]

Expanding in powers of \(\beta^{-1}\) after a rescaling \(\vec{\pi}_x \to \vec{\pi}_x / \sqrt{\beta}\),

\[
Z \sim \int \left[ \prod_x d^{N-1}\vec{\pi}_x \right] \exp \left\{ - \frac{1}{2} \sum_{(x,y)} (\vec{\pi}_x - \vec{\pi}_y)^2 - \frac{1}{8\beta} \sum_{(x,y)} (\vec{\pi}_x^2 - \vec{\pi}_y^2)^2 \right. \\
- \frac{1}{16\beta^2} \sum_{(x,y)} (\vec{\pi}_x^2 - \vec{\pi}_y^2) \left[ (\vec{\pi}_x^2)^2 - (\vec{\pi}_y^2)^2 \right] + \frac{1}{2\beta} \sum_x \vec{\pi}_x^2 + \frac{1}{4\beta^2} \sum_x (\vec{\pi}_x^2)^2 + O(\beta^{-3}) \right\} \tag{5}
\]

(terms containing a single sum over \(x\) come from the change in the measure).

2.1 Hasenfratz terms

If the boundary conditions are such that there is a continuum of classical vacuum configurations, obtained by rotation of \(\vec{S}_x^{(0)}\) (e.g. for FBC or PBC), the
corresponding zero modes have to be dealt with by introducing collective coordinates. As shown by Hasenfratz [5], this amounts to adding an extra term to the action,

\[- (N - 1) \ln \sum_x \sqrt{1 - \vec{\pi}^2}. \quad (6)\]

The integrand of the partition function (5) gets multiplied by

\[
\exp \left\{ - \frac{N - 1}{2V\beta} \sum_x \vec{\pi}_x^2 - \frac{N - 1}{8V^2\beta^2} \sum_x (\vec{\pi}_x^2)^2 - \frac{N - 1}{8V^2z^2\beta^2} \sum_x \sum_y \vec{\pi}_x^2 \vec{\pi}_y^2 + O(\beta^{-3}) \right\}. \quad (7)
\]

Notice that all terms in the exponent are suppressed in our notation by powers of $V$, the volume of the system.

2.2 Vertices

The quadratic part of (5) gives a propagator $\delta^{ij} G_{xy}$ (superindices denote ‘colour’, subindices denote lattice points). The precise form of $G_{xy}$ depends on the boundary conditions, and will be discussed in next section.

The vertices corresponding to (5) and (7) are:

- **Order $\beta^{-1}$, two-$\vec{\pi}$ vertex ($\circ$):**

\[
V_{zw}^{k\ell} = \frac{1}{\beta} \left( 1 - \frac{N - 1}{V} \right) \delta^{k\ell} \delta_{zw}. \quad (8)
\]

- **Order $\beta^{-1}$, four-$\vec{\pi}$ vertex (□):**

\[
V_{zwu}^{k\ell mn} = \frac{1}{\beta} \left[ \sum_n \delta_{zwu} \left( \delta^{k\ell} \delta_{mn} + \delta^{km} \delta^{\ell n} + \delta^{kn} \delta^{\ell m} \right) + \left( \delta^{n,m} \delta_{zwu} \delta^{k\ell} \delta_{mn} + \delta^{n,m} \delta_{zwu} \delta^{km} \delta^{\ell n} + \delta^{n,m} \delta_{zwu} \delta^{kn} \delta^{\ell m} \right) \right]. \quad (9)
\]

- **Order $\beta^{-2}$, four-$\vec{\pi}$ vertex (■):**

\[
W_{zwu}^{k\ell mn} = \frac{1}{\beta^2} \left[ \left( 2 - \frac{N - 1}{V} \right) \sum_n \delta_{zwu} \left( \delta^{k\ell} \delta_{mn} + \delta^{km} \delta^{\ell n} + \delta^{kn} \delta^{\ell m} \right) - \frac{N - 1}{V^2} \left( \delta_{zwu} \delta_{tu} \delta^{k\ell} \delta_{mn} + \delta_{zwu} \delta_{tu} \delta^{km} \delta^{\ell n} + \delta_{zwu} \delta_{tu} \delta^{kn} \delta^{\ell m} \right) \right]. \quad (10)
\]

- **Order $\beta^{-2}$, six-$\vec{\pi}$ vertex (●):**

\[
W_{zwu}^{k\ell mnab} = \frac{1}{\beta^2} \left\{ -3n_z \delta_{zwu} \delta_{pq} \left( \delta^{k\ell} \delta_{mn} \delta_{ab} + 14 \text{ terms} \right) + \left[ \left( \delta^{p,m} \delta_{zwu} \delta_{pq} \left( \delta^{k\ell} \delta_{mn} + \delta^{km} \delta_{\ell n} + \delta^{kn} \delta_{\ell m} \right) \delta_{ab} \right) + 14 \text{ terms} \right] \right\}. \quad (11)
\]
The meaning of the symbols used is the following: \( n_x \) is the number of nearest neighbours of site \( x \). The value of \( \delta_{x_1 x_2 \ldots x_n} \) is 1 for \( x_1 = x_2 = \ldots = x_n \), and zero otherwise. As for \( \delta^{n,n}_{xy} \), it is 1 if \( x \) and \( y \) are nearest neighbours, and zero otherwise (in particular, \( \delta^{n,n}_{xx} = 0 \)).

All terms explicitly dependent on the volume \( V \) are Hasenfratz terms, and should not be included in the perturbative calculations in absence of zero-modes.

3 Propagator, boundary conditions

The form of the \( \vec{\pi} \)-propagator \( G_{xy} \) depends on the boundary conditions imposed. The quadratic form in the exponent of the integrand in (5) has the form

\[
-\frac{1}{2} \sum_{x,y} \vec{\pi}_x \cdot M_{xy} \vec{\pi}_y, 
\]

with

\[
M_{x,y} = n_x \delta_{xy} - \delta^{n,n}_{xy},
\]

acting trivially on the internal \( O(N) \) space.

For DBC and SIBC, this quadratic form has no zero modes, and the matrix of propagators is just \( G = M^{-1} \). However, for FBC and PBC, configurations with \( \vec{\pi}_x = \vec{\pi}_0 \forall x \) constitute the kernel of \( M \). Let \( P \) be the projector onto this space, and \( P^\perp \) its orthogonal projector. Then

\[
M = M_0 P^\perp + 0 P, 
\]

where \( M_0 \) is regular in the space of nonzero-modes. The matrix \( G \) is defined as

\[
G = M_0^{-1} P^\perp + 0 P. 
\]

Let us discuss the form of \( M \) and \( G \) for the different boundary conditions mentioned.

3.1 Free boundary conditions

For definiteness, we work with a (strictly) 2-dimensional square lattice, with \( V = L \times T \) sites, \( T = L \). Rows are numbered from 0 to \( T - 1 \), and columns from 0 to \( L - 1 \). Lexicographically ordering sites in the lattice, and taking into account the different numbers of nearest neighbours lattice sites have, we write the \( V \times V \) matrix (13) in terms of blocks of size \( L \times L \) as

\[
M = \begin{pmatrix}
  a & -1 & & & \\
  -1 & b & -1 & & \\
  & -1 & b & -1 & \\
  & & \ddots & \ddots & \ddots \\
  & & & -1 & b \\
  & & & & -1 & a
\end{pmatrix},
\]
where 1 is the $L \times L$ unit matrix,

$$
a = \begin{pmatrix}
2 & -1 & & & \\
-1 & 3 & -1 & & \\
& -1 & 3 & & \\
& & & \ddots & \\
& & & & 3 & -1 \\
& & & & -1 & 2
\end{pmatrix},
$$

(17)

and $b = a + 1$.

Observe that $\ker \mathcal{M}$ is generated by $(1, 1, \ldots, 1)^T$.

Matrix $\mathcal{M}$ has a block tridiagonal structure, and its blocks are themselves tridiagonal matrices commuting with each other. By working within each eigenspace of the blocks, we can apply to the whole $\mathcal{M}$ an inversion procedure valid for tridiagonal matrices.

If $A$ is tridiagonal,

$$
A = \begin{pmatrix}
a_0 & -1 & & & \\
-1 & a_1 & -1 & & \\
& -1 & a_2 & & \\
& & & \ddots & \\
& & & & a_{r-2} & -1 \\
& & & & -1 & a_{r-1}
\end{pmatrix},
$$

(18)

its inverse is $A^{-1} = (\mu_{ab})$, with entries

$$
\mu_{ab} = \lambda_0 \lambda_{b+1} \cdots \lambda_a (1 + \lambda_0 \lambda_{a+1} (1 + \cdots (1 + \lambda_{r-2} \lambda_{r-1}) \cdots)), \quad a \geq b, \\
\mu_{ab} = \mu_{ba}, \quad a < b.
$$

(19)

constructed from numbers $\lambda_j$ which can be computed recursively from the diagonal elements of $A$:

$$
\lambda_0 = a_0^{-1}, \quad \lambda_j = (a_j - \lambda_{j-1})^{-1}, \quad j = 1, \ldots, r - 1.
$$

(20)

Possible divisions by zero can be avoided by rearranging the rows of $A$, as long as it is invertible.

If our matrix $\mathcal{M}$ of eq. (16) were invertible, we could apply this construction to each of the eigenspaces of matrices $a$ (eigenvalues $\alpha^{(h)}$, eigenvectors $v^{(h)}$, $h = 1, \ldots, L - 1$) and $b = a + 1$ (eigenvalues $\alpha^{(h)} + 1$, same eigenvectors). Procedure (20) to compute the ‘building blocks’ $\lambda_i^{(h)}$ of the inverse matrix can be written, for eigenvalue $\alpha^{(h)}$, as

$$
\lambda_0^{(h)} = \left(\alpha^{(h)}\right)^{-1},

\lambda_{j}^{(h)} = \left(\alpha^{(h)} + 1 - \lambda_{j-1}^{(h)}\right)^{-1}, \quad j = 1, \ldots, r - 2,

\lambda_{T-1}^{(h)} = \left(\alpha^{(h)} - \lambda_{T-2}^{(h)}\right)^{-1},
$$

(21)

and the $\mu_{ab}^{(h)}$ as

$$
\mu_{ab}^{(h)} = \lambda_0^{(h)} \lambda_{b+1}^{(h)} \cdots \lambda_a^{(h)} (1 + \lambda_0^{(h)} \lambda_{a+1}^{(h)} (1 + \cdots (1 + \lambda_{r-2}^{(h)} \lambda_{r-1}^{(h)}) \cdots)), \quad a \geq b, \\
\mu_{ab}^{(h)} = \mu_{ba}^{(h)}, \quad a < b.
$$

(22)
Then, all we would have to do is construct $G$ as

$$G = \mathcal{M}^{-1} = \sum_{h=0}^{L-1} \mu^{(h)} \otimes P^{(h)},$$

(23)

with $P^{(h)} = v^{(h)}v^{(h)T}$ the $L \times L$ projector onto the $h$-th eigenspace of $a, b$.

Now the eigenvalues of $a$ (resp. $b$) lie in the interval $[1, 3]$ (resp. $[2, 4]$), there existing just one eigenvector, $v^{(0)} \propto (1, 1, \ldots, 1)^T$, with eigenvalue 1 (resp. 2). Then (21) can be carried out without problems if $\alpha > 1$, but for the unit eigenvalue the last step is a division by zero, signalling the breakdown of the inversion procedure due to $\mathcal{M}$ being singular.

We need to generalise the procedure to obtain $G$ of the form (15). To do this, first we add a regulator:

$$\mathcal{M} \rightarrow \mathcal{M}_\varepsilon = \mathcal{M} + \varepsilon 1_{V \times V}.$$ 

(24)

The eigenvectors of $a_\varepsilon$ and $b_\varepsilon$ remain the same as for $a$ and $b$, and their eigenvalues are shifted by the small positive number $\varepsilon$. Procedure (21) can now be used for all eigenspaces. For eigenvalues strictly larger than $1 + \varepsilon$, the results are as before up to terms of order $\varepsilon$. For the lowest eigenvalue $\alpha^{(0)} = 1 + \varepsilon$ of $a_\varepsilon$, we obtain

$$\begin{align*}
\lambda^{(0)}_{\varepsilon j} &= 1 - (j + 1)\varepsilon + \frac{(j + 1)(j + 2)(2j + 3)}{6} \varepsilon^2 + \mathcal{O}(\varepsilon^3), \quad j = 0, \ldots, T - 2; \\
\lambda^{(0)}_{\varepsilon,T-1} &= \frac{1}{T\varepsilon} \left[ 1 + \frac{(T - 1)(2T - 1)}{6} \varepsilon + \mathcal{O}(\varepsilon^2) \right].
\end{align*}$$

(25)

The elements of the inverse, $\mu^{(0)}_{\varepsilon,ij}$, can be decomposed as

$$\mu^{(0)}_{\varepsilon,ij} = \frac{1}{T\varepsilon} + \tilde{\mu}_{ij} + \mathcal{O}(\varepsilon),$$

(26)

with

$$\begin{align*}
\tilde{\mu}_{ij} &= \frac{(T - i)(T - 1 - i)}{2} + \frac{j(j + 1)}{2} - \frac{T^2 - 1}{6}, \quad i \geq j, \\
\tilde{\mu}_{ij} &= \tilde{\mu}_{ji} \quad i < j.
\end{align*}$$

(27)

Now it suffices to observe that the divergent piece $\frac{1}{T\varepsilon}$ is just the contribution coming from the zero mode $\propto (1, 1, \ldots, 1)^T$ of $\mathcal{M}$ as a whole. Indeed, it can be checked that the sums of the contributions of all other $\mu^{(h)}$, and of $\tilde{\mu}$, to each row vanish. Then $G$ is constructed as

$$G = \tilde{\mu} \otimes P^{(0)} + \sum_{h=1}^{L-1} \mu^{(h)} \otimes P^{(h)},$$

(28)

which is the final result for FBC.
3.2 Periodic boundary conditions

For PBC, \( n_x = 4 \) at each site, hence

\[
\mathcal{M} = \begin{pmatrix}
  c & -1 & -1 \\
  -1 & c & \ddots \\
  \vdots & \ddots & \ddots & -1 \\
  -1 & -1 & c & \end{pmatrix},
\]

in terms of blocks of size \( L \times L \), with

\[
c = \begin{pmatrix}
  4 & -1 & -1 \\
  -1 & 4 & \ddots \\
  \vdots & \ddots & \ddots & 4 \\
  -1 & -1 & 4 & \end{pmatrix}.
\]

In this case, \( \mathcal{M} \) can be immediately diagonalised by observing that

\[
\mathcal{M} = \sum_{m=0}^{T-1} \left[ c - 2 \cos \left( \frac{2\pi m T}{L} \right) \right] \mathbb{1} \otimes P^{(m)},
\]

with the \( T \times T \) projector

\[
P^{(m)}_{ab} = \frac{1}{T} \omega_T^{m(a-b)}, \quad \omega_T = \exp \left( i \frac{2\pi}{T} \right).
\]

Now, of course,

\[
c = \sum_{n=0}^{L-1} \left[ 4 - 2 \cos \left( \frac{2\pi n}{L} \right) \right] Q^{(n)},
\]

with the \( L \times L \) projector

\[
Q^{(n)}_{cd} = \frac{1}{L} \omega_L^{n(c-d)}, \quad \omega_L = \exp \left( i \frac{2\pi}{L} \right).
\]

Inserting (33) into (31) and using symmetry properties, we obtain

\[
\mathcal{M} = \sum_{m=0}^{T-1} \sum_{n=0}^{L-1} \left[ 4 - 2 \cos \left( \frac{2\pi m T}{L} \right) - 2 \cos \left( \frac{2\pi n}{L} \right) \right] \mathbb{P}^{(mn)},
\]

with a total \( V \times V \) projector

\[
\mathbb{P}^{(mn)} = P^{(m)} \otimes Q^{(n)}, \quad (\mathbb{P}^{(mn)})_{ac, bd} = \frac{\cos \left[ \frac{2\pi}{T} m(a-b) + \frac{2\pi}{L} n(c-d) \right]}{V}.
\]

The \( \mathbb{P}^{00} \) contribution is zero, corresponding to the zero mode of \( \mathcal{M} \). This is just the decomposition (14). We can write directly \( G \) as in (15),

\[
G = \sum_{m=0}^{T-1} \sum_{n=0}^{L-1} \left[ 4 - 2 \cos \left( \frac{2\pi m T}{L} \right) - 2 \cos \left( \frac{2\pi n}{L} \right) \right] \mathbb{P}^{(mn)},
\]

the prime meaning omission of the \((m = 0, n = 0)\) term.
3.3 Dirichlet boundary conditions

For 0-Dirichlet boundary conditions, spins along the boundary of the system are frozen to \( \tilde{\pi}_x = \tilde{0} \forall x \in \partial \Lambda \).

All \( G_{xy} \) with \( x \) or \( y \) on the boundary thus vanish. This allows us to restrict the sums in the action and correlators (in terms of \( \pi_x \)) to the inner \( L \times T = (L-2) \times (T-2) \) lattice (matrices \( M \) and \( G \) will be \( \tilde{V} \times \tilde{V} = (L-2)(T-2) \times (L-2)(T-2) \)). All inner spins have 4 nearest neighbours, but the \( \delta^{n,m} \) piece in \( M \) makes its structure different from the periodic case:

\[
M = \begin{pmatrix}
    d & -1 & & \\
    -1 & d & & \\
    & & \ddots & \\
    & & -1 & d \\
    & & & -1 & d
\end{pmatrix},
\]

in terms of blocks of size \( \tilde{L} \times \tilde{L} \), with

\[
d = \begin{pmatrix}
    4 & -1 & & \\
    -1 & 4 & & \\
    & & \ddots & \\
    & & -1 & 4 \\
    & & & -1 & 4
\end{pmatrix}.
\]

The construction applied above to FBC can be used in this case without the complication due to zero modes, since \( M \) is regular here and all eigenvalues \( \delta^{(h)} \) of \( d \) are ‘safe’. The building blocks \( \lambda^{(h)} \) are computed as

\[
\lambda_j^{(h)} = (\delta^{(h)})^{-1}, \quad j = 1, \ldots, T - 1,
\]

and the \( \mu_{ab}^{(h)} \) as

\[
\mu_{ab}^{(h)} = \sum_{r=0}^{T-1} \lambda_a^{(h)} \lambda_{a+1}^{(h)} \cdots \lambda_{a+r}^{(h)} (1 + \lambda_{a+1}^{(h)} \lambda_{a+2}^{(h)} \cdots (1 + \lambda_{a+r-1}^{(h)} \lambda_{a+r}^{(h)}) \cdots), \quad a \geq b,
\]

\[
\mu_{ab}^{(h)} = \mu_{ba}^{(h)}, \quad a < b,
\]

to get

\[
G = M^{-1} = \sum_{h=0}^{L-1} \mu^{(h)} \otimes P^{(h)}
\]

with \( P^{(h)} = v^{(h)} v^{(h)\dagger} \), and \( v^{(h)} \) the \( b \)-th eigenvector of \( d \).

3.4 Superinstanton boundary conditions

Propagators for 0-superinstanton boundary conditions can be obtained from those for DBC by the following argument:

Freezing of \( \tilde{\pi}_0 = 0 \) can be attained by adding a term \( \frac{1}{2} \tilde{\pi}_0^2 \) to the action of the system with DBC, modifying the original quadratic form,

\[
\mathcal{M} \rightarrow \mathcal{M}_\lambda = \mathcal{M} - \lambda Y,
\]

where \( \lambda \) is a regularization parameter.
with \( Y_{ab} = \delta_{a0} \delta_{b0} \), and taking the limit \( \lambda \to +\infty \) after all calculations.

Then \( G^{SI} = \lim_{\lambda \to +\infty} G_{\lambda} \), with

\[
G_{\lambda} = (\mathcal{M} - \lambda Y)^{-1} = G(1 - \lambda Y G)^{-1} = G + \lambda Y \left( \sum_{n=0}^{\infty} \lambda^n (Y G)^n \right) Y. \tag{44}
\]

In components,

\[
(G_{\lambda})_{xy} = G_{xy} + \lambda G_{x0} \left( \sum_{n=0}^{\infty} \lambda^n G_{00} \right) G_{0y} = G_{xy} + \frac{\lambda G_{x0} G_{0y}}{1 - \lambda G_{00}}. \tag{45}
\]

Hence, taking the limit,

\[
G^{SI}_{xy} = \lim_{\lambda \to \infty} (G_{\lambda})_{xy} = G_{xy} - \frac{G_{x0} G_{0y}}{G_{00}}. \tag{46}
\]

### 4 The correlator

We are interested in the 2-point function of \( \vec{S}_x \), whose perturbative expansion can be expressed in terms of \( \vec{\pi} \) as

\[
\langle \vec{S}_x \cdot \vec{S}_y \rangle = 1 + \frac{1}{\beta} \left[ - \frac{1}{2} \left( \vec{\pi}_x - \vec{\pi}_y \right)^2 \right] + \frac{1}{\beta^2} \left[ - \frac{1}{8} \left( \vec{\pi}_x^2 - \vec{\pi}_y^2 \right) \right] + \frac{1}{\beta^3} \left[ - \frac{1}{16} \left( \vec{\pi}_x^2 - \vec{\pi}_y^2 \right) \right] \right. + \mathcal{O}(\beta^{-4}). \tag{47}
\]

We can write the perturbative expansion of \( \langle \vec{S}_x \cdot \vec{S}_y \rangle \) as follows:

\[
\langle \vec{S}_x \cdot \vec{S}_y \rangle \sim 1 + \sum_{i=1}^{r} \frac{c_i}{\beta^i} + \mathcal{O} \left( \beta^{-(r+1)} \right), \tag{48}
\]

with \( c_i \equiv \langle \vec{S}_x \cdot \vec{S}_y \rangle^{(i)} \) polynomials in \( N - 1 \),

\[
c_i = \sum_{j=1}^{i} c_{ij} (N - 1)^j, \quad i = 1, 2, \ldots \tag{49}
\]

#### 4.1 Feynman diagrams

\( \pi \pi \) processes (Feynman diagrams) contributing to \( \langle \vec{S}_x \cdot \vec{S}_y \rangle \) to order \( \beta^{-1} \), \( \beta^{-2} \) and \( \beta^{-3} \) are drawn in figure 1.

The \( \pi \pi \pi \pi \) contribution comes from the diagrams in figure 2 (which should be drawn for each channel):

Finally, figure 3 contains the unique Feynman diagram (up to channel reordering) representing the \( \pi \pi \pi \pi \pi \) contribution to the correlator:
4.2 Non-Hasenfratz terms

Coefficients $c_{ij}$ can be split into two terms, one coming from non-Hasenfratz contributions, the other term coming from Hasenfratz contributions:

$$c_{ij} = c_{ij}^{n,H} + c_{ij}^{H}.$$  \hfill (50)

Non-Hasenfratz contributions, in our notation, do not explicitly depend on the volume $V$.

We now list all these contributions, up to and including order $\beta^{-3}$. We write $c_{ij}$ instead of $c_{ij}^{n,H}$ when the corresponding Hasenfratz contribution vanishes identically.

We employ the following condensed notation:

$$
\begin{align*}
H_{ab}^c &= G_{ac} - G_{bc}, & J_{ab} &= G_{aa} - G_{bb}, \\
P_{ab}^{cd} &= G_{ac}G_{bd} - G_{ad}G_{bc}, & Q_{ab}^{cd} &= G_{ac}G_{bc} - G_{ad}G_{bd}, \\
R_{ab}^{cd} &= G_{ac}^2 + G_{bd}^2 - G_{ad}^2 - G_{bc}^2.
\end{align*}
$$

Order $\beta^{-1}$: there is only one contribution,

$$c_{11} = -\frac{1}{2} (G_{xx} + G_{yy} - 2G_{xy}) = -\frac{1}{2} (H^x_{xy} - H^y_{xy})$$  \hfill (52)

Order $\beta^{-2}$: There are contributions proportional to $N - 1$ and to $(N - 1)^2$,

$$c_{21} = -\frac{1}{4} R_{xy}^{zy} - \frac{1}{2} H_{xy}^z + \frac{1}{2} \sum_{(z,w)} (G_{zz}H_{xy}^{z} + G_{ww}H_{xy}^{w} - 2G_{zw}H_{xy}^{z}H_{xy}^{w}).$$  \hfill (53)
and
\[ c_{22}^{\text{H}} = -\frac{1}{8} (G_{xx}^2 + G_{yy}^2) + \frac{1}{4} \sum_{\langle z, w \rangle} J_{zw} (H^z_{xy} H^w_{xy}) \]  

Order \( \beta^{-3} \): there are contributions proportional to \( N - 1, (N - 1)^2 \) and \( (N - 1)^3 \),

\[ c_{31} = -\frac{1}{2} \left[ G_{xx}^3 + G_{yy}^3 - G_{xy}(G_{xx} + G_{yy}) \right] - \frac{1}{2} \sum_{z, w} G_{zw} H^z_{xy} H^w_{xy} \]
\[-\frac{1}{2} \sum_{z} (2 G_{zx} H^x_{xy} + G_{zz} G_{xx} - G_{yy} G_{yz} - 2 G_{xy} G_{zz} G_{yz}) \]
\[-\frac{1}{4} \sum_{\langle z, w \rangle} \left\{ \left[ 2 G_{zx} G_{xx} Q^w_{xz} - 2 G_{xy} G_{zz} Q^w_{yz} + G_{zw} (G_{zz} + G_{ww}) H^z_{xy} H^w_{xy} \right. \right. \]
\[ \left. \left. + \frac{1}{4} R^z_{xy} \right] + \frac{1}{2} P^z_{xy} + (-3 G_{zz}^2 + G_{zw}^2) H^z_{xy} + (z \leftrightarrow w) \right\} \]
\[ + \frac{1}{8} \sum_{\langle z, w \rangle, p} \left\{ \left[ 4 H^z_{xy} H^p_{xy} Q^w_{zp} + (G_{zp} H^z_{xy} - G_{wp} H^w_{xy})^2 \right] + (z \leftrightarrow w) \right\} + (x \leftrightarrow y) \]
\[ -\frac{1}{4} \sum_{\langle z, w \rangle, \langle p, q \rangle} \left\{ \left[ \left[ H^z_{xy} H^p_{xy} (G_{zz} Q^q_{zp} - G_{zw} Q^w_{zp} - G_{zp} R^q_{zp} + G_{wp} P^q_{zp}) \right. \right. \right. \]
\[ \left. \left. \left. + H^z_{xy} G_{zp} (H^w_{xy} Q^q_{zp} + H^w_{xy} Q^q_{zp}) \right] + (p \leftrightarrow q) \right\} + (z \leftrightarrow w) \right\} + (x \leftrightarrow y) \right\} \]
\[ + \frac{1}{8} \sum_{\langle z, w \rangle, p} \left\{ \left[ 2 H^z_{xy} H^p_{xy} J_{zw} + (G_{zp} - G_{wp}) H^z_{xy} \right] + (z \leftrightarrow w) \right\} + (x \leftrightarrow y) \]
\[ -\frac{1}{8} \sum_{\langle z, w \rangle, \langle p, q \rangle} \left\{ \left[ H^z_{xy} J_{zw} (G_{pp} (R^q_{zp} + G_{zp} - G_{wp}) + G_{pq} Q^z_{zp}) - H^z_{xy} H^w_{xy} G_{pp} Q^p_{zp} \right. \right. \]
\[ \left. \left. + H^z_{xy} H^p_{xy} (J_{zw} J_{pq} + G_{zz} G_{pp} - G_{ww} G_{qq}) \right. \right. \]
\[ \left. \left. - J_{zw} G_{pq} G_{zz} - J_{pq} G_{zw} G_{wp} \right] \right\} + (p \leftrightarrow q) + (z \leftrightarrow w) \right\} + (x \leftrightarrow y) \right\}. \]
Finally, the $O(\beta^{-3})$ contribution proportional to $(N-1)^3$ reads

$$c_{33}^{\text{H.}} = -\frac{1}{16} J_{zy}^2 (G_{xz} + G_{yy})$$

$$+ \frac{1}{32} \sum_{(z, w)} \left\{ J_{zy} J_{zw} R_{zy}^{zw} + (-J_{zw}^2 - 2G_{zz}^2 + 2G_{ww}^2) H_{xy}^2 + (z \leftrightarrow w) \right\} (x \leftrightarrow y)$$

$$- \frac{1}{16} \sum_{(z, w), (p, q)} \left\{ \left( J_{pq} H_{z}^z (H_{xy}^p G_{zp} J_{zw} + H_{xy}^z R_{zw}^{pq}) \right) \right.$$  

$$\left. + (p \leftrightarrow q) + (z \leftrightarrow w) \right\} (x \leftrightarrow y).$$

(57)

### 4.3 Hasenfratz terms

Hasenfratz terms, in our notation, come suppressed by powers of the volume $V$ of the system. They should be included for PBC and FBC, to deal properly with the rotation zero-mode of the vacuum manifold.

We list all Hasenfratz contributions which do not identically vanish.

Order $\beta^{-2}$: there is a contribution proportional to $(N-1)^2$.

$$c_{22}^{\text{H.}} = \frac{1}{2V} \sum_z H_{xy}^{z,2}$$

(58)

Order $\beta^{-3}$: contributions to $c_{32}$ and $c_{33}$.

$$c_{32}^{\text{H.}} = \frac{1}{2V} \sum_z \left\{ G_{zz} H_{xy}^z + G_{xx} G_{zz}^2 + G_{yy} G_{yz}^2 - 2 G_{xy} G_{xz} G_{yz} \right\}$$

$$+ \left( \frac{1}{2V^2} + \frac{1}{V} \right) \sum_{z, w} G_{zw} H_{xy}^z H_{xy}^w$$

$$- \frac{1}{2V} \sum_{(z, w), p} \left\{ 2H_{xy}^p (H_{xy}^z Q_{zp}^{zw} - H_{xy}^w Q_{wp}^{zw}) + (G_{zp} H_{xy}^z - G_{wp} H_{xy}^w)^2 \right\},$$

and

$$c_{33}^{\text{H.}} = \frac{1}{4V} \sum_z \left\{ G_{zz} H_{xy}^z + J_{zy} (G_{zz}^2 - G_{yz}^2) \right\}$$

$$+ \frac{1}{8V^2} \sum_{z, w} \left\{ G_{zz} H_{xy}^w + G_{ww} H_{xy}^z + 4G_{zw} H_{xy}^z H_{xy}^w \right\}$$

$$- \frac{1}{4V} \sum_{(z, w), p} \left\{ (G_{zp}^2 - G_{wp}^2)(H_{xy}^z - H_{xy}^w)^2 + 2 J_{zw} H_{xy}^p (G_{zp} H_{xy}^z - G_{wp} H_{xy}^w) \right\},$$

(60)
5 Results

C programs were written to compute the coefficients given by the above expressions for square lattices of sizes $2 \times 2$ through $120 \times 120$.

The main results were reported in [4], to wit: standard boundary conditions give rise to coefficients agreeing with each other in the infinite volume limit, while SIBC coefficients disagree with them in this limit, actually diverging at third order, as predicted in [2].

5.1 Standard boundary conditions

Figures 4 through 9 compare coefficients $c_1$, $c_{21}$, $c_{22}$, $c_{31}$, $c_{32}$ and $c_{33}$ for standard boundary conditions: FBC, PBC, DBC. Data is plotted only for lattices larger than $20 \times 20$ for ease of inspection, and the region $L \geq 100$ is showed separately.

The perturbative expansions for these boundary conditions can be shown to agree coefficient by coefficient in the thermodynamic limit, with limit values agreeing with [5]:

\[
\begin{align*}
\lim_{L \to \infty} & c^{F,P,D}_1 = -\frac{1}{4}, \\
\lim_{L \to \infty} & c^{F,P,D}_{21} = -\frac{1}{32}, \\
\lim_{L \to \infty} & c^{F,P,D}_{22} = 0, \\
\lim_{L \to \infty} & c^{F,P,D}_{31} = -0.00727, \\
\lim_{L \to \infty} & c^{F,P,D}_{32} = -0.006, \\
\lim_{L \to \infty} & c^{F,P,D}_{33} = 0.
\end{align*}
\]

(61)

5.2 SIBC: different thermodynamic limit

SIBC coefficients up to second order are plotted in figure 10. Their convergence is extremely slow compared with the previous cases. Yet their behaviour seems compatible with the conditions

\[
\begin{align*}
\lim_{L \to \infty} & c^{SI}_1 = -\frac{1}{4}, \\
\lim_{L \to \infty} & c^{SI}_{21} + c^{SI}_{22} = -\frac{1}{32},
\end{align*}
\]

(62)

necessary for the agreement, as $L \to \infty$, of the perturbative expansion of the Abelian ($N = 2$) model with the corresponding expansion for standard boundary conditions. This agrees with the results of [1], which used another method.

5.3 SIBC: infrared divergence at third order

Third order coefficients for SIBC are plotted, this time as a function of $\log L$, in figure 11. Both $c_{32}$ and $c_{33}$ are seen to diverge (logarithmically in $L$), a phenomenon predicted in [2]. The behaviour of $c_{31}$ is unclear, but the curve also
Figure 4: $c_1$ as a function of $L$ for FBC, PBC and DBC, and blow-up of the $L \geq 100$ region.
Figure 5: \( c_{21} \) as a function of \( L \) for FBC, PBC and DBC, and blow-up of the \( L \geq 100 \) region.
Figure 6: $c_{22}$ as a function of $L$ for FBC, PBC and DBC, and blow-up of the $L \geq 100$ region.
Figure 7: $c_{31}$ as a function of $L$ for FBC, PBC and DBC, and blow-up of the $L \geq 100$ region.
Figure 8: $c_{32}$ as a function of $L$ for FBC, PBC and DBC, and blow-up of the $L \geq 100$ region.
Figure 9: $c_{33}$ as a function of $L$ for FBC, PBC and DBC, and blow-up of the $L \geq 100$ region.
Figure 10: $c_1$, $c_{21}$ and $c_{22}$ as a function of $L$ for SIBC.
Figure 11: $c_{31}$, $c_{32}$ and $c_{33}$ as a function of log $L$ for SIBC.
suggests an infrared divergence. Thus, the $\beta^{-3}$ coefficient presumably diverges logarithmically in the infrared for all $N > 2$. However, the Abelian case $N = 2$ could yet prove convergent if the divergent parts of $c_{31}$, $c_{32}$ and $c_{33}$ cancel — in this case it would be interesting to check whether they agree with the corresponding coefficient with standard boundary conditions in the thermodynamic limit.

### 6 Conclusions and outlook

The perturbative expansion of observable $\langle \vec{S}_x \cdot \vec{S}_y \rangle$ for the vector O(N) model has been computed up to order $\beta^{-3}$ for different boundary conditions. Consistency of the usual infinite volume limit of the perturbative coefficients has been checked up to this order for standard boundary conditions (PBC, FBC, DBC). Divergence of the third order SIBC perturbative coefficient in the infrared limit, as predicted in [2], has been explicitly shown. It would be interesting to extend the analysis to larger lattice sizes (the current upper limit $L = 120$ was dictated by array storage requirements in available computers): the behaviour of the total $\beta^{-3}$ coefficient could have a thermodynamic limit for the Abelian case $N = 2$.

Expressions for Feynman diagrams have been computed exactly, and the $\pi$ propagator has been obtained exactly for all boundary conditions considered, using a method to diagonalise block tridiagonal matrices — computations being carried out by means of C programs. While the usefulness of this method depends critically on the particular boundary conditions used, a generalisation for other kinds of boundary conditions being thus unlikely, it is particularly well suited for exact computations in 2d rectangular systems. It could for instance prove useful to analyse the $1/N$ expansion of these models.

The long standing problem of the correct perturbative expansion of asymptotically free quantum field theories in the thermodynamic remains, all in all, unsolved. However much circumstantial evidence is gathered for the orthodox approach, for instance in the course of this work, a proof of the rule that standard boundary conditions provide the correct asymptotic series for these theories would be needed (which should involve a nonperturbative definition of the theories, since ‘asymptotic’ series need a definite function to be asymptotic to!).

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