pilot

Non-linear σ models on the lattice

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28th May 2020

Contents

1. Introduction

TO DO: Critical slowing down, brief intro to nl sigma models

$O(N)$ models

The $O(N)$ non-linear σ models are class of two-dimensional theories of real, N-dimensional fields $\sigma = (\sigma^1, \sigma^2, \ldots, \sigma^N)$, defined by the action

$$S = \frac{1}{2g} \int d^2x \, \partial_\mu \sigma(x) \cdot \partial_\mu \sigma(x) \tag{1}$$

together with the constraint

$$\sigma(x) \cdot \sigma(x) = 1 \tag{2}$$

CP^{N-1} models

The CP^{N-1} models are a class of two-dimensional theories of complex N-component fields $z = (z^1, z^2, \ldots, z^N)$, defined by the action

$$S = \frac{1}{g} \int d^2x (D_\mu z)^* \cdot (D_\mu z) \tag{3}$$

together with the constraint

$$z^*(x) \cdot z(x) = 1 \tag{4}$$

$D_\mu = \partial_\mu + iA_\mu$ is the usual covariant derivative due to a local $U(1)$ symmetry.

The gauge field is

$$A_\mu = \frac{i}{2}\big(z^* \cdot \partial_\mu z - (\partial_\mu z^*) \cdot z\big) \tag{5}$$

2. Preliminaries

2.1 Notation

The notation used to identify lattice positions and directions will be:

- A subscript n, m labels lattice sites, the total number of which is V. A sum over lattice sites is written as $\sum_n \equiv \sum_{n=1}^{V}$.
- Greek letters $\mu, \nu \ldots$ label lattice dimensions, with $\hat{\mu}$ representing a unit vector (in units of a) in the dimension μ. A sum over lattice dimensions is written as $\sum_\mu \equiv \sum_{\mu=1}^{d}$ where d is always 2.
- We will not adopt any special notation to denote a vector quantity. However, a vector (or multiplet) σ, z, ... is distinguished from its components $(\sigma^1, \sigma^2, \ldots)$, z^i, ... by the absence of a superscript number or Latin letter i, j.
- A subscript a, b labels field configurations in an ensemble, the total number of which is denoted N_{ens}.
- $\langle F \rangle$ denotes the ensemble average of F, which is defined by

$$\langle F \rangle \equiv \frac{1}{N_{\text{ens}}} \sum_{a=1}^{N_{\text{ens}}} F_a$$

2.2 Lattice

We will work exclusively with a two-dimensional tetragonal lattice of dimensions (aL, aL), where a is the lattice spacing.

For convenience, we will universally define $a \equiv 1$, so that the lattice length L and volume V count, respectively, the number of lattice sites along a single dimension and in the entire lattice.

The discrete versions of derivatives, for $a = 1$, are:

$$\delta_\mu f_n = f_{n+\hat{\mu}} - f_n \qquad \text{(forward difference operator)}$$
$$\delta^*_\mu f_n = f_n - f_{n-\hat{\mu}} \qquad \text{(backward difference operator)}$$
$$\bar{\delta}_\mu f_n = \frac{1}{2}\big(f_{n+\hat{\mu}} - f_{n-\hat{\mu}}\big) \qquad \text{(central difference operator)}$$

One possibility for the discrete Laplacian, which is Hermitian, is given by

$$\delta^2 f_n = \sum_\mu \delta^*_\mu \delta_\mu f_n = \sum_\mu \left(f_{n+\hat{\mu}} + f_{n-\hat{\mu}} - 2f_n \right) \tag{6}$$

As in the continuum, plane waves are eigenvectors of the Laplacian. However, the eigenvalues are different:

$$\delta^2 e^{ik\cdot x} = -\hat{k}^2 e^{ik\cdot x} \qquad\qquad \hat{k}_\mu = 2\sin\frac{k_\mu}{2} \tag{7}$$

For a function $F(x)$, the Fourier transform is

$$\tilde{F}(k) = \int \frac{d^d x}{(2\pi)^d} e^{ik\cdot x} F(x) \tag{8}$$

On a lattice, this becomes

$$\tilde{F}(k) = \frac{1}{V} \sum_x e^{ik\cdot x} F(x) \tag{9}$$

2.3 Observables

We consider the *connected* two point correlation function $G(x)$ as the basic building block for computing observables. Occasionally, we will refer to the *disconnected* version, which will have a subscript: $G(x)_{\text{disconn}}$.

We will be dealing with lattice field theories which possess translational and rotational invariance along the lattice dimensions.

Translation invariance means that observables should be independent of lattice position n in limit of infinite ensemble size. We may as well, therefore, choose to take the volume average of observables which have a dependence on n, such as the two point correlator: $G(x) = \frac{1}{V}\sum_n G(n, x)$.

In the same vein, rotational invariance means that, where an observable depends on the lattice sites on one particular dimension, we may as well average over all lattice dimensions. In particular, we do not designate a particular dimension as the time dimension, so any observable defined for a time slice will be averaged over each dimension.

2.4 Generalised spherical coordinates

Given that the non-linear σ models come with a unit norm constraint, parameterising the fields using generalised spherical coordinates [?] can be useful since the constraint is built in.

For the $O(N)$ models the parameterisation looks like:

$$\begin{aligned}
\sigma^1 &= \cos\phi^1 \\
\sigma^2 &= \sin\phi^1 \cos\phi^2 \\
\sigma^3 &= \sin\phi^1 \sin\phi^2 \cos\phi^3 \\
&\vdots \\
\sigma^{N-1} &= \sin\phi^1 \ldots \sin\phi^{N-2} \cos\phi^{N-1} \\
\sigma^N &= \sin\phi^1 \ldots \sin\phi^{N-1}
\end{aligned} \tag{10}$$

with the angles taking values in the range $\phi^1, \ldots, \phi^{N-2} \in [0, \pi], \phi^{N-1} \in [0, 2\pi)$.

In the CP^{N-1} case things are slightly different. Let us fix the gauge so that the N^{th} component of the field is real:

$$z = \begin{pmatrix} x^1 + ix^{N+1} \\ x^2 + ix^{N+1} \\ \vdots \\ x^{N-1} + ix^{2N-1} \\ x^N \end{pmatrix} \tag{11}$$

The x can then be parameterised using generalised spherical coordinates:

$$\begin{aligned}
x^1 &= \cos\phi^1 \\
x^2 &= \sin\phi^1 \cos\phi^2 \\
x^3 &= \sin\phi^1 \sin\phi^2 \cos\phi^3 \\
&\vdots \\
x^{D-2} &= \sin\phi^1 \ldots \sin\phi^{D-2} \cos\phi^{D-1} \\
x^{D-1} &= \sin\phi^1 \ldots \sin\phi^{D-1}
\end{aligned} \tag{12}$$

although this time there are $D = 2N-1$ angles, taking values in the range $\phi_1, \ldots, \phi_{D-2} \in [0, \pi], \phi^{D-1} \in [0, 2\pi)$.

3. Lattice actions

3.1 $O(N)$ action

The action can be discretised using the forward derivative, $\partial_\mu \sigma(x) \to \delta_\mu \sigma_n = \sigma_{n+\hat{\mu}} - \sigma_n$

$$\begin{aligned} S &= \frac{1}{2g} \sum_n \sum_\mu \delta_\mu \sigma_n \cdot \delta_\mu \sigma_n \\ &= -\frac{1}{g} \sum_n \sum_\mu \left(\sigma_{n+\hat{\mu}} \cdot \sigma_n - 1 \right) \end{aligned} \tag{13}$$

This has the same form as the Hamiltonian for a lattice of classical N-dimensional spin vectors with pure nearest-neighbour ferromagnetic interactions.

$$H_{\text{spin}} = -\sum_n \sum_\mu \sigma_{n+\hat{\mu}} \cdot \sigma_n \tag{14}$$

To relate them, we relabel the coupling $\frac{1}{g} \equiv \beta$, with β labelling, as is convention, the inverse temperature of the spin system. Then,

$$S = \beta H_{\text{spin}} + 2\beta V \tag{15}$$

The global shift of $2\beta V$ does not affect the dynamics of the system.

3.2 $O(2)$ action

Since the N-dimensional σ fields take values on the unit $(N-1)$-sphere, it can be convenient to use generalised spherical coordinates to parameterise them in terms of $N-1$ angles.

The $O(2)$ fields live on a circle and a parameterised by a single 'polar' angle θ.

$$\sigma_{O(2)} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \qquad \theta \in [0, 2\pi) \tag{16}$$

$$S_{O(2)} = -\beta \sum_n \sum_\mu \Big(\cos\theta_{n+\hat{\mu}} \cos\theta_n + \sin\theta_{n+\hat{\mu}} \sin\theta_n - 1 \Big)$$
$$= -\beta \sum_n \sum_\mu \Big(\cos(\theta_{n+\hat{\mu}} - \theta_n) - 1 \Big) \tag{17}$$

3.3 $O(3)$ action

For $O(3)$ we have the standard parameterisation of a unit sphere, in terms of polar angle θ and 'azimuthal' angle ϕ.

$$\sigma_{O(3)} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \qquad \theta \in [0,\pi],\ \phi \in [0, 2\pi) \tag{18}$$

$$S_{O(3)} = -\beta \sum_n \sum_\mu \Big(\cos\theta_{n+\hat{\mu}} \cos\theta_n + \sin\theta_{n+\hat{\mu}} \sin\theta_n \cos(\phi_{n+\hat{\mu}} - \phi_n) - 1 \Big) \tag{19}$$

3.4 CP^{N-1}: implicit gauge field

There are several possible CP^{N-1} lattice actions. The simplest choice is

$$S = -\frac{N}{g} \sum_n \sum_\mu \Big(\left| z^*_{n+\hat{\mu}} \cdot z_n \right|^2 - 1 \Big) \tag{20}$$

which clearly bears much resemblance to the $O(N)$ action.

In fact, for $N = 2$ this action is equivalent to the $O(3)$ lattice action given by eq. 13, up to a factor of $1/2$ in the coupling. We will sometimes denote the coupling by $\frac{N}{g} \equiv \beta$ to make contact with classical spin systems.

3.5 CP^1: implicit gauge field

A simple parameterisation for CP^1 is

$$z = \begin{pmatrix} \cos\frac{\theta}{2} e^{i\phi/2} \\ \sin\frac{\theta}{2} e^{-i\phi/2} \end{pmatrix} \tag{21}$$

with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$, yields a simple form for the action in terms of the polar angles:

$$S = -\frac{2}{g} \sum_n \sum_\mu \left(\cos\theta_n \cos\theta_{n+\mu} + \sin\theta_n \sin\theta_{n+\mu} \cos(\phi_n - \phi_{n+\mu}) - 1 \right) \tag{22}$$

which is the same as the $O(3)$ action in eq. 19 with $\beta = \frac{2}{g}$.

4. MCMC implementations

4.1 Local updates: $O(N)$

A local update comprises an alteration of the field variable at a single lattice site. Since the action is also local, we can efficiently compute the change in action due to a local update, without recalculating it for the entire lattice.

Let us define the local magnetisation at a site n as

$$M_n = \sum_{\mu} \left(\sigma_{n+\hat{\mu}} + \sigma_{n-\hat{\mu}} \right) = \sum_{\pm\mu} \sigma_{n+\hat{\mu}} \tag{23}$$

where the final sum over nearest neighbours is expressed as a sum over both positive and negative directions for each dimension.

The change in action due to an update at lattice site n is then

$$\delta S = -\beta \, \delta\sigma_n \cdot M_n \tag{24}$$

For $O(2)$ in terms of the polar angle this is

$$\delta S_{O(2)} = -\beta \sum_{\pm\mu} \Big(\cos(\theta_{n+\hat{\mu}} - \theta'_n) - \cos(\theta_{n+\hat{\mu}} - \theta_n) \Big) \tag{25}$$

4.2 Random walk Metropolis: $O(2)$

For $O(2)$, the most efficient approach is to work with the polar angle. We can tune the algorithm by choosing the maximum change in angle for a single proposal. The tunable parameter is denoted $\delta_{\mathsf{max}} \in [0, 1]$ and gives the fraction of the largest possible change.

The algorithm is then

Random walk Metropolis: $O(2)$

1. Randomly select a lattice site n
2. Generate a random number x from $[0, 1]$
3. Generate a proposal: $\theta'_n = \theta_n + (x - \frac{1}{2})\pi\delta_{\text{max}}$
4. Evaluate eq. 25 to obtain δS
5. Accept the proposal with probability $\exp(-\delta S)$
6. Return to step 1.

4.3 Random walk Metropolis: $O(3)$

For $O(3)$, we could also work with the spherical polar representation. However, the combination of the slightly more complicated action, and the fact that the parameterisation induces a Jacobian factor of $\sin\theta$ which needs to be accounted for in the Metropolis step, means it is more convenient to work with the spin vectors and rotation matrices.

The method for generating restricted $O(3)$ rotations is given as an appendix. To summarise, the spin vector is represented as a rotation matrix acting on a unit vector in the $\mathbf{z}$ direction. The proposal is generated by rotating the $\mathbf{z}$ axis and then re-applying the rotation matrix.

Random walk Metropolis: $O(3)$

1. Randomly select a lattice site n
2. Calculate its representation as a rotation matrix $R_{\theta\phi}$ acting on $\mathbf{z} = (0, 0, 1)$
3. Generate two random numbers x, y from $[0, 1]$
4. Use x, y to get a polar angle $0 \leq \gamma \leq \pi\delta_{\text{max}}$ and azimuthal angle $0 \leq \alpha < 2\pi$.
5. Rotate the coordinate system $\mathbf{z} \to \mathbf{z}'$ using α, γ
6. Generate a proposal: $\sigma'_n = R_{\theta\phi}\mathbf{z}'$
7. Evaluate eq. 24 to obtain δS
8. Accept the proposal with probability $\exp(-\delta S)$
9. Return to step 1.

4.4 Random walk Metropolis: $O(N)$

Generating restricted rotations in arbitrary dimensions is a generalisation of the $O(3)$ case. However, it becomes computationally expensive fairly quickly.

If we are willing to accept unrestricted rotations, there is an algorithm which generates $O(N)$ rotations (according to their Harr measure). We may not be able to tune the acceptance rate, but as a brute force approach this will work.

4.5 Heat bath: $O(2)$

TO DO:

4.6 Heat bath: $O(3)$

This closely resembles the Metropolis algorithm for $O(3)$, except that we generate restricted rotations according to the Gibbs measure and do away with the Metropolis acceptance step.

Instead of rotating the current spin vector, we take $\hat{M}_n$ as a reference vector and generate restricted rotations of this.

The azimuthal angle α which rotates the coordinate system $\mathbf{z} \to \mathbf{z}'$ is once again unconstrained. However, the polar angle should be generated according to

$$\cos\gamma = \frac{1}{\beta|M_n|}\log\left[(1-x)e^{\beta|M_n|} + x\,e^{-\beta|M_n|}\right] \tag{26}$$

where x is drawn from the standard uniform distribution $[0,1]$.

Heat bath: $O(3)$

1. Randomly select a lattice site n
2. Calculate the local magnetisation M_n, and the representation of $\hat{M}_n$ as a rotation matrix $R_{\theta\phi}$ acting on $\mathbf{z} = (0, 0, 1)$
3. Generate two random numbers x, y from $[0, 1]$
4. With y, obtain an azimuthal angle α from $[0, 2\pi]$
5. With x, obtain $\cos\gamma$ from eq. 26
6. Rotate the coordinate system $\mathbf{z} \to \mathbf{z}'$ using α, γ
7. Update the spin: $\sigma'_n = R_{\theta\phi}\mathbf{z}'$
8. Return to step 1.

5. Observables

5.1 Two point correlation functions

5.1.1 Two point correlator: $O(N)$

The two point correlation function is given by

$$G(n,x) = \langle \sigma_{n+x} \cdot \sigma_n \rangle = \frac{1}{N_{\text{ens}}} \sum_{a=1}^{N_{\text{ens}}} \sigma_{n+x,a} \cdot \sigma_{n,a} \tag{27}$$

Since $\langle \sigma \rangle = \vec{0}$, this is a connected correlation function.

Making use of the translation symmetry of eq. 13, we define the volume average of this quantity

$$G(x) = \frac{1}{V} \sum_n G(n,x) \tag{28}$$

Let us also make use of translational invariance to define the volume-averaged *disconnected*[1] two-point correlation function, which is defined for a single field 'a' rather than for an ensemble

$$G_V(x\,;a) = \frac{1}{V} \sum_n \sigma_{n+x,a} \cdot \sigma_{n,a} \tag{29}$$

This is a useful quantity since it allows us to study autocorrelations between field configurations generated with an MCMC algorithm, at different length scales.

In the interest of eliminating duplicated calculations, we can use the fact that

$$G(x) = \langle G_V(x) \rangle \tag{30}$$

5.1.2 Two point correlator: CP^{N-1}

CP^{N-1} observables are often defined in terms of the outer product

$$P_n \equiv z_n^* \otimes z_n \tag{31}$$

[1] The volume-average of σ is generally non-zero, so this is not a connected correlation function.

The disconnected correlation function is given by

$$G(n,x) = \langle \mathrm{Tr}\, P_{n+x} P_n \rangle = \langle |z^*_{n+x} \cdot z_n|^2 \rangle = \frac{1}{N_{\mathsf{ens}}} \sum_{a=1}^{N_{\mathsf{ens}}} |z^*_{n+x,a} \cdot z_{n,a}|^2 \tag{32}$$

where we have used the trace property $\mathrm{Tr}\, AB = \sum_i (AB)_{ii} = \sum_i \sum_j A_{ij} B_{ji}$.

The connected correlator is just $G(n,x) - 1$ since $\langle \mathrm{Tr}\, P_n \rangle = \langle z^*_n \cdot z_n \rangle = \langle 1 \rangle$.

As in the $O(N)$ case, we define

$$G_V(x\,;a) = \frac{1}{V} \sum_n |z^*_{n+x,a} \cdot z_{n,a}|^2 \tag{33}$$

$$G(x) = \frac{1}{V} \sum_n G(n,x) = \langle G_V(x) \rangle \tag{34}$$

5.1.3 Fourier space correlator

The Fourier transform of $G(x)$ on a periodic lattice is

$$\tilde{G}(k) = \frac{1}{V} \sum_x e^{ik\cdot x}\, G(x) \tag{35}$$

where $k = \frac{2\pi \mathrm{n}}{L}$ take discrete values in the first Brillouin zone, labelled by integers $\mathrm{n} = -\frac{L}{2}, -\frac{L}{2}+1, \ldots, \frac{L}{2}-1$.

5.2 Two point observables

5.2.1 Susceptibility

The susceptibility is given by the Fourier space correlator at zero momentum:

$$\chi = \tilde{G}(0) = \frac{1}{V} \sum_x G(x) \tag{36}$$

5.2.2 Ising energy density

The average of correlators at unit separation measures the energy density associated with a Hamiltonian that contains purely nearest-neighbour interactions. This is often called

the 'Ising energy density'.

$$E_{\text{ising}} = \frac{1}{d}\sum_{\mu} G(\hat{\mu}) \tag{37}$$

5.2.3 Zero momentum correlator

If we interpret one of the lattice dimensions as a time dimension, we can define a Fourier transformed correlator in each 'time slice'.

$$\tilde{G}(\vec{k}, t) = \frac{1}{L^{d-1}}\sum_{\vec{x}} e^{i\vec{k}\cdot\vec{x}}\, G(\vec{x}, t) \tag{38}$$

where $\vec{x}$ denotes the $d-1$ spatial dimensions (although this is just a single dimension in the $d = 2$ case).

The zero momentum correlator refers to the $\vec{k} = \vec{0}$ case. We will take advantage of rotational symmetry and define this as a dimensional average.

$$\tilde{G}_{\vec{0}}(t) = \frac{1}{d}\big(\tilde{G}(\vec{0}, t) + \tilde{G}(0, \ldots, t, 0) + \ldots + \tilde{G}(0, t, \ldots, 0) + \tilde{G}(t, \vec{0})\big) \tag{39}$$

5.2.4 Effective pole mass

For a periodic lattice, an effective pole mass can be defined by

$$m_p(t) = \cosh^{-1}\left(\frac{\tilde{G}_{\vec{0}}(t-1) + \tilde{G}_{\vec{0}}(t+1)}{2\tilde{G}_{\vec{0}}(t)}\right) \tag{40}$$

The quantity $m_p(t)^{-1}$ is also an estimator for the exponential correlation length. See appendix for details.

5.2.5 Second-moment correlation length

The second-moment correlation length can be defined for lattice two point correlators as

$$\xi^2_{(2m)} = \frac{1}{2d}\frac{\sum_x x^2\, G(x)}{\sum_x G(x)} \tag{41}$$

See appendix for details.

5.2.6 Low-momentum approximations for the correlation length

These definitions should coincide with the second-moment correlation length in the limit $V \to \infty$.

$$\xi^2_{(a)} = \frac{1}{d} \sum_{\mu} \frac{L_\mu^2}{(2\pi)^2} \left(1 - \frac{\mathbb{R}\mathrm{e}\, \tilde{G}(2\pi/L_\mu)}{\tilde{G}(0)} \right) \tag{42}$$

$$\xi^2_{(b)} = \frac{1}{d} \sum_{\mu} \frac{1}{4\sin^2(\pi/L_\mu)} \left(\frac{\tilde{G}(0)}{\mathbb{R}\mathrm{e}\, \tilde{G}(2\pi/L_\mu)} - 1 \right) \tag{43}$$

The notation $\tilde{G}(2\pi/L_\mu)$ means to imply that the μ^{th} component of the momentum vector is $2\pi/L_\mu$, and all other components are zero.

See appendix for details.

5.3 Classical spin observables

As previously mentioned, we can interpret σ as N-dimensional classical spin vectors. In the classical spin context, we can define observables as functions of the spin Hamiltonian and squared magnetisation, which are defined by

$$H_{\mathsf{spin}} = -\sum_n \sum_\mu \sigma_{n+\hat{\mu}} \cdot \sigma_n \qquad\qquad M^2 = \sum_n \sum_m \sigma_m \cdot \sigma_n$$

5.3.1 Energy density

The energy density is defined as the expectation value of the Hamiltonian density:

$$\begin{aligned} E_{\mathsf{spin}} &= \frac{1}{V} \langle H_{\mathsf{spin}} \rangle \\ &= -\frac{1}{V} \frac{1}{N_{\mathsf{ens}}} \sum_{a=1}^{N_{\mathsf{ens}}} \sum_n \sum_\mu \sigma_{n+\hat{\mu},a} \cdot \sigma_{n,a} \\ &= -\sum_\mu G(\hat{\mu}) \end{aligned} \tag{44}$$

This should be equal to $-d$ times the Ising energy.

5.3.2 Magnetic susceptibility

The magnetic susceptibility is defined in an analogous way[2]

$$\begin{aligned}\chi_m &= \frac{1}{V}\langle M^2\rangle \\ &= \frac{1}{V}\frac{1}{N_{\text{ens}}}\sum_{a=1}^{N_{\text{ens}}}\sum_n\sum_m \sigma_{m,a}\cdot\sigma_{n,a} \\ &= \sum_x G(x) \\ &= \tilde{G}(0)\end{aligned} \tag{45}$$

This should be equal to the susceptibility defined previously.

5.3.3 Heat capacity

At the next order there is the specific heat capacity[3]

$$c = \frac{\beta^2}{V}\Big[\langle H^2_{\text{spin}}\rangle - \langle H_{\text{spin}}\rangle^2\Big] = \beta^2\frac{\langle H^2_{\text{spin}}\rangle}{V} - \beta^2 V E^2_{\text{spin}} \tag{46}$$

5.4 Definitions involving the $O(N)$ action

The $O(N)$ lattice action is

$$S = \frac{\beta}{2}\sum_n\sum_\mu \delta_\mu\sigma_n\cdot\delta_\mu\sigma_n = -\beta\sum_n\sum_\mu\big(\sigma_{n+\hat{\mu}}\cdot\sigma_n - 1\big)$$

[2]This is also equivalent to the definition in ref. [**?**], which is $\chi_m = \frac{1}{V}\sum_n\sum_m\langle\sigma_m\cdot\sigma_n\rangle$, by just swapping the order of sums.

[3]The factors of β in the definition stem from the fact that the heat capacity is conventionally defined as a derivative of with respect to temperature, the inverse of β. To be explicit, $c = \frac{1}{V}\frac{\partial E_{\text{spin}}}{\partial T} = \frac{\beta^2}{V}\frac{\partial^2}{\partial\beta^2}\log\mathcal{Z}$

5.4.1 Alternative definition of energy density

Another definition of energy density, found in e.g. ref. [?]

$$\begin{aligned} E_{\text{deriv}} &= \frac{1}{V}\sum_{n}\sum_{\mu}\langle \delta_\mu \sigma_n \cdot \delta_\mu \sigma_n \rangle \\ &= \frac{2}{\beta V}\langle S \rangle \\ &= 2E_{\text{spin}} + 4 \end{aligned} \tag{47}$$

5.4.2 Equivalent definition of heat capacity

Eq. 46 is simply the variance of the $O(N)$ action, divided by volume.

$$c = \frac{1}{V}\Big[\langle S^2 \rangle - \langle S \rangle^2\Big] \tag{48}$$

5.5 Topological observables

5.5.1 Charge density: geometrical, $O(3)$

A geometrical definition of topological charge density q for the $O(3)$ non-linear σ model on the $d = 2$ lattice was provided by Berg and Luscher in [?]. The general intuition is that the topological charge for a field configuration should count the number of times the field 'wraps around' the unit 2-sphere.

The charge density is defined for sites n^* on the 'dual lattice' – a point on the dual lattice is the midpoint of a square whose corners are adjacent sites on the lattice – and is a function of the four σ's surrounding n^*. By imagining that the four spin vectors define points on the same unit 2-sphere, we can interpret the surface area enclosed by geodesic paths connecting the points as a measure of topological charge density. TO DO: Diagram, types of magnetic skyrmions.

The definition consists of the following set of equations. Firstly,

$$q_{n^*} = \frac{1}{4\pi}\Big(\Delta(\sigma_n, \sigma_{n+\hat{\mu}_1}, \sigma_{n+\hat{\mu}_1+\hat{\mu}_2}) + \Delta(\sigma_n, \sigma_{n+\hat{\mu}_1+\hat{\mu}_2}, \sigma_{n+\hat{\mu}_2})\Big) \tag{49}$$

defines the topological charge density in terms of a function of three of the four spins

surrounding n^*. The function $\Delta(\vec{a},\vec{b},\vec{c})$ is the *signed*[4] area of a (unit radius) spherical triangle with corners given by the vectors $\vec{a},\vec{b},\vec{c}$.

If we instead parameterise Δ by three angles on the surface of the 2-sphere,

$$\begin{aligned}\cos\alpha &= \vec{a}\cdot\vec{b}\\ \cos\beta &= \vec{b}\cdot\vec{c}\\ \cos\gamma &= \vec{c}\cdot\vec{a}\end{aligned}$$

then Δ is given very simply by

$$\Delta(\alpha,\beta,\gamma) = \pm(\alpha+\beta+\gamma-\pi) \tag{50}$$

with the sign given by the sign of $\vec{a}\cdot(\vec{b}\times\vec{c}) = \sin\beta$.

In terms of the vectors, Δ may be given explicitly, including the sign, by

$$\exp\left(i\frac{\Delta(\vec{a},\vec{b},\vec{c})}{2}\right) = \frac{1+\vec{a}\cdot\vec{b}+\vec{b}\cdot\vec{c}+\vec{c}\cdot\vec{a}+i\vec{a}\cdot(\vec{b}\times\vec{c})}{\left[2(1+\vec{a}\cdot\vec{b})(1+\vec{b}\cdot\vec{c})(1+\vec{c}\cdot\vec{a})\right]^{1/2}} \tag{51}$$

This leads to

$$\Delta(\vec{a},\vec{b},\vec{c}) = 2\tan^{-1}\left(\frac{\vec{a}\cdot(\vec{b}\times\vec{c})}{1+\vec{a}\cdot\vec{b}+\vec{b}\cdot\vec{c}+\vec{c}\cdot\vec{a}}\right) \tag{52}$$

Since we always take the smaller of the two possible spherical triangles, we require that $\Delta(\vec{a},\vec{b},\vec{c}) \in (-2\pi, 2\pi)$, with extremal values corresponding to half of the surface area of the sphere being enclosed. However, note that eq. 52 runs into problems when two of the vectors lay on a great circle.

An important technical point is that we must use the variant of the $\tan^{-1}$ function, known as *arctan2*, which maps values to $(-\pi,\pi)$.

5.5.2 Charge density: geometrical, CP^{N-1}

For CP^{N-1} the geometrical approach results in the following definition of lattice topological charge density [?]

$$q_{n^*} = \frac{1}{2\pi}\,\mathbb{I}\mathrm{m}\left[\log\mathrm{Tr}(P_{n+\hat{\mu}+\hat{\nu}}P_{n+\hat{\mu}}P_n) + \log\mathrm{Tr}(P_{n+\hat{\nu}}P_{n+\hat{\mu}+\hat{\nu}}P_n)\right] \tag{53}$$

[4]This is just so that 'winds' in opposite directions cancel out rather than add. It helps to picture the case for $\mathbb{S}^1$.

5.5.3 Charge

Topological charge is defined in terms of the charge density by

$$Q = \sum_{n^*} q_{n^*} \tag{54}$$

5.5.4 Susceptibility

Hence, the topological susceptibility is

$$\chi_t = \frac{1}{V}\langle Q^2 \rangle \tag{55}$$

5.6 Deterministic approach for small lattices

TO DO:

6. Appendices

6.1 Generating restricted $O(3)$ rotations

To generate restricted $O(3)$ rotations is a two-step process. First, we can represent a spin vector as a rotation matrix acting on $\hat{\mathbf{z}} = (0, 0, 1)$:

$$\sigma = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} = \begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{56}$$

These components can be calculated as

$$\cos\theta = \sigma^3 \tag{57}$$

$$\sin\theta = \sqrt{1 - \cos^2\theta} \tag{58}$$

$$\cos\phi = \sigma^1 / \sin\theta \tag{59}$$

$$\sin\phi = \sigma^2 / \sin\theta \tag{60}$$

The next step is to apply a random, restricted rotation $\hat{\mathbf{z}} \to \hat{\mathbf{z}}'$, which effectively amounts to rotating the coordinate system. The $\hat{\mathbf{z}}'$ can be made to be arbitrarily close to $\hat{\mathbf{z}}$ by generating a new polar angle $0 \leq \gamma \leq \pi\delta_{\mathsf{max}}$, and azimuthal angle $0 \leq \alpha < 2\pi$. By applying the matrix representation of σ to $\hat{\mathbf{z}}'$, we end up with a vector that is a restricted rotation of σ.

$$\sigma' = \begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} \sin\gamma\cos\alpha \\ \sin\gamma\sin\alpha \\ \cos\gamma \end{pmatrix} \tag{61}$$

6.2 Correlation lengths

The exponential correlation length ξ marks a transition between power law and exponential behaviour in the two point correlation function. For separations much larger than the correlation length,

$$G(x) \sim \frac{e^{-|x|/\xi}}{|x|^{\vartheta}} \qquad\qquad |x| \gg \xi \tag{62}$$

where ϑ is an exponent which depends on the system under study; for Gaussian models (at most quadratic in the fields and their derivatives), $\vartheta = \frac{d-1}{2}$.

The second-moment correlation length, defined by

$$\xi^2_{(2m)} = C\frac{\int d^d x\, x^2\, G(x)}{\int d^d x\, G(x)} \tag{63}$$

can be shown to coincide with ξ^2 for a suitable proportionality constant C, by switching to spherical coordinates and performing the one-dimensional integral over $|x|$ by parts. For one-dimensional Gaussian systems ($\vartheta = 0$), $C = \frac{1}{2}$.

We can note that $\xi^2_{(2m)}$ may equivalently be expressed as

$$\xi^2_{(2m)} = -\frac{C}{\tilde{G}(0)}\frac{\partial^2}{\partial k^2}\tilde{G}(k)\bigg|_{k_\mu=0} \tag{64}$$

A related quantity is the 'physical' or 'pole' mass, resulting from the pole of the propagator at zero spatial momentum (the 'wall-wall' propagator).

$$\tilde{G}(\vec{0}, t) \sim e^{-mt} \qquad\qquad t \gg m^{-1} \tag{65}$$

The reciprocal of the mass can be seen as a correlation length in one dimension.

Lattice definitions

This is all well and good for infinite systems, but we would like to be able to define a correlation length on a finite lattice, which matches ξ in the $V \to \infty$ limit.

We will take the constant of proportionality to be $(2d)^{-1}$ so that, when a dimensional average is taken over the lattice, the result is consistent with a one-dimensional Gaussian model.

The most obvious thing to do is replace eq. 63 with its discrete, finite volume analogue, although we must remember to account for periodic boundary conditions since the separation x appears explicitly.

$$\xi^2_{(2m)} = \frac{1}{2d}\frac{\sum_x x^2\, G(x)}{\sum_x G(x)} \tag{66}$$

Low momentum approximations to the correlation length

Another option is to take the discrete, finite volume analogue of eq. 64:

$$\begin{aligned}\xi^2_{(a)} &= -\frac{1}{2d\tilde{G}(0)}\sum_\mu \frac{\tilde{G}(2\pi/L_\mu)+\tilde{G}(-2\pi/L_\mu)-2\tilde{G}(0)}{(2\pi/L_\mu)^2} \\ &= \frac{1}{d}\sum_\mu \frac{L_\mu^2}{(2\pi)^2}\left(1-\frac{\mathbb{R}\mathrm{e}\,\tilde{G}(2\pi/L_\mu)}{\tilde{G}(0)}\right)\end{aligned} \tag{67}$$

The notation $\tilde{G}(2\pi/L_\mu)$ means to imply that the μ^{th} component of the momentum vector is $2\pi/L_\mu$, and all other components are zero. In the second line, we have used the fact that $\tilde{G}(-k)=\tilde{G}(k)^*$ since $G(x)$ is real.

Using the form of the lattice propagator $\tilde{G}(k)\propto\left(\sum_\mu \hat{k}_\mu^2+\xi^{-2}\right)^{-1}$ (where the proportionality hides renormalisation effects),

$$\frac{2\tilde{G}(0)}{\tilde{G}(2\pi/L_\mu)+\tilde{G}(-2\pi/L_\mu)} = \frac{\tilde{G}(0)}{\mathbb{R}\mathrm{e}\,\tilde{G}(2\pi/L_\mu)} = \xi^2\left(4\sin^2(\pi/L_\mu)+\frac{1}{\xi^2}\right) \tag{68}$$

Hence, we have a third expression for the correlation length:

$$\xi^2_{(b)} = \frac{1}{d}\sum_\mu \frac{1}{4\sin^2(\pi/L_\mu)}\left(\frac{\tilde{G}(0)}{\mathbb{R}\mathrm{e}\,\tilde{G}(2\pi/L_\mu)}-1\right) \tag{69}$$

Pole mass

On a periodic lattice with extent T in the time dimension, it can be shown that the zero-momentum correlator takes the following form (for a single particle, or in the long-t limit)

$$\tilde{G}(\vec{0},t)\sim e^{-mt}+e^{-m(T-t)} = 2e^{-m\frac{T}{2}}\cosh(mt') \tag{70}$$

with $t'\equiv\frac{T}{2}-t$.

We can obtain m as follows:

$$\begin{aligned}\frac{\tilde{G}(\vec{0},t+1)+\tilde{G}(\vec{0},t-1)}{2\tilde{G}(\vec{0},t)} &= \frac{\cosh\left(m(t'+1)\right)+\cosh\left(m(t'-1)\right)}{2\cosh(mt')} \\ &= \frac{2\cosh(mt')\cosh(m)}{2\cosh(mt')} \\ &= \cosh(m)\end{aligned} \tag{71}$$

The dimensional averaging has already been taken care of in the definition of the zero-momentum correlator.