`pilot` documentation

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10th May 2020

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2.1 The 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 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.

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

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

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

$$\tilde{F}(k) = \int \frac{d^d x}{(2\pi)^d} e^{ik\cdot x} F(x) \tag{1}$$

On a lattice, this becomes

$$\tilde{F}(k) = \frac{1}{V} \sum_x e^{ik\cdot x} F(x) \tag{2}$$

Translational symmetry. Ensemble averages can be then averaged over volume. Due to the translational symmetry of the theory, we expect $G(n, x)$ to be independent of the base lattice site n in the infinite-ensemble limit. We may as well, therefore, choose to define $G(x)$ as where we have chosen to define $G(x)$ so that it is also a volume-average on top of being an ensemble average. We may as well do this, since translational symmetry

means G depends only on separations (x) and not on absolute coordinates.

2.2 The fields

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.

2.3 Observables

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

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

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: $G(x)_{\mathsf{disconn}}$.

3. $O(N)$ non-linear σ models

3.1 Background

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

$$S = \frac{1}{2g} \int d^2x \, \partial_\mu \sigma(x) \cdot \partial_\mu \sigma(x) \tag{3}$$

together with the constraint

$$\sigma(x) \cdot \sigma(x) = 1 \tag{4}$$

The individual components of σ transform as space-time scalars. However, the constraint, which restricts the fields to take values on the $(N-1)$-dimensional unit sphere $\mathbb{S}^{N-1}$, means that, as a whole, σ transforms as an $O(N)$ multiplet.[1]

The action has a global $O(N)$ symmetry, but may otherwise strike you as being fairly uninteresting. However, if we absorb the constraint into the definition of the fields, so that $\sigma = (\tilde{\sigma}, \rho)$ where $\tilde{\sigma}$ is an $(N-1)$-dimensional object and $\rho(x)^2 = 1 - \tilde{\sigma}(x) \cdot \tilde{\sigma}(x)$, then we can write the action as [1]

$$\begin{aligned} S &= \frac{1}{2g} \int d^2x \left(\partial_\mu \tilde{\sigma}(x) \cdot \partial_\mu \tilde{\sigma}(x) + \partial_\mu \rho(x) \partial_\mu \rho(x) \right) \\ &= \frac{1}{2g} \int d^2x \left(\partial_\mu \tilde{\sigma}(x) \cdot \partial_\mu \tilde{\sigma}(x) + \frac{\left[\tilde{\sigma}(x) \cdot \partial_\mu \tilde{\sigma}(x) \right]^2}{1 + \tilde{\sigma}(x) \cdot \tilde{\sigma}(x)} \right) \end{aligned}$$

which is an interacting theory of the $\tilde{\sigma}$ field, without any external constraints. Clearly, the interesting dynamics of the non-linear σ models originate from eq. 4.

Another interesting facet of $O(N)$ non-linear σ models is that the fields can sustain topological excitations – i.e. ones which cannot be created or destroyed by local fluctuations. We can assign a given field a topological charge based on how many times it 'winds' around the unit $(N-1)$-sphere.

[1] I.e. the components transform into one another under N-dimensional orthogonal transformations.

3.2 Lattice formulation

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

$$\begin{aligned} S &= \frac{1}{2g} \sum_n \sum_\mu \delta_\mu \sigma_n \cdot \delta_\mu \sigma_n \\ &= -\frac{1}{g} \sum_n \sum_\mu \left(\sigma_{n+\hat{\mu}} \cdot \sigma_n - 1 \right) \end{aligned} \tag{5}$$

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

$$H_{\text{spin}} = -\sum_n \sum_\mu \sigma_{n+\hat{\mu}} \cdot \sigma_n \tag{6}$$

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,

$$S = \beta H_{\text{spin}} + 2\beta V \tag{7}$$

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

3.3 Spherical parameterisation

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.

$$\sigma_{O(2)} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \qquad\qquad \theta \in [0, 2\pi) \tag{8}$$

$$\begin{aligned} S_{O(2)} &= -\beta \sum_n \sum_\mu \Big(\cos\theta_{n+\hat{\mu}} \cos\theta_n + \sin\theta_{n+\hat{\mu}} \sin\theta_n - 1 \Big) \\ &= -\beta \sum_n \sum_\mu \Big(\cos(\theta_{n+\hat{\mu}} - \theta_n) - 1 \Big) \end{aligned} \tag{9}$$

For $O(3)$ we have the standard parameterisation of a unit sphere, in terms of polar angle

θ and 'azimuthal' angle ϕ.

$$\sigma_{O(3)} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \qquad \theta \in [0,\pi],\ \phi \in [0,2\pi) \tag{10}$$

$$S_{O(3)} = -\beta \sum_n \sum_\mu \Big(\cos\theta_{n+\hat{\mu}} \cos\theta_n + \sin\theta_{n+\hat{\mu}} \sin\theta_n \cos(\phi_{n+\hat{\mu}} - \phi_n) - 1 \Big) \tag{11}$$

For higher N we can use generalised spherical coordinates [2]

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

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

3.4 MCMC implementations

3.4.1 Local updates

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

$$M_n = \sum_\mu \left(\sigma_{n+\hat{\mu}} + \sigma_{n-\hat{\mu}} \right) = \sum_{\pm\mu} \sigma_{n+\hat{\mu}} \tag{13}$$

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

$$\delta S = -\beta\, \delta\sigma_n \cdot M_n \tag{14}$$

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

$$\delta S_{O(2)} = -\beta \sum_{\pm\mu} \Big(\cos(\theta_{n+\hat{\mu}} - \theta'_n) - \cos(\theta_{n+\hat{\mu}} - \theta_n) \Big) \tag{15}$$

3.4.2 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 $\delta_{\text{max}} \in [0, 1]$ 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. 15 to obtain δS
5. Accept the proposal with probability $\exp(-\delta S)$
6. Return to step 1.

3.4.3 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. 14 to obtain δS
8. Accept the proposal with probability $\exp(-\delta S)$
9. Return to step 1.

3.4.4 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.

3.4.5 Heat bath: $O(2)$

TO DO:

3.4.6 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

$$\cos\gamma = \frac{1}{\beta|M_n|}\log\left[(1-x)e^{\beta|M_n|} + x\,e^{-\beta|M_n|}\right] \tag{16}$$

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. 16
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.

3.5 Two point observables

3.5.1 Two point correlator

The *connected* two point correlation function is given by

$$\begin{aligned} G(n,x) &= \langle\sigma_{n+x}\cdot\sigma_n\rangle - \langle\sigma_{n+x}\rangle\cdot\langle\sigma_n\rangle \\ &= \frac{1}{N_{\text{ens}}}\sum_{a=1}^{N_{\text{ens}}}\sigma_{n+x,a}\cdot\sigma_{n,a} - \left(\frac{1}{N_{\text{ens}}}\sum_{a=1}^{N_{\text{ens}}}\sigma_{n+x,a}\right)\cdot\left(\frac{1}{N_{\text{ens}}}\sum_{a=1}^{N_{\text{ens}}}\sigma_{n,a}\right) \end{aligned} \tag{17}$$

Making use of the translation symmetry of eq. 5, we define the volume average of this quantity

$$G(x) = \frac{1}{V}\sum_n G(n,x) \tag{18}$$

3.5.2 Volume averaged two point correlator

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

$$G_V(x\,;a) = \frac{1}{V}\sum_n \sigma_{n+x,a}\cdot\sigma_{n,a} - \left(\frac{1}{V}\sum_n \sigma_{n,a}\right)^2 \tag{19}$$

This is a useful quantity since it allows us to study autocorrelations at different length scales.

3.5.3 Fourier space correlator

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

$$\tilde{G}(k) = \frac{1}{V}\sum_x e^{ik\cdot x}\, G(x) \tag{20}$$

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

3.5.4 Susceptibility

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

$$\chi = \tilde{G}(0) = \frac{1}{V}\sum_x G(x) \tag{21}$$

3.5.5 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'.

$$E_{\text{ising}} = \frac{1}{d}\sum_\mu G(\hat{\mu}) \tag{22}$$

3.5.6 Zero momentum correlator

If we interpret one of the lattice dimensions as a time dimension, we can restrict the Fourier transform to the spatial dimensions only.

$$\tilde{G}(k,t) = \frac{1}{L^{d-1}} \sum_{x} e^{ik\cdot x}\, G(x,t) \tag{23}$$

where x now denotes all $d-1$ spatial dimensions (just a single dimension in the $d=2$ case).

The zero momentum correlator refers to the $k=0$ case, which is just

$$\tilde{G}(0,t) = \frac{1}{L^{d-1}} \sum_{x} G(x,t) \tag{24}$$

3.5.7 Effective pole mass

The pole mass is given in the continuum by

$$m_p = -\partial_t \log\langle \tilde{G}(0,t)\rangle \tag{25}$$

An effective pole mass can be defined by [3]

$$m_p^{\text{eff}}(t) = \cosh^{-1}\left(\frac{\tilde{G}(0,t-1)+\tilde{G}(0,t+1)}{2\tilde{G}(0,t)}\right) \tag{26}$$

The effective pole mass and zero momentum correlator are the only two quantities which will require treating the lattice dimensions differently.

3.6 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

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

3.6.1 Energy density

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

$$\begin{aligned} E_{\text{spin}} &= \frac{1}{V}\langle H_{\text{spin}}\rangle \\ &= -\frac{1}{V}\frac{1}{N_{\text{ens}}}\sum_{a=1}^{N_{\text{ens}}}\sum_{n}\sum_{\mu}\sigma_{n+\hat{\mu},a}\cdot\sigma_{n,a} \\ &= -\sum_{\mu}G(\hat{\mu})_{\text{disconn}} \end{aligned} \tag{27}$$

In the high temperature limit where $\langle\sigma\rangle = 0$, making the connected correlators equal to the disconnected, this energy density should be $-d$ times the Ising energy density defined previously.

3.6.2 Magnetic susceptibility

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

$$\begin{aligned} \chi_m &= \frac{1}{V}\langle M^2\rangle \\ &= \frac{1}{V}\frac{1}{N_{\text{ens}}}\sum_{a=1}^{N_{\text{ens}}}\sum_{n}\sum_{m}\sigma_{m,a}\cdot\sigma_{n,a} \\ &= \sum_{x}G(x)_{\text{disconn}} \\ &= \tilde{G}(0)_{\text{disconn}} \end{aligned} \tag{28}$$

In the high temperature limit this should be equal to the susceptibility defined previously.

[2]This is also equivalent to the definition in ref. [4], 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.

3.6.3 Heat capacity

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

$$c = \frac{\beta^2}{V}\left[\langle H_{\text{spin}}^2\rangle - \langle H_{\text{spin}}\rangle^2\right] = \beta^2 \frac{\langle H_{\text{spin}}^2\rangle}{V} - \beta^2 V E_{\text{spin}}^2 \tag{29}$$

3.7 Definitions involving the $O(N)$ action

The $O(N)$ lattice action is

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

3.7.1 Alternative definition of energy density

Another definition of energy density, found in e.g. ref. [4]

$$\begin{aligned} E_{\text{deriv}} &= \frac{1}{V}\sum_n \sum_\mu \langle \delta_\mu \sigma_n \cdot \delta_\mu \sigma_n \rangle \\ &= \frac{2}{\beta V}\langle S \rangle \\ &= 2E_{\text{spin}} + 4 \end{aligned} \tag{30}$$

3.7.2 Equivalent definition of heat capacity

Eq. 29 is simply the variance of the $O(N)$ action, divided by volume.

$$c = \frac{1}{V}\left[\langle S^2\rangle - \langle S\rangle^2\right] \tag{31}$$

[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, $c = \frac{1}{V}\frac{\partial E_{\text{spin}}}{\partial T} = \frac{\beta^2}{V}\frac{\partial^2}{\partial \beta^2}\log \mathcal{Z}$

3.8 Topological observables for $O(3)$

3.8.1 Topological charge density: geometric definition

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 [4]. 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,

$$q_{n^*} = \frac{1}{4\pi}\Big(\Delta(\sigma_n, \sigma_{n+\hat{\mu}_1}, \sigma_{n+\hat{\mu}_1+\hat{\mu}_2}) + \Delta(\sigma_n, \sigma_{n+\hat{\mu}_1+\hat{\mu}_2}, \sigma_{n+\hat{\mu}_2})\Big) \tag{32}$$

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

$$\Delta(\alpha, \beta, \gamma) = \pm(\alpha + \beta + \gamma - \pi) \tag{33}$$

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

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

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

$$\exp\left(i\frac{\Delta(\vec{a},\vec{b},\vec{c})}{2}\right) = \frac{1+\vec{a}\cdot\vec{b}+\vec{b}\cdot\vec{c}+\vec{c}\cdot\vec{a}+i\vec{a}\cdot(\vec{b}\times\vec{c})}{\left[2(1+\vec{a}\cdot\vec{b})(1+\vec{b}\cdot\vec{c})(1+\vec{c}\cdot\vec{a})\right]^{1/2}} \tag{34}$$

This leads to

$$\Delta(\vec{a},\vec{b},\vec{c}) = 2\tan^{-1}\left(\frac{\vec{a}\cdot(\vec{b}\times\vec{c})}{1+\vec{a}\cdot\vec{b}+\vec{b}\cdot\vec{c}+\vec{c}\cdot\vec{a}}\right) \tag{35}$$

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. 35 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 $(-\pi, \pi)$.

3.8.2 Topological charge

Topological charge is defined in terms of the charge density by

$$Q = \sum_{n^*} q_{n^*} \tag{36}$$

3.8.3 Topological susceptibility

Hence, the topological susceptibility is

$$\chi_t = \frac{1}{V}\langle Q^2\rangle \tag{37}$$

3.9 Deterministic approach for small lattices

TO DO:

4. Appendices

4.1 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 $\hat{\mathbf{z}} = (0, 0, 1)$:

$$\sigma = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} = \begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{38}$$

These components can be calculated as

$$\cos\theta = \sigma^3 \tag{39}$$

$$\sin\theta = \sqrt{1 - \cos^2\theta} \tag{40}$$

$$\cos\phi = \sigma^1 / \sin\theta \tag{41}$$

$$\sin\phi = \sigma^2 / \sin\theta \tag{42}$$

The next step is to 'perturb' this vector, which effectively amounts to rotating the coordinate system $\hat{\mathbf{z}} \to \hat{\mathbf{z}}'$. The result can be made to be arbitrarily close to $(0, 0, 1)$ 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.

$$\sigma' = \begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} \sin\gamma\cos\alpha \\ \sin\gamma\sin\alpha \\ \cos\gamma \end{pmatrix} \tag{43}$$

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