Chapter 3

RANDOM VARIABLES

Having in hand the definition of the probability model from chapter 2, the next logical step is to define random variables. In particular, we seek *order parameters* — random variables which allow us to identify the phase transition to long cycles. Specific random variables used in this dissertation are as follows. For each, the relevant theory sections (in this chapter) and experiment sections (in chapter 9) are pointed to.

- System energy and energy density: these are as discussed in section 2.1; explicit computation is discussed in section 9.8.
- The number of ℓ -cycles in the permutation for $\ell = 1, 2, ..., N$: the definitions are familiar from elementary algebra; computation is discussed in section 9.9.
- Cycle length, spatial cycle length, and correlation length: sections 3.2 and 9.10.
- Mean jump length and maximum jump length: sections 3.3 and 9.11. These are used to confirm the hypothesis of short jump lengths as mentioned in section 3.6.
- Fraction of sites in cycles of specified lengths, and fraction of sites in long cycles: section 3.4 and (theory) and 9.12 (experiment).
- Longest cycle length and macroscopic-cycle quotient: sections 3.5 and 9.13.
- Winding numbers, scaled winding number, and fraction of sites in winding cycles: sections 3.6 and 9.14.

A word on notation: given a random variable X, let $Q = \mathbb{E}[X]$. For each quantity Q, one should distinguish between the finite-volume value $Q_L(T)$ and the infinite-volume limit $Q_{\infty}(T) = \lim_{L \to \infty} Q_L(T)$. For this chapter, omitted subscripts are disambiguated by context. The difference becomes significant in chapter 9; at that point, we will carefully distinguish between $Q_L(T)$ and $Q_{\infty}(T)$.

3.1 Differences and distances on the torus

We first define the natural difference-vectors and distances on the 3-torus. Namely, for $\mathbf{z} \in \Lambda$, we define a zero-centered modulus vector $\mathbf{m}_L(\mathbf{z})$. For $\mathbf{x}, \mathbf{y} \in \Lambda$, this gives rise to a difference vector $\mathbf{d}_{\Lambda}(\mathbf{x}, \mathbf{y})$ and a distance $\|\mathbf{x} - \mathbf{y}\|_{\Lambda}$. The former are needed

for winding numbers (section 3.6); the latter are needed for the Hamiltonian (section 2.1), spatial cycle length and correlation length (section 3.2), and jump length (section 3.3). Specifically, we have the following:

$$\mathbf{m}_{L}(\mathbf{z}) = \begin{pmatrix} m_{L}(z_{1}) \\ m_{L}(z_{2}) \\ m_{L}(z_{3}) \end{pmatrix}$$
(3.1.1)

$$n_L(z) = n \in \mathbb{Z}$$
 which minimizes $|z + nL|$ (3.1.2)

$$m_L(z) = z + n_L(z)L$$
 (3.1.3)

$$\mathbf{d}_{\Lambda}(\mathbf{x}, \mathbf{y}) = \mathbf{m}_{\Lambda}(\mathbf{x} - \mathbf{y}) \tag{3.1.4}$$

$$\|\mathbf{z}\|_{\Lambda} = \|\mathbf{m}_{\Lambda}(\mathbf{z})\|. \tag{3.1.5}$$

For example, suppose L = 20, $\mathbf{x} = (0, 0, 18)$, and $\mathbf{y} = (0, 0, 1)$. Then $\mathbf{d}_{\Lambda}(\mathbf{x}, \mathbf{y}) = (0, 0, -3)$ and $\|\mathbf{x} - \mathbf{y}\|_{\Lambda} = 3$. This is called a zero-centered modulus since $m_L(z)$ takes values from -L/2 to L/2. There is an antipodal problem when L is even: the distance is well-defined on the torus, but differences are ambiguous at L/2 in any of the three slots. For example, if L = 20, $\mathbf{x} = (0, 0, 18)$, and $\mathbf{y} = (0, 0, 8)$, then $\|\mathbf{x} - \mathbf{y}\|_{\Lambda} = 10$ but $\mathbf{d}_{\Lambda}(\mathbf{x}, \mathbf{y}) = (0, 0, 10)$ or (0, 0, -10). However, as mentioned in sections 2.3, 3.6, 6.2, and 9.11, we work in the short-jump-length regime. Specifically, in section 9.11 we find that for T near T_c , jump length remains below 5, with probability very near 1, regardless of how big L is.

We now show that equation (3.1.5) is compatible with the definition of $\|\cdot\|_{\Lambda}$ from equation (2.1.2) on page 21. namely,

$$\|\mathbf{x} - \mathbf{y}\|_{\Lambda} = \min_{\mathbf{n} \in \mathbb{Z}^3} \{\|\mathbf{x} - \mathbf{y} + L\mathbf{n}\|\}.$$

Proposition 3.1.6. We have

$$\|\mathbf{x} - \mathbf{y}\|_{\Lambda} = \|\mathbf{d}_{\Lambda}(\mathbf{x}, \mathbf{y})\|.$$
(3.1.7)

Proof. For brevity, let $\mathbf{z} = \mathbf{x} - \mathbf{y}$. Since the square-root function is one-to-one and increasing on non-negative reals, it suffices to show

$$\|\mathbf{m}_{\Lambda}(\mathbf{z})\|^{2} = \min_{\mathbf{n}\in\mathbb{Z}^{3}}\{\|\mathbf{z}+\mathbf{n}L\|^{2}\}.$$

Starting with the right-hand side, we have

$$\begin{split} \min_{\mathbf{n}\in\mathbb{Z}^{3}}\{\|\mathbf{z}+\mathbf{n}L\|^{2}\} &= \min_{n_{1}\in\mathbb{Z}}\min_{n_{2}\in\mathbb{Z}}\min_{n_{3}\in\mathbb{Z}}\left\{(z_{1}+n_{1}L)^{2}+(z_{2}+n_{2}L)^{2}+(z_{3}+n_{3}L)^{2}\right\}\\ &= \min_{n_{1}\in\mathbb{Z}}\left\{(z_{1}+n_{1}L)^{2}\right\}+\min_{n_{2}\in\mathbb{Z}}\left\{(z_{2}+n_{2}L)^{2}\right\}+\min_{n_{3}\in\mathbb{Z}}\left\{(z_{3}+n_{3}L)^{2}\right\}\\ &= m_{L}(z_{1})^{2}+m_{L}(z_{2})^{2}+m_{L}(z_{3})^{2}\\ &= \|\mathbf{m}_{\Lambda}(\mathbf{z})\|^{2}. \end{split}$$

31

3.2 Cycle lengths and correlation length ξ

Definition 3.2.1. Fixing $\pi \in S_N$ and $\mathbf{x} \in \Lambda$, the cycle length $\ell_{\mathbf{x}}(\pi)$ is the smallest positive integer *a* such that $\pi^a(\mathbf{x}) = \mathbf{x}$. This is nothing more than the length of the cycle containing \mathbf{x} : if \mathbf{x} is in a 3-cycle, then $\ell_{\mathbf{x}}(\pi) = 3$. We define the spatial cycle length

$$s_{\mathbf{x}}(\pi) = \sum_{j=1}^{\ell_{\mathbf{x}}(\pi)} \|\pi^{j}(\mathbf{x}) - \pi^{j-1}(\mathbf{x})\|_{\Lambda}.$$

This is simply the sum of Euclidean jump distances for all permutation jumps in the cycle containing \mathbf{x} . We may at times instead write, respectively,

$$\ell_i(\pi) = \ell_{\mathbf{x}_i}(\pi)$$
 or $s_i(\pi) = s_{\mathbf{x}_i}(\pi)$.

For example, for the point configuration **X** and the permutation π in figure 3.1, we have

$$\ell_1(\pi) = \ell_2(\pi) = \ell_3(\pi) = \ell_4(\pi) = 4, \quad \ell_5(\pi) = \ell_6(\pi) = \ell_7(\pi) = 3, \text{ and } \ell_8(\pi) = 1.$$



FIGURE 3.1. A configuration of **X** and π with N = 8.

Definition 3.2.2. If **x** and **y** are in a common cycle of π , we say that **x** is connected to **y**; otherwise we say that **x** is not connected to **y**. These are written

$$\mathbf{x} \circ \mathbf{y}$$
 and $\mathbf{x} \circ \mathbf{y}$.

In the former case, we write

$$\ell_{\mathbf{x},\mathbf{y}}(\pi)$$

for the smallest positive integer a such that $\pi^a(\mathbf{x}) = \mathbf{y}$. This is the number of permutation jumps from \mathbf{x} to \mathbf{y} .

Definition 3.2.3. We may average cycle lengths and spatial cycle lengths (definition 3.2.1) over all points **x**:

$$\overline{\ell}(\pi) = \frac{1}{N} \sum_{\mathbf{x} \in \Lambda} \ell_{\mathbf{x}}(\pi) \qquad \overline{s}(\pi) = \frac{1}{N} \sum_{\mathbf{x} \in \Lambda} s_{\mathbf{x}}(\pi).$$

Now, $\mathbb{E}[\ell_{\mathbf{x}}] = \mathbb{E}[\ell_{\mathbf{y}}]$ for all $\mathbf{x}, \mathbf{y} \in \Lambda$, and both are the same as $\mathbb{E}[\overline{\ell}]$ as shown in the lemma below. Experimentally, however, as discussed at the beginning of chapter 4, we cannot compute expectations over all $\pi \in \mathcal{S}_N$; we must content ourselves with sample means over some sequence of M permutations π_1, \ldots, π_M , obtained in an MCMC simulation. We may increase the sample size by a factor N (thereby decreasing the sample variance by a factor of N, by the central limit theorem) if we average over all points \mathbf{x} . For each permutation, we may compute $\overline{\ell}(\pi)$ by averaging $\ell_{\mathbf{x}}(\pi)$ over all N point positions, and likewise for $s_{\mathbf{x}}(\pi)$ and \overline{s} .

Lemma 3.2.4. For all $\mathbf{x} \in \Lambda$, $\mathbb{E}[\overline{\ell}] = \mathbb{E}[\ell_{\mathbf{x}}]$.

Proof. The left-hand side is

$$\mathbb{E}[\overline{\ell}] = \sum_{\pi \in \mathcal{S}_N} P_{\text{Gibbs}}(\pi) \overline{\ell}(\pi).$$

Since both sums are finite, we have

$$\mathbb{E}[\overline{\ell}] = \sum_{\pi \in \mathcal{S}_N} P_{\text{Gibbs}}(\pi) \overline{\ell}(\pi) = \sum_{\pi \in \mathcal{S}_N} P_{\text{Gibbs}}(\pi) \frac{1}{N} \sum_{\mathbf{x} \in \Lambda} \ell_{\mathbf{x}}(\pi)$$
$$= \frac{1}{N} \sum_{\mathbf{x} \in \Lambda} \sum_{\pi \in \mathcal{S}_N} P_{\text{Gibbs}}(\pi) \ell_{\mathbf{x}}(\pi) = \overline{\mathbb{E}[\ell_{\mathbf{x}}]}.$$
(3.2.5)

The equality $\overline{\mathbb{E}[\ell_{\mathbf{x}}]} = \mathbb{E}[\ell_{\mathbf{x}}]$ follows from translation invariance on the 3-torus.

In summary, we have

$$\ell_{\mathbf{x}}(\pi) = \min\{a > 0 : \pi^{a}(\mathbf{x}) = \mathbf{x}\} \qquad s_{\mathbf{x}}(\pi) = \sum_{j=1}^{\ell_{\mathbf{x}}(\pi)} \|\pi^{j}(\mathbf{x}) - \pi^{j-1}(\mathbf{x})\|_{\Lambda}$$
$$\mathbb{E}[\ell_{\mathbf{x}}] = \sum_{\pi \in S_{N}} P_{\text{Gibbs}}(\pi)\ell_{\mathbf{x}}(\pi) \qquad \mathbb{E}[s_{\mathbf{x}}] = \sum_{\pi \in S_{N}} P_{\text{Gibbs}}(\pi)s_{\mathbf{x}}(\pi)$$
$$\overline{\ell}(\pi) = \frac{1}{N}\sum_{\mathbf{x} \in \Lambda} \ell_{\mathbf{x}}(\pi) \qquad \overline{s}(\pi) = \frac{1}{N}\sum_{\mathbf{x} \in \Lambda} s_{\mathbf{x}}(\pi)$$
$$\mathbb{E}[\overline{\ell}] = \sum_{\pi \in S_{N}} P_{\text{Gibbs}}(\pi)\overline{\ell}(\pi) \qquad \mathbb{E}[\overline{s}] = \sum_{\pi \in S_{N}} P_{\text{Gibbs}}(\pi)\overline{s}(\pi).$$

The quantities on the second line are convenient for theoretical use; the quantities on the fourth line (due to the larger sample size) are preferable for experimental use.

We define a correlation length ξ to be

$$\xi = \mathbb{E}[\overline{s}]. \tag{3.2.6}$$

Computational details are in section 9.10.

3.3 Mean and maximum jump length

Definition 3.3.1. Let

$$j_{\mathbf{x}}(\pi) = \|\pi(\mathbf{x}) - \mathbf{x}\|_{\Lambda}$$

be the length of the permutation jump starting at site \mathbf{x} ; let

$$j(\pi) = \frac{1}{N} \sum_{i=1}^{N} j_{\mathbf{x}_i}(\pi).$$

The mean jump length at site \mathbf{x} is simply

$$\mathbb{E}[j_{\mathbf{x}}] = \sum_{\pi \in \mathcal{S}_N} P_{\text{Gibbs}}(\pi) \| \pi(\mathbf{x}) - \mathbf{x} \|_{\Lambda}.$$

By linearity of expectation, this is the same as the average over all sites:

$$\mathbb{E}[j(\pi)] = \mathbb{E}[j_{\mathbf{x}_1}(\pi)].$$

As was the case for $\overline{\ell}$ and \overline{s} in section 3.2, we approximate the uncomputably large sum over all N! permutations by a random sequence of M permutations, and the sample mean is random. By the central-limit theorem argument in section 3.2, the variance of the sample mean of j is a factor of N smaller than the variance of the sample mean of $j_{\mathbf{x}}$, since the sample size is MN instead of M. Additional computational details are discussed in section 9.11.

3.4 Fraction of sites in infinite cycles f_I

If one wants to quantify the temperature-dependent onset of long cycles (section 2.3), then one can define a random variable which counts the fraction of sites in long cycles. In the infinite limit, one looks for infinite cycles. One could define

$$f_I(\infty) = 1 - \sum_{k \ge 1} P_{\text{Gibbs}}(\ell_0 = k)$$
 (3.4.1)

where $\ell_0(\pi)$ is as defined in section 3.2. For finite volume, where simulations are done, the right-hand side of (3.4.1) is always 0: every site is in a cycle of some finite length. One might then define

$$f_I(N) = 1 - \sum_{k < \varepsilon(N)} P_{\text{Gibbs}}(\ell_0 = k)$$
(3.4.2)

where $\varepsilon(N)$ is such that $\varepsilon(N) \to \infty$ as $N \to \infty$ but $\varepsilon(N)/N \to 0$. For example, one may take $\varepsilon(N) = \sqrt{N}$. This is chosen so that as $N \to \infty$, one obtains $f_I(\infty)$. In [BU07] it is found, among other results, that mesoscopic cycles are unimportant: for $T > T_c$, there are only microscopic cycles; for $T < T_c$, there are only microscopic and macroscopic cycles. The $\varepsilon(N)$ cutoff is designed to separate the former from the latter.

For practical computation, [GRU] begin by defining

$$\rho = \frac{N}{V},$$

where $V = L^3$ is the volume, i.e. ρ is the particle density. For $1 \le m \le n \le N$, define

$$\varrho_{m,n}(\pi) = \frac{1}{V} \# \{ i = 1, \dots, N : m \le \ell_i(\pi) \le n \}$$

This random variable, taking values between 0 and ρ , is the density of sites in cycles of specified length. One may also consider the related random variable

$$f_{m,n}(\pi) = \frac{1}{N} \# \{ i = 1, \dots, N : m \le \ell_i(\pi) \le n \}$$

which is $\rho_{m,n}/\rho$. (Of course, on the unit lattice where $N = L^3$ and $\rho = 1$, the two random variables $f_{m,n}(\pi)$ and $\rho_{m,n}(\pi)$ are identical.) This runs from 0 to 1 and is the fraction of sites in cycles of specified length. For figure 3.1 on page 32, we have $f_{2,3}(\pi) = 3/8$. Then $\mathbb{E}[f_{\varepsilon(N),N}]$ matches equation (3.4.2) as follows:

$$\mathbb{E}[f_{\varepsilon(N),N}(\pi)] = \frac{1}{N} \mathbb{E}\left[\#\{i=1,\ldots,N:\ell_i(\pi) \ge \varepsilon(N)\}\right]$$
$$= \frac{1}{N} \mathbb{E}\left[\sum_{i=1}^N \mathbb{1}_{\ell_i(\pi) \ge \varepsilon(N)}(\pi)\}\right] = \frac{1}{N} P_{\text{Gibbs}}(\ell_i(\pi) \ge \varepsilon(N)).$$

This is the same as $P_{\text{Gibbs}}(\ell_0(\pi) \ge \varepsilon(N))$ by translation invariance. Then

$$P_{\text{Gibbs}}(\ell_0(\pi) \ge \varepsilon(N)) = \sum_{k \ge \varepsilon(N)} P_{\text{Gibbs}}(\ell_0 = k) = 1 - \sum_{k < \varepsilon(N)} P_{\text{Gibbs}}(\ell_0 = k) = f_I(N).$$

In practice, a single cutoff of the form $\varepsilon(N)$ is not used; one estimates the infinitelimit behavior in a different way. To see how to do this, we next invoke results of [Sütő2] and [BUV09] regarding the behavior of $\mathbb{E}[f_{1,k}]$ as a function of k/N in the infinite limit. The former, [Sütő2], applies in the non-interacting case; the latter, [BUV09], applies in the Ewens case but with non-spatial permutations, which are equivalent to random spatial permutations with T = 0. For the non-interacting case, $\mathbb{E}[f_{1,k}]$ is a straight line of slope 1 as shown in the upper left of figure 3.2. At T = 0, it fills the full diagonal; cycle lengths have uniform distribution. At $T > T_c$, the diagonal vanishes into the upper-left corner; there are no long cycles. The transition to criticality occurs at T such that the diagonal becomes visible. See also [Lugo].



FIGURE 3.2. Qualitative behavior of $\lim_{N\to\infty} \mathbb{E}[f_{1,k}]$ as a function of k/N in the non-interacting (upper left) and non-spatial large- α Ewens-interacting (upper right) cases. Lower left and lower right show the behavior for finite N.

In finite volume, $\mathbb{E}[f_{1,k}]$ is rounded as shown in the bottom left of figure 3.2. Thus, one wishes to draw a tangent-line approximation for the infinite-volume behavior, and take f_I to be one minus the vertical intercept. This avoids use of a specific, arbitrary cutoff $\varepsilon(N)$, replacing it instead with a graphical estimator which makes use of all available data. See also section 9.12 for computational details, including the handling of sampling variability.

For Ewens interactions, the diagonals are curved as shown in the upper right of figure 3.2. For the small α values considered in this dissertation, however, this Betz-

Ueltschi-Velenik sag in the curve is less than the sampling variability in the data itself (see the plots in section 9.12). Thus, the sag is not relevant to our discussion. It should also be remarked that the author has performed larger- α simulations for which the sag is indeed observed simulationally.

3.5 Macroscopic-cycle quotient f_{max}/f_I

Definition 3.5.1. For a permutation π in S_N , define

$$\ell_{\max}(\pi) = \max_{1 \le i \le N} \ell_i(\pi).$$
(3.5.2)

For a spatial permutation, this is precisely the same as

$$\ell_{\max}(\pi) = \max_{\mathbf{x} \in \Lambda} \ell_{\mathbf{x}}(\pi). \tag{3.5.3}$$

We write

$$f_{\max} = \mathbb{E}[\ell_{\max}]/N. \tag{3.5.4}$$

Definition 3.5.5. The macroscopic cycle quotient, written f_{max}/f_I for brevity, is given by

macroscopic cycle quotient =
$$\begin{cases} \frac{\mathbb{E}[\ell_{\max}]}{Nf_I}, & f_I \neq 0\\ 0, & f_I = 0. \end{cases}$$
(3.5.6)

Intuition was discussed in sections 2.4 and 2.5; computational details are discussed in section 9.13.

3.6 Winding numbers, f_S , and f_W

The box $\Lambda = [0, L]^3$ with periodic boundary conditions is topologically equivalent to the 3-torus. Permutation cycles wind around the 3-torus some number of times in the x, y, and/or z directions. The sub- T_c onset of long cycles corresponds to the appearance of cycles which wrap around the torus in one or more of the three axes. If a cycle goes around once in the clockwise direction, we want to say it has sign +1; likewise, we want sign -1 for the counterclockwise direction. The following definition formalizes this intuition.

Definition 3.6.1. The *winding number* (really a 3-tuple of numbers) of a permutation π is

$$\mathbf{W}(\pi) = (W_x(\pi), W_y(\pi), W_z(\pi)) = \frac{1}{L} \sum_{i=1}^{N} \mathbf{d}_{\Lambda}(\pi(\mathbf{x}_i), \mathbf{x}_i)$$
(3.6.2)

where \mathbf{d}_{Λ} is the difference vector defined in equation (3.1.4). This simply counts the integer number of wraps of π 's cycles around the 3-torus in each of the three directions. We also write

$$\mathbf{W}^{2}(\pi) = \mathbf{W}(\pi) \cdot \mathbf{W}(\pi) = W_{x}(\pi)^{2} + W_{y}(\pi)^{2} + W_{z}(\pi)^{2}.$$
 (3.6.3)

Definition 3.6.4. The scaled winding number is

$$f_S = \frac{\mathbb{E}[\mathbf{W}^2]L^2}{3\beta N} = \frac{\mathbb{E}[\mathbf{W}^2]T}{3L}.$$

See [PC87] for the physical derivation. For us, it simply needs to be scaled by $L^2/N = 1/L$ in order to be an intensive parameter.

Definition 3.6.5. Let $c_{\mathbf{x}}(\pi)$ consist of all sites in the same cycle as \mathbf{x} :

$$c_{\mathbf{x}}(\pi) = \{ \mathbf{y} \in \Lambda : \mathbf{y} = \pi^{a}(\mathbf{x}), a = 0, 1, 2, \dots, N-1 \}.$$

Let $\mathbf{w}_{\mathbf{x}}(\pi)$ be the *winding vector* for \mathbf{x} (which is clearly the same for all sites in the same cycle as \mathbf{x}):

$$\mathbf{w}_{\mathbf{x}}(\pi) = \frac{1}{L} \sum_{\mathbf{y} \in c_{\mathbf{x}}(\pi)} \mathbf{d}_{\Lambda}(\pi(\mathbf{y}), \mathbf{y}),$$

where the difference vectors are again interpreted as in section 3.1. Note that all three slots of $\mathbf{w}_{\mathbf{x}}(\pi)$ are necessarily integer-valued. We say that π winds through \mathbf{x} if \mathbf{x} has a non-zero winding vector:

$$t_{\mathbf{x}}(\pi) = \begin{cases} 1, & \mathbf{w}_{\mathbf{x}}(\pi) \neq (0, 0, 0); \\ 0, & \mathbf{w}_{\mathbf{x}}(\pi) = (0, 0, 0). \end{cases}$$

We use these to define the *fraction of sites in winding cycles*:

$$f_W(\pi) = \mathbb{E}\left[\frac{1}{N}\sum_{\mathbf{x}\in\Lambda} t_{\mathbf{x}}(\pi)\right].$$

Computational details are discussed in section 9.14.

3.7 Order parameters: quantifying long cycles

Of the random variables presented in this chapter, the following, referred to as order parameters, may be used to locate the critical temperature $T_c(\alpha)$ below which long cycles begin to appear. The first four are non-zero for $T < T_c$ and zero for $T > T_c$. Since ξ blows up below T_c , $1/\xi$ goes to zero below T_c . See also figure 3.3.

- $f_{\max} := \mathbb{E}[\ell_{\max}]/N.$
- Fraction of sites in long ("infinite") cycles f_I .
- Scaled winding number f_S .
- Fraction f_W of sites in cycles which wind.
- Reciprocal correlation length $1/\xi$.



FIGURE 3.3. Behavior of order parameters as functions of L and T, for the noninteracting model. Each of the following occurs at a critical temperature T_c , in the limit $L \to \infty$: onset of N-scaling of the length of the longest cycle (f_{max}) , onset of long cycles (f_I) , onset of winding cycles $(f_S \text{ and } f_W)$, and blow-up of correlation length (vanishing of $1/\xi$). For finite L, the transitions are smooth; they sharpen toward non-analyticity as $L \to \infty$. Interactions increase the critical temperature, shifting these graphs to the right.