Chapter 2

The model of random spatial permutations

Here we review concepts from [BU07, BU08], fixing notation and intuition to be used in the rest of the paper.

2.1 The probability model

Our state space is

$$\Omega_{\Lambda,N} = \Lambda^N \times \mathcal{S}_N$$

where $\Lambda = [0, L]^3$ with periodic boundary conditions and $\mathcal{S}_N$ is the group of permutations of N points[1]. Point positions are $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$ for $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \Lambda$. These are called *spatial permutations* in that they involve the permutation π as well as the N point positions $\mathbf{x}_1, \ldots, \mathbf{x}_N$. See figure 2.1.

The probability measure on this state space will be constructed via Gibbs measure, $P_{\text{Gibbs}} = e^{-H}/Z$, on a Hamiltonian H. The background probability measure is discrete (uniform) in π and continuous (Lebesgue) in $\mathbf{X}$. The Hamiltonian takes one of two forms. In the first, relevant to the Bose gas, we have

$$H(\mathbf{X}, \pi) = \frac{T}{4} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|_\Lambda^2 + \sum_{1 \le i < j \le N} V(\mathbf{x}_i, \mathbf{x}_{\pi(i)}, \mathbf{x}_j, \mathbf{x}_{\pi(j)}) \tag{2.1.1}$$

where $T = 1/\beta$ and the V terms are interactions between permutation jumps. The notation $\|\cdot\|_\Lambda$ indicates the natural distance on the 3-torus:

$$\|\mathbf{x} - \mathbf{y}\|_\Lambda = \min_{\mathbf{n} \in \mathbb{Z}^3} \{\|\mathbf{x} - \mathbf{y} + L\mathbf{n}\|\} \tag{2.1.2}$$

For the V terms in equation (2.1.1), the permutation jump $\mathbf{x}_i \mapsto \mathbf{x}_{\pi(i)}$ interacts with the permutation jump $\mathbf{x}_j \mapsto \mathbf{x}_{\pi(j)}$. The temperature scale factor $T/4$, not $\beta/4$, is atypical in statistical mechanics. For purposes of the current work, this may be considered an ansatz; in [BU07], this choice of scale factor is shown to be appropriate for permutation representation of the Bose gas. In particular, as will be explained in more detail below, only the identity permutation appears at high T, and (with $V \equiv 0$) uniformly weighted permutations appear at zero T.

[1] One may of course consider $\Lambda = [0, L]^d$ for $d = 1, 2$, but for this paper, $d = 3$ only.

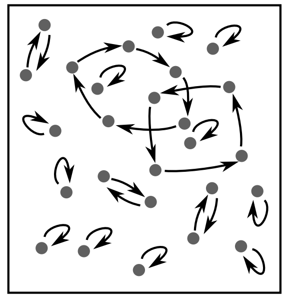

FIGURE 2.1. A spatial permutation on $N = 26$ points. There are 11 one-cycles, three two-cycles, one four-cycle, and one five-cycle. We say $r_1(\pi) = 11$, $r_2(\pi) = 3$, $r_4(\pi) = 1$, $r_5(\pi) = 1$, and $r_\ell(\pi) = 0$ for all other ℓ.

In the second form of the Hamiltonian, considered in this paper, we use interactions which are dependent solely on cycle lengths:

$$H(\mathbf{X}, \pi) = \frac{T}{4} \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|_\Lambda^2 + \sum_{\ell=1}^{N} \alpha_\ell r_\ell(\pi), \tag{2.1.3}$$

where $r_\ell(\pi)$ is the number of ℓ-cycles in π, for ℓ from 1 and N, and the α_ℓ's are free parameters, called *cycle weights*. One ultimately hopes to choose the α_ℓ's appropriately for the Bose gas; even if not, the model is well-defined and of its own mathematical interest.

The first contribution to the energy[2] is the sum of squares of permutation jump lengths. Since we will use a Gibbs distribution with $P_{\text{Gibbs}} = e^{-H}/Z$, the highest-probability permutations will be the ones with lowest energy. Thus, permutations with long jumps will be disfavored; permutations with many short jumps will be less strongly disfavored. The second contribution to the energy involves cycle weights. We consider only small cycle weights, which perturb the critical temperature but which do not qualitatively modify the effects of the distance-related terms. More intuition for the model will be presented in section 2.3.

Choices of point positions $\mathbf{x}_1, \ldots, \mathbf{x}_N$ yield two cases: (1) In the *annealed model*, point positions are variable in the continuum and are averaged over. One has a particle density $\rho = N/L^3$. This model is examined analytically in [BU07, U07, BU08]. (2) In the *quenched model*, point positions are held fixed. Specifically, we consider $N = L^3$ points on the fully occupied integer-indexed sites of the $L \times L \times L$ cubic lattice. This model is examined simulationally in [GRU] and in this dissertation. We often write

[2]The papers [BU07] and [U07] generalize from $\|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|_\Lambda$ to $\xi(\mathbf{x}_i, \mathbf{x}_{\pi(i)})$ where ξ is a spherically symmetric non-negative-valued function on $\mathbb{R}^d$ having integrable $e^{-\xi}$. This generalization is not of interest in this dissertation.

$H(\pi)$ in place of $H(\mathbf{X},\pi)$ since we either work on a lattice where the $\mathbf{x}_i$'s are held fixed, or on the continuum where the $\mathbf{x}_i$'s are integrated out. Thus, the system energy H (as well as all other random variables we consider) is a function of the permutation π.

We consider two partition functions, for a fixed point configuration $\mathbf{X}$ and for an average over point configurations, respectively:

$$Y(\Lambda,\mathbf{X}) = \sum_{\sigma\in\mathcal{S}_N} e^{-H(\mathbf{X},\sigma)} \quad \text{and} \quad Z(\Lambda,N) = \frac{1}{N!}\int_{\Lambda^N} Y(\Lambda,\mathbf{X})\, d\mathbf{X}.$$

Fixing point positions $\mathbf{X}$, we have a discrete distribution on π:

$$Y(\Lambda,\mathbf{X}) = \sum_{\sigma\in\mathcal{S}_N} e^{-H(\mathbf{X},\sigma)}, \qquad P_{\text{Gibbs}}(\pi) = P_{\Lambda,\mathbf{X}}(\pi) = \frac{e^{-H(\mathbf{X},\pi)}}{Y(\Lambda,\mathbf{X})}. \tag{2.1.4}$$

For varying point positions (e.g. for considerations of the Bose gas), we have a joint distribution which is continuous in $\mathbf{X}$ and discrete in π:

$$P_{\Lambda,N}(\mathbf{X},\pi)\, d\mathbf{X} = \frac{e^{-H(\mathbf{X},\pi)} d\mathbf{X}}{Z(\Lambda,N)}.$$

From this we obtain two marginal distributions. If we integrate over point configurations $\mathbf{X}$, then we obtain a discrete distribution on $\mathcal{S}_N$:

$$P_{\Lambda,N}(\pi) = \frac{1}{N!}\int_{\Lambda^N} d\mathbf{X}\, P_{\Lambda,N}(\mathbf{X},\pi) = \frac{\frac{1}{N!}\int_{\Lambda^N} d\mathbf{X}\, e^{-H(\mathbf{X},\pi)}}{\frac{1}{N!}\int_{\Lambda^N} d\mathbf{X}\, \sum_{\sigma\in\mathcal{S}_N} e^{-H(\mathbf{X},\sigma)}} = \frac{\int_{\Lambda^N} d\mathbf{X}\, e^{-H(\mathbf{X},\pi)}}{Z(\Lambda,N)\, N!}.$$

If, on the other hand, we sum over permutations, then we obtain a continuous distribution for point configurations:

$$P_{\Lambda,N}(\mathbf{X})\, d\mathbf{X} = \sum_{\pi\in\mathcal{S}_N} P_{\Lambda,N}(\mathbf{X},\pi)\, d\mathbf{X} = \frac{Y(\Lambda,\mathbf{X})\, d\mathbf{X}}{Z(\Lambda,N)}. \tag{2.1.5}$$

This continuous distribution is certainly of interest: it is the point distribution for the Bose gas, when the Hamiltonian is appropriately chosen. However, it is very difficult to compute: this is but one of several results in [LLS]. From here on, we consider the two discrete distributions on $\mathcal{S}_N$, namely, $P_{\Lambda,\mathbf{X}}(\pi)$ and $P_{\Lambda,N}(\pi)$.

For a random variable $X(\pi)$, we have

$$\mathbb{E}_{\Lambda,\mathbf{X}}[X] = \frac{\sum_{\pi\in\mathcal{S}_N} X(\pi) e^{-H(\mathbf{X},\pi)}}{Y(\Lambda,\mathbf{X})} \quad \text{and} \quad \mathbb{E}_{\Lambda,N}[X] = \frac{\int_{\Lambda^N} d\mathbf{X} \sum_{\pi\in\mathcal{S}_N} X(\pi) e^{-H(\mathbf{X},\pi)}}{Z(\Lambda,N) N!}.$$

In either case, we also write the probability as $P_{\text{Gibbs}}(\pi)$ and the expectation as

$$\mathbb{E}[X] = \sum_{\pi\in\mathcal{S}_N} P_{\text{Gibbs}}(\pi) X(\pi). \tag{2.1.6}$$

2.2 Model variants by choice of cycle weights

The model of random spatial permutations is in fact a family of models. As described in the previous section, point positions may be annealed or quenched, the latter being the case for this dissertation. Likewise, various constraints may be placed on the cycle weights. Recall from equation (2.1.3) that

$$H(\mathbf{X},\pi) = \frac{T}{4}\sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{x}_{\pi(i)}\|_\Lambda^2 + \sum_{\ell=1}^{N} \alpha_\ell r_\ell(\pi). \tag{2.2.1}$$

There are N free parameters α_ℓ, and thus many models of spatial permutations. (See also figure 2.2.)

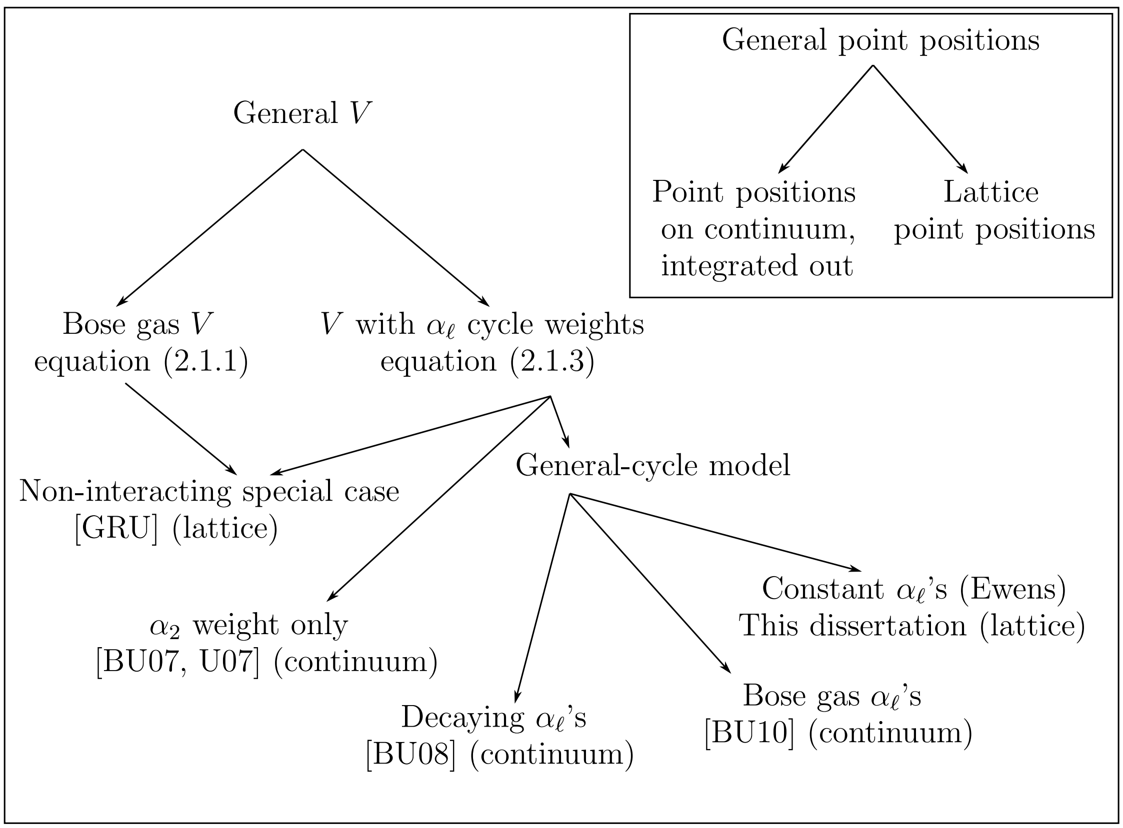

Figure 2.2. Model variants by choice of point positions and choice of cycle weights.

If $\alpha_\ell = 0$ for all ℓ, one obtains the *non-interacting case*. When $\alpha_2 = \alpha$ and $\alpha_\ell = 0$ for $\ell \neq 2$, we have the *two-cycle model* [BU07, U07] in which two-cycles are discouraged as α is increased. Otherwise, we have the *general-cycle model*. This splits into (at least) three submodels: Betz and Ueltschi, in [BU08], consider the case where α_ℓ tend toward zero faster than $1/\log(\ell)$. (Note that this includes the two-cycle model as a special case.) Ideally, one would have α_ℓ's which match the Brownian-bridge interactions for the Bose gas (appendix A). Work in this direction has recently been done by Betz and Ueltschi [BU10], but is beyond the scope of this dissertation.

For this dissertation, we consider the case where $\alpha_\ell = \alpha$ is constant in ℓ. We call this the *spatial Ewens distribution* [Ewens]. In summary, the model considered in this dissertation uses point positions held fixed on the fully occupied cubic unit lattice, with small non-negative Ewens cycle weights.

2.3 Qualitative characterization of long cycles

Having seen definitions for the probability model, one next asks what a typical random spatial permutation looks like. In this section we develop intuition; in section 3.7, we construct quantitative descriptions of the ideas presented here.

FIGURE 2.3. Points and permutation jumps, for a typical permutation at high T (there are only small cycles of short jumps), medium but subcritical T (all jump lengths are short, with occasional long cycles thereof), and low T (jump lengths are arbitrary).

As $T \to \infty$, the probability measure becomes supported only on the identity permutation: the distance-dependent terms in equation (2.1.3) are large whenever any jump has non-zero length. For large but finite T, the length-dependent terms penalize permutation jumps from a site to any site other than itself. Thus, for large T we expect the identity permutation to be the most likely, with occasional 2-cycles, 3-cycles, etc. which involve nearby points. On the other extreme, as $T \to 0$, length-dependent terms go to zero and the probability measure approaches the uniform distribution on $\mathcal{S}_N$: the distance-dependent terms all go to zero. For intermediate T, one observes that the length $\|\pi(\mathbf{x}) - \mathbf{x}\|_\Lambda$ of each permutation jump remains small, increasing smoothly as T drops. See figure 9.8 on page 99 for more precise information.

The intermediate-temperature regime is the one of interest. As is found in theoretical and simulational work, as detailed through the rest of this dissertation, this regime has the following properties. There is a phase transition: for T below a critical temperature T_c, while individual jump lengths remain short (i.e. we work in the short-jump-length regime), *arbitrarily long cycles form.* See figure 2.3 for depictions of typical permutations at high T, subcritical T, and low T. In the non-interacting case, $T_c(0)$ is approximately 6.87; interactions — in the form of positive α terms — increase $T_c(\alpha)$. Quantifying that dependence, i.e.

$$\Delta T_c(\alpha) = \frac{T_c(\alpha) - T_c(0)}{T_c(0)}, \tag{2.3.1}$$

as a function of α for small positive α, is the central goal of this dissertation.

From figures such as 2.3, one can detect long cycles visually. How do we measure them numerically? Let $\ell_{\max}(\pi)$ be the length of the longest cycle in π, with $\mathbb{E}[\ell_{\max}]$ its mean over all permutations. We take $N = L^3$ points on the $L \times L \times L$ unit lattice with periodic boundary conditions. We observe that for T above T_c, $\mathbb{E}[\ell_{\max}]$ increases only perhaps as fast as $\log L$. That is to say, $\mathbb{E}[\ell_{\max}]/N$ goes to zero as $L \to \infty$. For T below T_c, the length of the longest cycle does increase as L increases — we find that $\mathbb{E}[\ell_{\max}]$ scales with N. (This is one of the results of [Sütő1]; it is perhaps surprising that the scaling is by $N = L^3$ rather than, say, L^2.) That is to say, $\mathbb{E}[\ell_{\max}]/N$ approaches a temperature-dependent constant as $L \to \infty$; there are arbitrarily long cycles, or infinite cycles, in the infinite-volume limit. See figure 2.4 for plots of $\mathbb{E}[\ell_{\max}]/N$ as a function of T for various system sizes with $N = L^3$. See also figure 9.10 on page 101. Precise information about $\mathbb{E}[\ell_{\max}]/N$ and other quantities is found in section 3.7.

2.4 Known results

In this dissertation we study chiefly the α-dependent shift in critical temperature for Ewens cycle weights and cubic-lattice point positions. We will also consider an α-dependent macroscopic-cycle quotient, to be defined below. Here we survey known results for related models — namely, other cycle weights as described in section 2.2, and point positions integrated over the continuum — before stating our conjectures for our model in section 2.5.

Known results for point locations averaged over the continuum (as discussed in section 2.1) are obtained largely using Fourier methods [BU08] which are unavailable for point positions held fixed on the lattice. Betz and Ueltschi have determined $\Delta T_c(\alpha)$, to first order in α, for two-cycle interactions [BU07] and decaying cycle weights [BU08]. The critical (ρ, T, α) manifold relates ρ_c to T_c. Specifically, they obtain the following, with the decaying-cycle-weight constraint on the cycle weights

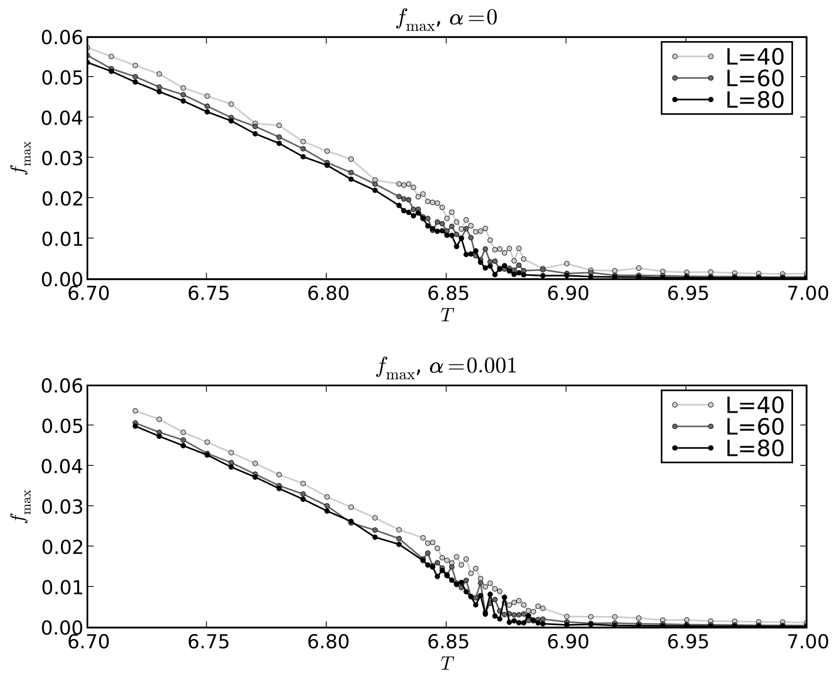

FIGURE 2.4. Order parameter $f_{\max} = \mathbb{E}[\ell_{\max}]/N$ for finite systems, with $\alpha = 0, 0.001$. Interactions increase the critical temperature.

$\{\alpha_\ell\}$:

$$\rho_c(\alpha_1, \alpha_2, \ldots) = \frac{1}{(4\pi\beta)^{3/2}} \sum_{\ell \geq 1} e^{-\alpha_\ell} \ell^{-3/2}. \tag{2.4.1}$$

In the non-interacting special case, all cycle weights are zero, and we have

$$\rho_c(0) = \frac{1}{(4\pi\beta)^{3/2}} \sum_{\ell \geq 1} \ell^{-3/2} = \frac{\zeta(3/2)}{(4\pi\beta)^{3/2}} \tag{2.4.2}$$

where ζ is the Riemann zeta function. For the two-cycle special case [BU07], α_2 is non-zero, and the other cycle weights are zero. We have

$$\rho_c(\alpha) = \frac{1}{(4\pi\beta)^{3/2}} \left(e^{-\alpha} 2^{-3/2} + \sum_{\ell \neq 2} e^{-\alpha_\ell} \ell^{-3/2} \right) = \rho_c(0) + \frac{(e^{-\alpha} - 1)}{(8\pi\beta)^{3/2}}.$$

In addition to our main interest on the shift in critical temperature (here, phrased in terms of critical density), we also examine the fraction of sites in macroscopic cycles. As will be discussed in more detail in sections 3.4 and 3.5, $\ell_{\max}$ is the length of the longest cycle of a permutation; f_I will quantify the fraction of sites participating in long cycles. For $\alpha_\ell \equiv 0$ (the non-interacting model), one observes empirically that the *macroscopic-cycle quotient* $\mathbb{E}[\ell_{\max}]/N f_I$ is constant for T below but near T_c. (That is, the two order parameters f_I and $\mathbb{E}[\ell_{\max}]/N$ have the same critical exponent.) For uniform-random (non-spatial) permutations, Shepp and Lloyd 1966 [SL] solved Golomb's 1964 question [Golomb]: $\mathbb{E}[\ell_{\max}]/N \approx 0.6243$. Unpublished work of Betz and Ueltschi has found $\mathbb{E}[\ell_{\max}]/N f_I$ holds that same value for random spatial permutations in the non-interacting case $\alpha_\ell \equiv 0$. The intuition is that long cycles are uniformly distributed within the zero Fourier mode.

2.5 Conjectures

Equation (2.4.1) gives ρ_c as a function of $\beta = 1/T$. For the cubic unit lattice, we fix $\rho \equiv 1$ and thus obtain β_c, or equivalently T_c:

$$T_c(\alpha_1, \alpha_2, \ldots) = \frac{4\pi}{\left(\sum_{\ell \geq 1} e^{-\alpha_\ell} \ell^{-3/2}\right)^{2/3}}. \tag{2.5.1}$$

For the non-interacting special case, this is

$$T_c(0) = \frac{4\pi}{\zeta(3/2)^{2/3}} \approx 6.625. \tag{2.5.2}$$

The Ewens-cycle-weight case does not satisfy the decaying-cycle-weight constraint where the α_ℓ's must go to zero in ℓ faster than $1/\log(\ell)$; all the α_ℓ's are the same. Nonetheless, using equation (2.5.1), we obtain

$$T_c(\alpha) = \frac{4\pi}{\left[e^{-\alpha}\zeta(3/2)\right]^{2/3}} \approx 6.625 e^{2\alpha/3}.$$

Taylor-expanding in the small parameter α, the shift in critical temperature is then

$$\Delta T_c(\alpha) = \frac{T_c(\alpha) - T_c(0)}{T_c(0)} = e^{2\alpha/3} - 1 \approx \frac{2\alpha}{3} \quad \text{and} \quad c \approx 0.667. \tag{2.5.3}$$

(Note that this is not in conflict with the constant c in section 1.4, which through abuse of notation we also called c. There, one examines $\Delta T_c(a)$ where a is the scattering length of the interacting Bose gas; here, one has $\Delta T_c(\alpha)$ for free parameter α.)

As the primary goal of this dissertation, we inquire whether this result, obtained for decaying cycle weights with point positions varying on the continuum, holds for Ewens weights with point positions held fixed on the lattice. We suspect that the fine details of point positions are unimportant for the shift in critical temperature. For Ewens interactions, $\Delta T_c(\alpha)$ is theoretically unknown for points either on the continuum or on the lattice. The simulational treatment in this dissertation is the only known attack on this question.

Secondarily, we conjecture that $\mathbb{E}[\ell_{\max}]/Nf_I$, as discussed in section 2.4, is α-dependent but constant in T (for T below but near T_c) for our model of lattice point positions and Ewens cycle weights.