The Ideal Glass and the Ideal Disk Packing in Two Dimensions: Appendix

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In this appendix we develop an argument that a maximal graph with periodic boundary conditions on a torus (genus 1) has zero specific entropy in support of our manuscript. Enumerating circle packings is a much more difficult problem than enumerating graphs, but as we will see, this is an appropriate proxy for predicting the specific entropy of circle packings. The core of the argument is that in the limit of the number of nodes going to infinity, the proportion of graphs that are maximal goes to zero. We will outline why this is true and then demonstrate how it relates to packings of circles in periodic boundary conditions.

We limit our argument to graphs which are 2-connected because this is what is available in the literature.

Put in simple terms, a k-connected graph is a graph where a path exists between every vertex even after removing any set of $k-1$ vertices and their edges. From this definition, any k-connected graph is 2-connected for $k >= 2$. It is wise, in this analysis, to omit graphs which are not 2-connected as these will never represent jammed configurations. A graph which is not 2-connected has at least one vertex for which multiple disconnected clusters will form upon its removal. Such a vertex is termed an articulation point and the independent clusters can pivot about this point. Such a graph is floppy and we should not consider it among the set of jammed packings. However, it is worth noting that the inverse is not necessarily true: a specific k-connected graph for $k >= 2$ does not necessarily have corresponding jammed packings with the underlying graph structure.

We further restrict our analysis to packings of hard disks with at least 3 contacts per disk. It is easy to see that this is required for local rigidity. However, it is worth noting again that having three contacts per particle is not a sufficient condition for jamming. To better reduce our search space, we consider the Maxwell-Calladine index theorem which states that a two dimensional elastic network with n nodes (vertices), m contacts (edges), n_{floppy} floppy modes, and S states of self stress has the property that

$$n_{\text{floppy}} - S = 2n - m. \tag{1}$$

If we define the average number of edges per node, $\mu \equiv m/n$ for a network and note that we require 1 state of self stress (from the fact that our boundaries are fixed) and 2 trivial floppy modes, we find that Eqn. 1 sets a lower bound on μ for a jammed packing as

$$n_{\text{floppy}} - S = 2n - m \implies 2 - 1 = 2n - m \implies \mu_{\text{min}} = 2 - 1/n. \tag{2}$$

Note that this ignores the possibility of non-linearly rigid jammed packings, which can generally be ignored for large system sizes [1].

If we consider triangulated packings, we have the condition that every face of our network must have exactly 3 edges. If we factor in the double-counting, then for a maximal graph, $3F = 2m$. The Euler characteristic for a toroidal graph is $\chi = n - m + F = 2 - 2g = 0$, where F is the number of faces and $g = 1$ is the genus of a torus. Using $3F = 2m$, the relation between the number of faces and edges for a maximal graph, the maximal value of μ is

$$\mu_{\max} = 3. \tag{3}$$

Note again that there exist packings of hard disks that are not jammed and yet may satisfy the property $\mu >= \mu_{\min}$.

Now that we have defined our search space, we begin our derivation with equation 4 from Chapuy et. al.[2]. The number of graphs, $b_{n,m}^{(g)}$, with n nodes, m edges, and of genus g has the following asymptotic form

$$b_{n,m}^{(g)} \sim d_{\mu}^{(g)} n^{5g/2-4} \left(\delta_{\mu}\right)^{n} n! \tag{4}$$

with n vertices and $m = \lfloor \mu n \rfloor$ edges, where $d_{\mu}^{(g)}$ is a prefactor that depends on surface genus and δ_{μ} is the base of the exponential growth with n and does not depend on genus.

This work by Chapuy et al. is an extension of the work by Bender et al. [3] which is valid for planar graphs (genus $g = 0$). In Bender et al., the authors have the following theorem for planar graphs (in the notation of [2]): *For $m_0/n \in J$, there is a unique $t \in (0, 1)$, such that $\mu(t) = m_0/n$, and*

$$b_{n,m}^{(0)} = \frac{3x_0(t)^2 y_0(t) D_3(t) n!}{8\sqrt{2}\pi \left(1 + y_0(t)\right) \sigma(t) n^3 m} x_0(t)^{-n} y_0(t)^{-m} \left(\exp\left\{ -\frac{(m - m_0)^2}{2n\sigma^2(t)} \right\} + o(1) \right), \tag{5}$$

uniformly as $n \to \infty$ and $m_0/n \in J$. In this expression x_0, y_0, and σ are all pure functions of a variable t. We work to massage the equation into the form given by 4. Without loss of generality, the authors of Bender et al. [3] choose t such that $t = t(1) \approx 0.62637$ and $y_0(t) = 1$. This value of t gives

$$\sigma = 0.618431, \; x_0 = 0.03819, \; \text{and} \; \mu_0 = 2.2629. \tag{6}$$

If we let $\mu \equiv m/n$, then

$$b^{(0)}_{n,m} = \frac{3x_0^2 D_3 n!}{16\sqrt{2}\pi\sigma n^4 \mu} x_0^{-n} \left(\exp\left\{ -\frac{n\left(\mu - \mu_0\right)^2}{2\sigma^2} \right\} + o(1) \right). \tag{7}$$

This can be rewritten asymptotically as

$$b^{(0)}_{n,m} \sim d^{(0)}_{\mu} n^{-4} \left(\delta_\mu\right)^n n! \tag{8}$$

by gathering the prefactor into $d^{(g)}_{\mu}$ and defining the base of the exponential as

$$\delta_\mu \equiv \left(\frac{1}{x_0} \exp\left\{ \frac{\left(\mu - \mu_0\right)^2}{2\sigma^2} \right\} \right). \tag{9}$$

We now consider the ratio of $b^{(1)}_{n,\mu_2 n}$ and $b^{(1)}_{n,\mu_1 n}$ which we define as

$$R_{\mu_1,\mu_2} \equiv \frac{b^{(1)}_{n,\mu_2 n}}{b^{(1)}_{n,\mu_1 n}} = \left(\frac{d^{(1)}_{\mu_2}}{d^{(1)}_{\mu_1}} \right) \left(\frac{\delta_{\mu_2}}{\delta_{\mu_1}} \right)^n \tag{10}$$

$$= C_{1,2} \exp\left\{ -\frac{1}{2\sigma^2} \left(\mu_2 - \mu_1\right)\left(\mu_2 + \mu_1 - 2\mu_0\right) \right\}^n, \tag{11}$$

where $C_{1,2}$ is the ratio of prefactors and relatively unimportant. We compute the ratio of the number of maximal toroidal graphs to the number of toroidal graphs for any value of $\mu_1 < 3$. Let $\mu_2 = 3$ represent the case of maximal toroidal graph. We see that in the limit as $n \to \infty$, this ratio tends to 0 when

$$3 > \mu_1 > 2\mu_0 - 3 \approx 1.5258. \tag{12}$$

Since these equations do not apply to graphs for which $\mu < 2 - 1/n$, we have shown that the ratio of maximal toroidal graphs to any other type of 2-connected toroidal graph tends to 0 in the thermodynamic limit.

ZERO SPECIFIC ENTROPY

From the circle packing theorems [4], we know that maximal graphs correspond uniquely to circle packings. However, this is not true for graphs with lower coordination. In fact, from the circle packing theorems, we know that there is at least one circle packing for every graph. Given these two facts, we know that $R_{\mu,3}$ is an upper bound for the ratio of the number of triangulated circle packings to circle packings with a fixed μ value where $3 > \mu \geq 2$. Since this upper bound tends to 0 in the thermodynamic limit, the specific entropy of maximal circle packings is 0 in the thermodynamic limit. We note that there are many pairs $\mu_1 \neq \mu_2$ for which R_{μ_1,μ_2} will also tend to zero. However, $\mu_2 = 3$ is the only value for which this ratio will *always* tend to zero.

CONFIGURATIONAL ENTROPY

It is true that the specific entropy of maximal graphs goes to 0 in the thermodynamic limit, but one may also be interested in the behavior of the configurational entropy.

For this, we use equation 4 in reference [2] which is the formula for the total number of 2-connected graphs on a torus (for all possible values of μ),

$$b_n^{(1)} \sim d^{(1)} n^{-1} \delta^n n! \tag{13}$$

and reference [3] tells us that

$$\delta = 1/x_0. \tag{14}$$

We define a new ratio Q_μ as the fraction of *all* graphs with n nodes that happen to have a particular value of μ to be

$$Q_\mu \equiv \frac{b_{n,\mu n}^{(1)}}{b_n^{(1)}} \tag{15}$$

$$= \frac{d_\mu^{(1)}}{d^{(1)}} n^{-1/2} \exp\left\{-\frac{1}{2\sigma^2}\left(\mu-\mu_0\right)^2\right\}^n . \tag{16}$$

From this it is clear that any μ other than $\mu = \mu_0$ is rare in the thermodynamic limit.

Next we define the asymptotic probability of finding a graph with a given μ and n

$$P(\mu, n) \sim P_0 n^{-1/2} \exp\left\{-\frac{1}{2\sigma^2}\left(\mu-\mu_0\right)^2\right\}^n . \tag{17}$$

From this, we define the asymptotic configurational entropy of our system,

$$S(\mu, n) \sim -k_B P(\mu, n) \ln P(\mu, n). \tag{18}$$

After substituting,

$$S(\mu, n) \sim -k_B P_0 \exp\left\{-\frac{1}{2\sigma^2}\left(\mu-\mu_0\right)^2\right\}^n \left[\ln P_0 n^{-1/2} - \frac{1}{2} n^{-1/2} \ln n - \frac{1}{2\sigma^2} n^{1/2} \left(\mu-\mu_0\right)^2\right]. \tag{19}$$

We wish to know the value of μ which gives the lowest configurational entropy. We first consider the boundaries by substituting the numerical values found earlier in (6) :

$$S(3,n) \sim k_B P_0 \left(0.491475\right)^n \left[-\ln P_0 n^{-1/2} + \frac{1}{2} n^{-1/2} \ln n + 0.710344 n^{1/2}\right] \tag{20}$$

and

$$S(2,n) \sim k_B P_0 \left(0.913619\right)^n \left[-\ln P_0 n^{-1/2} + \frac{1}{2} n^{-1/2} \ln n + 0.0903418 n^{1/2}\right] \tag{21}$$

For large n, $S(3,n)$ is lower than $S(2,n)$ therefore, $S(2,n)$ is not a minimum in the limit of large n. We check if there are any critical points which may correspond to minima. By differentiating S, this condition is satisfied when

$$\exp\left\{-\frac{1}{2\sigma^2}\left(\mu-\mu_0\right)^2\right\}^n \left(\mu-\mu_0\right)\left(-2\sigma^2 + n(\mu-\mu_0)^2 + \sigma^2 \ln n - 2\sigma^2 \ln P_0\right) = 0 \tag{22}$$

The exponential term can never be 0 so we have critical points at $\mu = \mu_0$ and $\mu = \mu_0 \pm \sqrt{\frac{\sigma^2}{n}\left[2 - \ln\left(\frac{n}{P_0^2}\right)\right]}$.

We define this last solution as $\mu_{1\pm}$. The critical point for μ_0 is

$$S(\mu_0, n) \sim k_B P_0 \frac{1}{2\sqrt{n}} \ln \frac{n}{P_0^2}. \tag{23}$$

This decays very slowly with n so we can easily rule this out as a minimum for large n. Finally, we check

$$S(\mu_{1\pm}, n) \sim \frac{k_B}{e} \tag{24}$$

This entropy is constant with n and will therefore never be the lowest entropy state.

From this, we can conclude that the configurational entropy of $\mu = 3$ approaches 0 for 2-connected toroidal graphs faster than any other value. For sufficiently large n, it will be the lowest entropy state. Similarly from before, if we set $\mu = 3$, we see that this is a lower bound for the configurational entropy of maximal circle packings.

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[2] G. Chapuy, E. Fusy, O. Giménez, B. Mohar, and M. Noy, Asymptotic enumeration and limit laws for graphs of fixed genus, Journal of Combinatorial Theory, Series A **118**, 748 (2011).

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[4] K. Stephenson, *Introduction to circle packing: the theory of discrete analytic functions* (Cambridge University Press, New York, 2005).