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Thomas P. Hayes
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SFI WORKING PAPER: 2014-07-023

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SFI WORKING PAPER: 2014-06-023

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Lower Bounds on the Critical Density in the Hard Disk Model via Optimized Metrics

Thomas P. Hayes* Cristopher Moore†

July 9, 2014

Abstract

We prove a new lower bound on the critical density ρ_c of the hard disk model, i.e., the density below which it is possible to efficiently sample random configurations of n non-overlapping disks in a unit torus. We use a classic Markov chain which moves one disk at a time, but with an improved path coupling analysis. Our main tool is an optimized metric on neighboring pairs of configurations, i.e., configurations that differ in the position of a single disk: we define a metric that depends on the difference in these positions, and which approaches zero continuously as they coincide. This improves the previous lower bound $\rho_c \geq 1/8$ to $\rho_c \geq 0.154$.

1 Introduction

The hard disk model is one of the simplest physical models of a non-ideal gas; yet it displays surprisingly complex behavior, including multiple phase transitions. A *configuration* in this model consists of an arrangement of n disks of radius r on a unit torus, so that no two of the disks overlap. At sufficiently high density, configurations tend to have a solid, or crystalline form. At sufficiently low densities, there is a gaseous phase, in which individual disks have plenty of room to move around. A more complex *hexatic* phase has been observed in a narrow range of intermediate densities [2].

Markov chain Monte Carlo algorithms have been used extensively to sample from this model's configuration space. Indeed, it was precisely this system that was studied in the classic paper of Metropolis et al. [11], who used Los Alamos' MANIAC computer to study a system with $n = 224$ disks. The simplest such algorithms choose a disk and attempt to move it to a new position. These algorithms work well at low densities, where the proposed position doesn't overlap with the other disks too often. However, as with many other MCMC algorithms, our theoretical guarantees lag well behind practice. While it is believed that these algorithms mix in polynomial time throughout the gaseous phase, we can only prove this up to a density well below the experimental critical point.

The present work gives improved upper bounds on the mixing time for *single-disk global-move dynamics*, which attempts to move a uniformly random disk to a uniformly random position anywhere in the torus. As a corollary, we obtain a new rigorous lower bound on the critical density at which the gaseous phase ends.

One of the challenging aspects of this particular Markov chain is that its state space is *continuous*, whereas many of the existing techniques for analyzing mixing times of Markov chains are fundamentally discrete. In particular, previous work [7] used path coupling with the Hamming metric, where the distance between two configurations is 1 whenever they differ in the position of a single disk. Our approach is to define a metric that depends continuously on the difference between the two positions. In particular, our metric goes to zero continuously as the two positions coincide, fitting our intuition that two configurations should be very close if a single disk has only been displaced a small amount.

*Department of Computer Science, University of New Mexico. hayes@cs.unm.edu

†Santa Fe Institute. moore@santafe.edu

2 Preliminaries

2.1 Configurations of Hard Disks

Let Ω denote the set of n -tuples of points in the d -dimensional unit torus, $[0, 1]^d$, that satisfy the constraint that no two of the points are at distance less than $2r$ from one another. For now, let us assume n and r are such that Ω is non-empty, and moreover, of positive Lebesgue measure. As a measurable subset of $[0, 1]^d$, Ω inherits the Lebesgue measure, and hence can be viewed as a probability space. We will refer to this as the “uniform distribution.”

Alternatively but equivalently, we can view each element of Ω as an arrangement, or configuration, of n labelled, non-overlapping disks of radius r . The combined volume of these disks is $\rho = nf(d, r)$ where $f(d, r)$ denotes the volume of a d -dimensional ball of radius r . This can be given in closed form as

$$f(d, r) = \frac{\pi^{d/2} r^d}{\Gamma(d/2 + 1)}.$$

We will focus on the case $d = 2$, where $f(d, r) = \pi r^2$.

Since the volume of the torus $[0, 1]^d$ is one, we call ρ the *density* of each configuration in Ω . A two-dimensional close packing of disks has density

$$\rho_{\text{packing}} = \frac{\pi\sqrt{3}}{6} \approx 0.9069.$$

At this point the disks form a triangular lattice, and the state is a perfect crystal. In contrast, at low enough densities the system is in a liquid or gaseous phase, where the disks have enough space between them to move freely. Numerical results (e.g. [10, 12]) suggest a phase transition to a solid with long-range correlations at a critical density $\rho_c \approx 0.7$. In addition, in between the solid and liquid phases there appears to be a *hexatic* phase, with a rather subtle type of correlation. Namely, if we draw lines between nearby pairs of disks, the orientations of these lines are correlated at large distances, even though the disks’ positions are not [2, 1, 5].

2.2 The Single-Particle Global-Move Dynamics

Viewing the elements of Ω as arrangements of n disks, there is a natural Markov chain on Ω that moves at most one disk at each timestep. Namely, choose a disk at random, and a uniformly random location in $[0, 1]^d$. If it would result in a valid configuration, remove the chosen disk, and replace it by a new disk centered at the chosen location. If not, because the chosen location is within distance $2r$ of one or more of the other disk centers, then reject the move and leave the configuration unchanged. This Markov chain is known as the *single-particle global-move dynamics*.

It is easy to see that this Markov chain is reversible, and hence the uniform distribution is stationary. The main question we are interested in is: for what densities ρ does this Markov chain mix rapidly, in poly(n) steps? In physical terms, up to what density can it be proved that the system is in its gaseous phase?

It is worth mentioning that a number of other dynamics have been proposed for Ω , many of which are based on local moves of one or more disks at a time. The most efficient seems to be a non-reversible Markov chain called *event chain dynamics*, due to Bernard, Krauth, and Wilson [2]. Unfortunately, we have even less rigorous understanding of these other dynamics than of single-disk dynamics.

Kannan, Mahoney, and Montenegro [7, Theorem 2] proved the following.

Theorem 1. *For n hard-core particles in dimension d , the single-disk global-move dynamics has mixing time τ bounded by*

$$\tau = \begin{cases} O(n \log n) & \text{if } 2^{d+1} \rho < 1 - \gamma \text{ for any constant } \gamma \\ O(n^2 \log n) & \text{if } 2^d \rho = 1. \end{cases}$$

In particular, this shows that the critical density marking the end of the gaseous phase is bounded below by $\rho_c \geq 2^{-(d+1)}$, or $\rho_c \geq 1/8$ for $d = 2$.

We review the proof of [7], which is based on path coupling [3]. Assume that $X_t, Y_t \in \Omega$ differ only in the position of a single disk, say disk 1. Couple the dynamics so that, in the next timestep, both X and Y make the same choice of disk j to move. If $j = 1$, which occurs with probability $1/n$, we choose the same proposed position in both chains. The chains will coalesce if the proposed position is valid; otherwise, the Hamming distance remains 1. Since a fraction ρ of the total volume is within distance r of a center, a fraction at most $2^d \rho$ is within distance $2r$ of a center. Thus coalescence occurs with probability at least $(1 - 2^d \rho)/n$.

If $j \neq 1$, we define the coupling so that the proposed position is identical if it is valid in both chains. Otherwise, we choose the proposed position uniformly for X , and obtain the proposed position for Y by reflecting around the line bisecting the two positions of disk 1. This guarantees that for at least half of these scenarios, the attempted update will fail in both chains. (This is reminiscent of Jerrum’s coupling for graph coloring, which matches forbidden colors with each other to increase the probability that a move will be rejected in both chains [6].) For the other half, one or both updates may succeed, increasing the Hamming distance to 2. Since a ρ/n fraction of the total volume is covered by disk 1, the probability of the Hamming distance increasing is at most $2^d \rho/n$.

Comparing these probabilities, we see that the expected change in Hamming distance $d(X_t, Y_t)$ is negative whenever $1 - 2^d \rho > 2^d \rho$, or equivalently, when $\rho < 2^{-(d+1)}$. When $\rho = 2^{-(d+1)}$, the proof is completed by lower bounding the expected squared change in $d(X_t, Y_t)$.

3 Related Work

Our work is different than most previous work on Markov chains in two respects. First, the state space is continuous. Second, we improve a path coupling argument not by optimizing the coupling or expanding the set of moves, but by optimizing the metric we use to define the distance between neighboring configurations.

Markov chains with continuous state spaces have received relatively little attention in computer science. An important recent exception is Randall and Winkler [14, 13], who analyzed the problem of arranging n dots in an interval, or on a circle. Indeed, their work can be thought of as the one-dimensional version of the hard disk model.

Vigoda [15] was one of the first to use an adaptively weighted Hamming metric to improve a path coupling argument. Earlier work by Dyer and Greenhill [4] and Luby and Vigoda [9] had established that the Glauber dynamics for the hard-core model on graphs of maximum degree Δ mixes in polynomial time when the fugacity λ is bounded below $2/(\Delta - 2)$. Both of these works proceeded by proving $O(n \log n)$ mixing for a related Markov chain with an expanded set of moves, which they related to Glauber dynamics with a comparison argument: namely, they added a “slide” transition that can move a particle between two adjacent sites. By suitably balancing the probabilities for single-site updates against those for the slide moves, they showed that a greedy coupling is contractive for the Hamming metric.

Rather than adding a slide transition or altering the coupling, Vigoda [15] obtained the same bound by defining a metric in which a single disagreement counts as distance $1 - c|B_v|$ where B_v denotes the set of “blocked” neighbors of the disagreeing vertex v , and c is a suitably chosen parameter. (A vertex is blocked if any of its neighbors, excluding v , is occupied.) Each such blocked neighbor corresponds to a move which will be rejected rather than driving the two configurations apart. Thus Vigoda’s metric “rewards” pairs of configurations, considering them closer than the Hamming metric would suggest, whenever the probability that the simple coupling would increase the disagreement them is relatively low. Our approach is similar in spirit: we define the distance between two neighboring configurations as small whenever the disagreeing disk is only displaced slightly from one configuration to the other.

4 Main Result

We prove the following.

Theorem 2. *For n hard-core particles in $d = 2$ dimensions, the single-disk global-move dynamics has mixing time $\tau = O(n \log n)$ whenever*

$$\rho \leq 0.154483\dots$$

Thus the critical density below which the system is in its gaseous phase is bounded by $\rho_c \geq 0.154483\dots$

Our results represents a modest improvement over the previous lower bound on the critical density, $\rho_c \geq 1/8$, and remain far below the experimental value $\rho_c \approx 0.7$. However, we believe that our bound can be improved further by combining our continuous metric with other geometrical ideas.

Like [7], our proof works by path coupling. Indeed, we use precisely the same coupling they do; our improvement is entirely due to the choice of metric. For two configurations X, Y with Hamming distance 1, i.e., that disagree only in the location of one disk, if the two differing locations are at a Euclidean distance ℓ , we define the distance between the two configurations as $D(X, Y) = d(\ell)$, for a suitable subadditive function d with $d(\ell) = d_{\max} = 1$ for ℓ sufficiently large. We then optimize the function $d(\ell)$ to obtain the largest possible ρ such that the coupling is contractive, i.e., so that $\mathbb{E}[\Delta d(X, Y)]$ is bounded below zero for all pairs X, Y with Hamming distance 1.

As usual in path coupling, we extend this metric to pairs X, Y with Hamming distance $h > 1$ by considering paths through Ω of length h : that is, $Z_0 = X, Z_1, Z_2, \dots, Z_{h-1}, Z_h = Y$, where each pair (Z_i, Z_{i+1}) differ in the position of a single disk. Then we define

$$D(X, Y) = \min \sum_{i=0}^{h-1} D(Z_i, Z_{i+1})$$

where the minimum is taken over all the possible paths Z_1, \dots, Z_{h-1} . If $\mathbb{E}[\Delta d(X, Y)]$ is bounded below zero for all X, Y with Hamming distance 1, it follows that $\mathbb{E}[\Delta D(X, Y)] < 0$ for all $(X, Y) \in \Omega \times \Omega$. Since the maximum Hamming distance is n , this is enough to establish mixing in $O(n \log n)$ time.

There are two differences between our metric and that used in [7]. The first is that our function $d(\ell)$ depends continuously on ℓ , and $d(\ell) \rightarrow 0$ as $\ell \rightarrow 0$. In contrast, they used Hamming distance, where $d(\ell) = 1$ for all $\ell > 0$.

Secondly, their notion of Hamming distance is slightly different. They use a fixed labelling of the n disks, so that Hamming distance means the number of disks i whose positions differ in the two configurations. However, when we speak of the Hamming distance between two configurations, we always think of unlabelled or adaptively labelled disks, so that as few disks as possible are in differing positions under the two configurations. In general, these adaptively chosen labellings will change from timestep to timestep as the configurations evolve. In particular, if two configurations differ only in that two disks have been switched, we consider them identical rather than having Hamming distance 2. This further reduces the shortest-path metric between two configurations that differ on two disks; if disk i in X is close to disk j in Y and vice versa, our metric considers X and Y to be close, even if i and j are distant from each other in both configurations. As we will see, it is this switching of two labels that lets us take advantage of our continuous metric to prove contractivity at a higher density.

4.1 Path Coupling in Continuous State Spaces

The following version of Bubley and Dyer's path-coupling theorem is taken from the textbook of Levin, Peres and Wilmer [8, Theorem 14.6, Corollary 14.7].

Theorem 3. *Suppose the state space Ω of a Markov chain is the vertex set of a graph with length function $d \geq 1$ defined on edges. Let ρ be the corresponding shortest-path metric. Suppose that for each edge $\{x, y\}$, there exists a coupling (X_1, Y_1) of the distributions $P(x, \cdot)$, $P(y, \cdot)$ such that*

$$\mathbb{E}_{x,y}[\rho(X_1, Y_1)] \leq \rho(x, y) e^{-\alpha} = d(x, y) e^{-\alpha}.$$

Then

$$t_{\text{mix}}(\epsilon) \leq \left\lceil \frac{-\log(\epsilon) + \log(\text{diam}(\Omega))}{\alpha} \right\rceil.$$

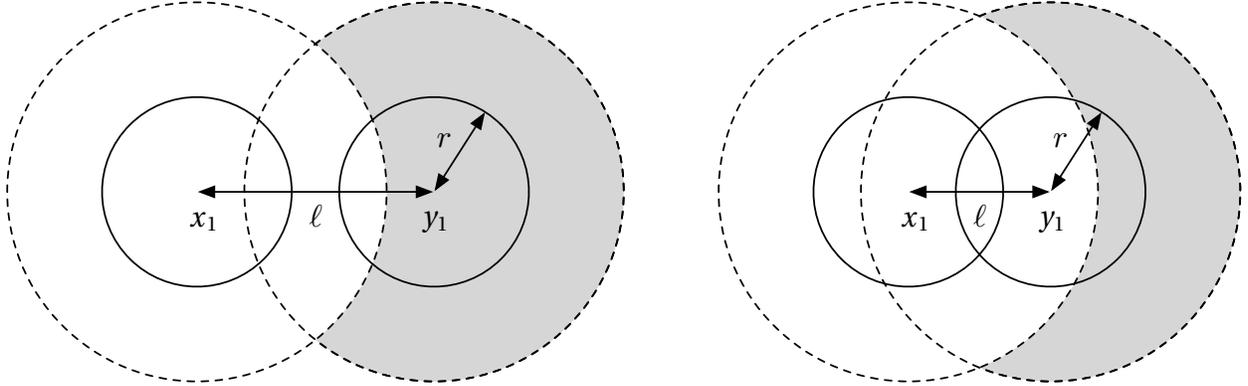


Figure 1: A disk centered at x_j is surrounded by a “danger zone” $Z(x_j)$ of radius $2r$. If two configurations differ at disk 1, a bad move only occurs if we try to move a disk into the “danger crescent” (shaded) $Z(y_1) \setminus Z(x_1)$, which we couple to its mirror image. On the left, $\ell > 2r$ and the crescent includes the center y_1 of the disk on the right. On the right, $\ell < 2r$ and the crescent excludes y_1 .

In our continuous setting, the length function d that is not bounded away from zero, so we cannot apply this theorem directly. However, the idea behind its proof immediately yields the following variant.

Theorem 4. *Suppose the state space Ω of a Markov chain is the vertex set of a graph with length function d defined on edges. Let ρ be the corresponding shortest-path metric. Suppose that for each edge $\{x, y\}$, there exists a coupling (X_1, Y_1) of the distributions $P(x, \cdot)$, $P(y, \cdot)$ such that*

$$\mathbb{E}_{x,y}(\rho(X_1, Y_1)) \leq \rho(x, y) e^{-\alpha} = d(x, y) e^{-\alpha}.$$

Then, for all X_0, Y_0 , all $\epsilon > 0$ and all $t \geq 1$,

$$\mathbb{P}[\rho(X_t, Y_t) > \epsilon] \leq \text{diam}(\Omega) e^{-\alpha t}.$$

Once we have a pair of configurations whose distance is sufficiently small, say $\epsilon/(n \log n)$, we can argue that over the course of the next $O(n \log n)$ updates, every disk that is successfully moved in one chain is moved to the same position in the other chain. By coupon collecting, this is enough steps to almost surely move each disk, so the two chains have coalesced with probability $1 - O(\epsilon)$. Combining this with Theorem 4, setting $\epsilon = O(1/(n \log n))$, $\text{diam}(\Omega) = O(n)$, $\alpha = O(1/n)$, we obtain a mixing time of $O(n \log n)$.

The above argument is not new; it was used by Randall and Winkler [14, Lemma 3] to analyze a local-move Markov chain for a one-dimensional version of the hard-core model.

4.2 Analysis of the Path Coupling

Let X, Y be two configurations differing in the position of one disk, which we call disk 1. Denote the disks’ centers as $X = (x_1, x_2, \dots, x_n)$ and $Y = (y_1, y_2, \dots, y_n)$, where $x_1 \neq y_1$ and $x_j = y_j$ for all $j \geq 2$. We write $\ell = \|x_1 - y_1\|$, so the distance between X and Y in our metric is $d(\ell)$.

If disk 1 is chosen for the move, then the distance will decrease to zero if the proposed position is legal. Each disk x_j is surrounded by a “danger zone” $Z(x_j)$ of radius $2r$, which has area $4\pi r^2$. As in [7], we pessimistically assume that these danger zones are disjoint; equivalently, we use the union bound for the probability that the proposed position falls into any of them. Thus X and Y coalesce with probability at least $1 - 4\pi r^2 n = 1 - 4\rho$.

If any other disk $j \geq 2$ is chosen for the move, then the update will ordinarily succeed or fail in both chains. The one case where it may not is when the proposed position z is in the danger zone of y_1 but outside

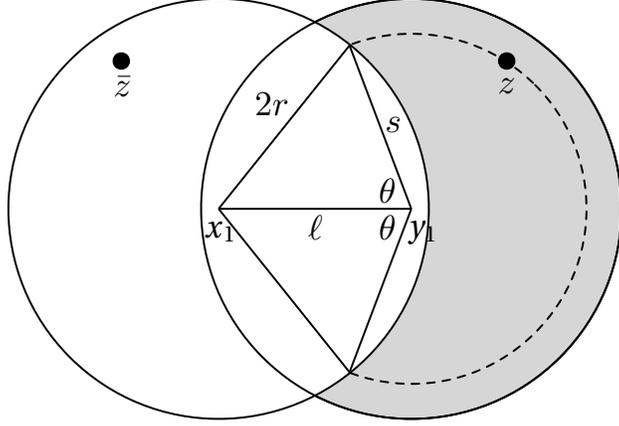


Figure 2: We attempt to move a disk to z in the X chain, and to its mirror image \bar{z} in the Y chain. If $\|z - y_1\| = s$, then the danger crescent (shaded) ranges over a circular arc (dashed) centered at y_1 and subtending an angle $2(\pi - \theta)$ where $\theta = \theta(s, \ell)$ is given by (2).

the danger zone of x_1 . We will call this set $Z(y_1) \setminus Z(x_1)$ the *danger crescent*, or simply the “crescent,” since, at least when $d = 2$, its shape is known as a crescent or lune.

When the X chain proposes a position z in the danger crescent, the Y chain proposes the mirror image position in $Z(x_1) \setminus Z(y_1)$, which we denote \bar{z} . If the update succeeds in either or both chains, our metric will generally change, either increasing or decreasing, as we will investigate more closely below.

The above cases are the only ways that $d(X, Y)$ can change. In particular, note that when X proposes a move into the mirror image of the crescent, the proposed move is always rejected in both chains, being blocked by disk 1 in both cases.

When one or both updates succeed, we need to decide whether the two disks formerly labelled “disk j ” should remain paired together, or whether one of them should swap places with disk 1 in our pairing. This is done greedily, minimizing the new distance between the configurations.

As shown in Fig. 2, let $s = \|z - y_1\|$. We will distinguish two cases. When $s \geq \ell$ and the move succeeds in at least one of the two chains, we call it a “far move.” In this case we keep the original indexing of the disks, so that on the next step we have $x'_1 = x_1$ and $x'_j = z$ if the move succeeds in the X chain, and similarly in the Y chain. Since the x_j is distant from x_1, y_1 , and z with probability $1 - O(1/n)$, we use the trivial upper bound $d(x'_j, y'_j) \leq d_{\max} = 1$ on the change in distance.

When $s < \ell$ and the move succeeds in at least one of the two chains, we call it a “near move.” Suppose without loss of generality that the move succeeds in the X chain, i.e., z is not blocked in the X chain. In this case, we swap the labels 1 and j in the X chain, setting $x'_1 = z$ and $x'_j = x_1$. Since the actual distance is the minimum over all relabelings, this choice, like any other, will imply an upper bound on the expected distance. There are then two cases: either the mirror image \bar{z} is blocked in the Y chain or not. If it is not, so that the move succeeds in both chains, we set $y'_j = \bar{z}$; in either case, we set $y'_1 = y_1$. Thus the change in our metric is at most

$$\begin{aligned} & d(\|x'_j - y'_j\|) + d(\|x'_1 - y'_1\|) - d(\|x_1 - y_1\|) \\ & \leq d_{\max} + d(\|z - y_1\|) - d(\|x_1 - y_1\|) \\ & = d_{\max} + d(s) - d(\ell), \end{aligned}$$

where again $d_{\max} = 1$.

Combining the above formulas, our upper bound on the expected change in the metric due to new disagreements becomes d_{\max} times the area of the danger crescent, minus the integral of the potential “savings” $d(\ell) - d(s)$ over the subregion $s \leq \ell$ corresponding to near moves.

L	8	16	32	64	128	256
ρ_c	0.150024	0.152182	0.153373	0.153999	0.154320	0.154483

Table 1: Lower bounds on ρ_c obtained by dividing the interval $[0, 4r]$ into L subintervals.

Now, using a formula for the area of intersection of two circles, we find the area of the danger crescent equals

$$A_{\mathfrak{D}}(\ell) = r^2 \left(8 \sin^{-1} \left(\frac{\ell}{4r} \right) + \frac{\ell}{r} \sqrt{4 - \frac{\ell^2}{4r^2}} \right). \quad (1)$$

Integrating the savings $d(\ell) - d(s)$ is more difficult, because we don't know the right choice of d . However, we can still set up the integral. For $0 \leq s \leq \ell$, let $\theta(s, \ell)$ denote the angle shown in Fig. 2. When the triple $(s, \ell, 2r)$ satisfies the triangle inequality, θ is given by the law of cosines:

$$\theta(s, \ell) = \cos^{-1} \left(\frac{s^2 + \ell^2 - 4r^2}{2\ell s} \right) \quad (2)$$

Otherwise, let $\theta = 0$ when $s < \ell - 2r$, and $\theta = \pi$ when $s < 2r - \ell$.

Note that when $\ell \leq r$, we have $\theta(s, \ell) = \pi$ for all $s \leq \ell$. This means there is never any savings in this case, so the correct setting of $d(\ell)$ for $0 \leq \ell \leq r$ satisfies

$$d(\ell) = \frac{n}{1 - 4\rho} A_{\mathfrak{D}}(\ell) = \frac{\rho}{\pi(1 - 4\rho)} \left(8 \sin^{-1} \left(\frac{\ell}{4r} \right) + \frac{\ell}{r} \sqrt{4 - \frac{\ell^2}{4r^2}} \right). \quad (3)$$

So, in the interval $0 \leq \ell \leq r$ we can determine the optimal metric analytically.

Now, integrating in polar coordinates, the expected savings equals

$$\int_{s=0}^{\ell} 2(\pi - \theta(s, \ell)) (d(\ell) - d(s)) s \, ds.$$

Putting this all together, our coupling will be ϵ -contractive relative to our chosen metric if, for all $0 < \ell \leq 4r$, we have

$$\left(\frac{1 - 4\rho}{n} - \epsilon \right) d(\ell) \geq A_{\mathfrak{D}}(\ell) - \int_0^{\ell} 2(\pi - \theta(s, \ell)) (d(\ell) - d(s)) s \, ds. \quad (4)$$

We set $d(\ell) = 1$ for all $\ell \geq 4r$.

Now, for any fixed choice of ρ and ϵ , we can consider various families of metrics. In particular, if we divide the interval $[0, 4r]$ into L subintervals of width $4r/L$ each, and assume that $d(\ell)$ is constant within each subinterval, the integral in (4) becomes a finite Riemann sum. For each ρ this gives a linear program with m variables. We then perform a binary search, finding the largest ρ for which this LP is feasible. Setting $\epsilon = 10^{-6}/n$ and using a numerical software package to determine LP feasibility, we obtain the results shown in Table 4.2. It seems unlikely that increasing L will improve the first three digits of ρ_c .

The metric $d(\ell)$ we obtain is shown in Fig. 3. It appears to have a piecewise analytic form, but we have made only desultory attempts to determine it except for (3) in the range $0 \leq \ell \leq r$ (with which there is excellent agreement). Interestingly, the constraints in 4 seem to be tight for $0 \leq \ell \leq 2r$, and slack for $2r < \ell \leq 4r$.

5 Further Improvement

Our new lower bound on the critical density is still very far from the experimental value $\rho_c \approx 0.7$. Our analysis of the coupling of single-disk global-move dynamics can undoubtedly be improved significantly, even

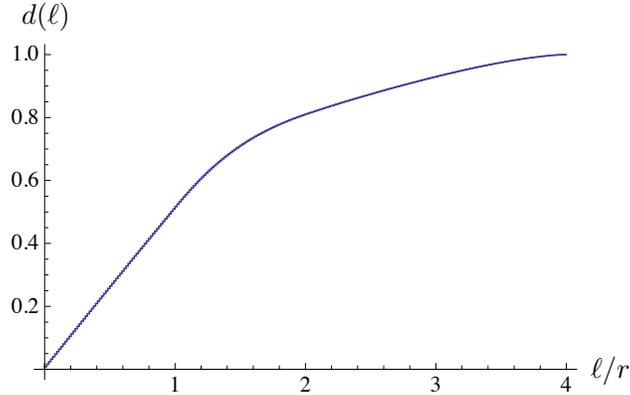


Figure 3: The optimal metric resulting from dividing $[0, 4]$ into $L = 256$ equal subintervals, setting $d(\ell)$ equal to a constant in each subinterval, and solving the resulting LP.

if we stick with the current coupling. It seems especially important to reduce the probability that a good move is rejected, i.e., reduce the term 4ρ on the left side of (4). Equivalently, we need to use the fact that, at least after a warm start, many of the danger zones overlap with high probability, so that the expected area of their union is less than 4ρ . We believe that this and other ideas will let us push the lower bound on ρ_c above $1/4$.

Another direction for improvement would be to increase the probability of savings from modifying the pairing. In particular, the worst case for our current analysis has all new disagreements come from moves that are blocked in exactly one of the two chains. Perhaps by accounting for the possibility that some of the blocking disks can be moved away, this worst case could be avoided.

Acknowledgments

We benefited from the Workshop on Disorder, Algorithms, and Complexity at the Aspen Center for Physics, and from conversations with Werner Krauth. This work was supported by NSF grant CCF-1219117.

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