

Hard Disk Model: Overview

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Description of the Problem

There is a two dimensional box (can be higher dimensions) where the edges wrap around to each other (i.e. a toroid). Within this box there are N disks with radius r that cannot overlap one another. The percentage of the area that this disks take up within the box is represented by ρ . In other words,

$$\rho = \frac{N * \pi r^2}{Area\ of\ Box}.$$

The goal of this problem is to determine when it is possible to efficiently sample random configurations below some critical density ρ_c .

Importance of the Problem

The hard disk model has applications in physics; more specifically it can show multiple phase transitions if the problem is mapped to an ideal-gas model. When the density ρ is sufficiently high, the configurations represent a more solid or crystalline form. For lower densities, the configurations are more gas like. There is a small range of densities where a hexatic phase occurs [1].

Approaches to the Problem

Markov chain Monte Carlo algorithms have been used in the past to sample configurations from this model. Experimental results suggest that $\rho_c \approx 0.7$ [2][3].

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Old Approach

One of the easiest ways is to pick up a disk and attempt to move it to a random location within the box. This process is referred to as *single-disk global-move dynamics*. More precisely a disk i is pick uniformly at random and a location x in the box is also picked uniformly at random. If the disk i can be placed at location x without overlapping another disk then we do it, otherwise we leave disk i in its original location. Using this dynamic and a path coupling argument the result yields $\rho_c \leq 1/8 = 0.125$ [4] for when the box is two dimensions.

Hayes and Moore [5] later improved the bound to $\rho_c \leq 0.154483...$ To accomplish this they used the same single-disk global-move dynamics and path coupling arguments, but modified the Hamming metric. The normal Hamming metric is 0 if the disks are in the same location in both chains, and 1 if the disks are in different locations. Hayes and Moore designed a Hamming metric that depends continuously on the difference between the two positions. More importantly it goes to zero continuously as the two positions coincide.

New Approach

Instead of using single-disk global-move dynamics one could use a *single-disk sliding-move dynamics*. The idea behind this is to pick a disk and direction uniformly at random. The disk attempts to move in the picked direction a distance ϵ . If the disk bumps into another disk while moving, the picked disk stops moving and the bumped into disk begins moving in the same direction for the remainder of the distance. If this new moving disk bumps into another disk, the process is repeated.

The intuition that this dynamic might perform better is that it is used in practice. By empirical observations this approach appears to mix well.

Other Ideas

There is a variation of this model where disks are allowed to enter and leave the box (i.e. toroid). This adds an extra variable λ to the system which controls to probability of a disk entering or leaving the system. Since N is not constant, neither is the density ρ . A question that could be asked about this model would be how ρ and λ are related to each other. Given some fixed λ value, what would ρ converge to after a sufficient amount of time steps? Or is there some critical range for λ where the density never converges?

References

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