Computational topology for configuration spaces of hard disks

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Authors: Gunnar Carlsson, Jackson Gorham, Matthew Kahle, and Jeremy Mason

Recommended and a commentary by Randall D. Kamien, University of Pennsylvania

Free volume theory is a successful approach to studying the entropy of crystalline phases of hard spheres and disks (free *area* theory in the latter); a periodic structure is chosen, the Voronoi cells of each lattice site are found, and then the volume accessible to each sphere or disk confined to their cells is calculated to estimate the entropy and the free energy, $F = -TS$ [1]. This approach strictly prevents overlaps of the particles at the cost of neglecting cooperative motion of groups of particles. For instance, if we fix the volume fraction of hard spheres and compare the FCC and BCC lattices, free volume theory predicts that the FCC lattice has a higher entropy. At first, this may seem paradoxical – the volume fraction is the same, so there is precisely as much unused volume in both lattices. But the volume is not used as efficiently in the case of BCC. Recall that the FCC lattice (or one of its stacking faults) gives the densest packing of hard spheres [2]. Compare a fixed number, N, of spheres close-packed into an FCC lattice and a BCC lattice. The former starts smaller than the latter; upon expansion to the same volume fraction, the FCC lattice had to expand more than the BCC lattice and so there must be more room for the spheres to move.

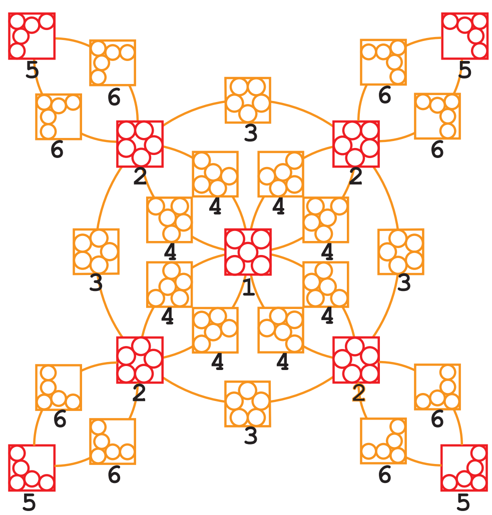

Figure 1. The dendrogram connecting different packing topologies. As the disk radius shrinks, new regions of configuration space open up in the numerical order specified on the dendrogram. Figure from arXiv:1108.5719.

In the paper by Carlsson, Gorham, Kahle, and Mason, the authors have delved significantly deeper into these subtleties. Considering only five hard disks in a square, they find the space of configurations of the disks and show that this space is not always one piece. In other words, "you can't get there from here" - there are classes of hard disk configurations with the same area fraction which are not connected to each other. In statistical mechanics we might say that these simple systems break ergodicity. They have presented their results in a dendrogram, shown in Figure 1. Each square depicts a class of packings. The numbers correspond to the order in which they become available as the disk size decreases. First, only the very symmetric configuration 1 is allowed as soon as the radius r_1^* is small enough for the disks to fit. As the disk size shrinks, configuration 2 is allowed at a critical radius r_2^*, but *it is not possible to move from configuration 1 to 2 at that radius!* In fact, the four different orientations of the disks in configuration 2 are not connected either until the disks shrink to r_3^* and the four separate classes all become one class, still separated from configuration 1. And so this pattern continues: as the radius shrinks below r_4^* configurations 1-4 are all in the same part of phase space and any configuration can become any other configuration. Counterintuitively, at a still smaller r_5^* a **new** class of configurations appear that are not connected to the others, an island of configurations that only upon further reduction of the radius combines with the other configurations.

Not only is this surprising, but it suggests that the jamming transition may proceed through a cascade of ergodicity-breaking changes in phase space. Compare this to the Ising model where the order-disorder transition is characterized by breaking the phase space into two disconnected pieces (up and down) in the thermodynamic limit. Can we learn something from only *five* disks? Recall that the hard sphere melting transition can be (and was) ascertained with only 32 spheres [3,4]. Like the disks, we are getting close.

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[2] T.C. Hales, Annals of Math. **162** (2005) 1063; T.C. Hales and S.P. Ferguson, Discrete Comput. Geom. **36** (2006) 21.
[3] W.W. Wood and J.D. Jacobson, J. Chem. Phys. **27** (1957) 1207.
[4] B.J. Alder and T.E. Wainwright, J. Chem. Phys. **27** (1957) 1208.