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LETTER TO THE EDITOR

Is a local description of stable 2D random packing possible?

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Abstract. Local models of stable 2D random packing by Williams and by Uhler and Schilling are discussed in terms of car parking and equilibrium fluid 1D distributions. A numerical simulation of a simple 2D model is also presented, whose results are different from the previous two. It is concluded that those simple-minded approaches to the problem of random 2D packing are questionable and accurate answers to the problem will have to come from more realistic models.

In a recent paper (Burgos and Bonadeo 1986), we have discussed the behaviour of periodic one-dimensional systems of hard rods, characterising the differences between an equilibrium fluid and a system where the sample is generated by sequential introduction of rods whose position has been randomly chosen, corresponding to the so-called car parking problem (CPP). It was shown that for the CPP the successive rods 'remember' the order in which they were introduced in the sample, say i , and different radial distribution functions $G_i(R)$ appear. In the equilibrium fluid (EF) the distribution of points in the configuration space of the rod's positions is uniform, whereas the conditional probabilities for successive rods destroy this uniformity in the CPP.

The random packing of equal 2D discs has been studied by a series of authors (Bideau *et al* 1983, Onoda and Liniger 1985, Wojciechowski *et al* 1981) and, in particular, the stability of these packings within the framework of a local cluster description is discussed in two very recent letters (Williams 1985, Uhler and Schilling 1985).

The systems under study are defined as n -clusters, composed of a central disc with n contacting neighbours; the central disc is considered to be stable if it cannot be moved without moving its neighbours. The stability of these n -clusters is supposed to represent that of the whole assembly of discs in a mean-field type of approach. It is immediately seen that the problem of the n -cluster is trivially mapped into that of a one-dimensional periodic system of hard rods, with period 2π and the length of the rods $\sigma = 2\pi/6$. It is clear that all clusters with $n < 3$ are unstable, some three-clusters are stable and some are not, all four- and five-clusters are stable; six-clusters are possible, but have zero probability of occurring in a random process, as do unstable four-clusters. The aim of this letter, which is to find the mean coordination number of the stable clusters, is achieved by counting the number of three-, four- and five-clusters or equivalently calculating the corresponding probabilities.

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We will now briefly describe the contents of the two aforementioned letters. The reasoning of Uhler and Schilling (1985) goes as follows: let us consider three-clusters first: the unstable ones will be transformed necessarily, by definition, into four-clusters. Of the stable ones, it is possible to calculate the probability of a *radially* incoming disc to get to the central one without touching those around it; the corresponding fraction will also transform into four-clusters; the same procedure is repeated to calculate the fraction of four-cluster which will transform into five-clusters. These authors impose the condition that, at each stage, the peripheral discs are uniformly distributed, equating this to maximum randomness. As a result they calculate the ratio of stable to unstable three-clusters to be $P_s/P_u = 2$ and obtain the probabilities for finding an n -cluster, P_n , as

$$P_3 = 0.592 \quad P_4 = 0.399 \quad P_5 = 0.009$$

leading to a mean coordination number $n_c = 3.416$.

Williams (1985) only considers the ratio of stable to unstable three-clusters to obtain a lower bound to the coordination number r_{\min} . To do this, he calculated the conditional probability of, once the two first peripheral discs are located, a third radially incoming one stabilising the cluster or not. Had he not miscounted the configurations, he would have gotten $P_s/P_u = 2.18$ and $r_{\min} = 3.314$. All these facts were correctly recognised by Uhler and Schilling.

It is clear that, at each stage, Uhler and Schilling condition the sample to have a one-dimensional equilibrium fluid distribution: it is easy to obtain their results by using the corresponding radial distribution functions (Burgos and Bonadeo 1986). The procedure of Williams, instead, corresponds to the sequential CPP. If we assume that at each stage the peripheral discs follow the CPP distribution, we may follow the steps to calculate the probabilities for the n -clusters as above by using the corresponding radial distribution functions, given by Burgos and Bonadeo. We obtain

$$P_3 = 0.6342 \quad P_4 = 0.3592 \quad P_5 = 0.0066 \quad n_c = 3.3724.$$

It could be discussed whether EF or CPP are more 'random' systems, and in any case the results are not that much different; one would have to decide from physical arguments to what extent the relaxation occurs by which equilibrium is attained. But it is our opinion that the whole procedure is inconsistent and physically unrealistic.

Let us now imagine how such a cluster, either equilibrium fluid or sequential CPP, would be constructed or numerically simulated. We start with two peripheral discs; a third one comes in, radially, from a random direction. If it hits an existing disc, it bounces off and new random discs (or numbers in the simulation) are generated until one gets to the central disc; the three-cluster is shaken to attain equilibrium for EF or left as it is for CPP. Now we look to see if it is stable or not; if it is, we just try to add one more disc. If this one fits, we have a four-cluster; if it does not, the three-cluster is left alone forever. The unstable three-clusters, instead, are bombarded until a fourth disc finds its way in; all four-clusters are shaken for EF or left as they are. To decide if a four-cluster gets to be a five-cluster, we just try once to see if a random disc does or does not hit an existing peripheral one.

The description above reflects exactly the assumption of the models but in our view clarifies their inconsistency: in the EF, for instance, the clusters are completely relaxed, by definition. Instead they behave as completely rigid in accepting additional discs or not—except if they are unstable; in both EF and CPP, the clusters have just one chance of growing. Once it has passed, they remain as they were. Why do they not

have a second, a third, maybe a twenty-seventh chance? Of course, by trying hard enough, all (local) clusters, in this picture, would eventually get to be five-membered, which is known to be the wrong answer.

Uhler and Schilling (1985) consider that the mean coordination number they arrived at, $n_c = 3.416$, is an upper bound because of non-local effects caused by hindrances originated in non-adjacent discs. We have made a numerical simulation of another simple local model. In this model, successive randomly generated discs are directed radially towards the central one; the system is completely rigid, and the incoming discs stick to the first disc they come into contact with, staying at this place and therefore partially shielding the central one. In this picture, one- and two-clusters are possible, macroscopic stability being provided by the environment. Our simulation with 40 000 samples yields the following results:

$$P_1 = 0.000 \quad P_2 = 0.029 \quad P_3 = 0.464 \quad P_4 = 0.476$$
$$P_5 = 0.031 \quad n_c = 3.510 \pm 0.010.$$

The model is at least internally consistent and two dimensional, but certainly not physically realistic: the most obvious shortcoming is the rigidity of the systems. In this sense, $n_c = 3.51$ should be considered a *lower* bound, because relaxation should allow more discs to reach the central one.

In conclusion we believe that simple-minded models, including the last one, give results of questionable value at best: we know that the coordination number must be between 3 and 4. Accurate answers will have to come from more realistic models, probably based on molecular dynamics-like calculations.

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