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Universal properties of Voronoi tessellations of hard discs

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Abstract. We describe a 2D mosaic obtained by the Voronoi tessellation of a monosize assembly of discs at different packing fractions. The experimental device (hard discs moving on an air table) produces, for every packing fraction, a succession of mosaics in statistical equilibrium, which constitutes a statistical ensemble. This ensemble is large enough for fluctuations from the most probable distributions to be negligible. We use the maximum entropy principle to get the distribution of the polygons in 2D mosaics generated from an assembly of hard discs. Steric exclusion yields an extra conservation law, which is sufficient to give a good agreement with the experimental data. A similar behaviour in the six-fold parameter seems to hold for other mosaics.

1. Introduction

Bidimensional mosaics have been extensively studied because of their importance in metallurgy (grain aggregates), biology (tissues), geology (fracture patterns, jointings), etc. Their structure is, to first order, universal, apart from a length scale specific to the physical system, and is the archetype of a random, space filling cellular pattern or froth (Weaire and Rivier 1984). As in statistical mechanics, a particular dilute gas at a particular instant is one representative of an ensemble, the ideal gas under given macroscopic conditions; here, a particular mosaic is a representative of a statistical ensemble. The problems are how to extract from a few, often small samples, the average properties of the ensemble and the distribution of microstates, and how to explore the whole ensemble to minimize or control fluctuations within the ensemble. The last problem has so far only been solved on the computer, by Monte Carlo simulations (Peshkin *et al* 1991 and references therein). This paper presents an experimental solution to these problems, and extracts some conclusions on the characteristics of the ensemble. The method is new, and should lead to reliable conclusions once a large set of data has been collected.

Bidimensional mosaics can be represented in a simplified way by convex polygons covering the plane and their general properties are described in a satisfactory manner with few characteristics of the constitutive n -sided polygons; typically we need:

- the relative frequency p_n ($n \geq 3$) of n -sided polygons: practically, p_n is maximum for $n \approx 5-6$, then decreases monotonously at larger n ;
- the average number of sides $m(n)$ of the nearest neighbours of n -sided polygons, which appears to be a linear function of $1/n$ (Aboav's law, Aboav 1980);

• the average area A_n of n -sided polygons. In many cases, it was verified that A_n behaves linearly with n

$$A_n = A_0(n - n_0) \quad n \geq 3. \quad (1)$$

This is the well known Lewis law (Lewis 1928), which has been more or less justified in evolutive processes (Weaire *et al* 1986).

Actually, the Lewis law is not the only possibility and in the present paper we shall show a mosaic issued from a tessellation in an assembly of hard discs where steric exclusion is responsible for a different behaviour. In that case (Lemaître *et al* 1992a), A_n is well fitted by

$$A_n = an + b + c/n \quad (2)$$

where a , b , c are constants. The extra $1/n$ term is not a small correction and it is precisely that term which allows us to get most quantities of interest, such as the p_n or variance μ_2 . In the next section, we explain how our mosaics are made, how they are continuously changing while remaining in statistical equilibrium, and present our mosaics and their experimental characteristics. In section 3, we recall the Rivier-Lissowski approach (MAXENT principle) (Rivier and Lissowski 1982, Rivier 1992) and show how it works in our case. In the last section, we compare those results to our experimental data and initiate a brief discussion on hidden constraints.

2. Disc assemblies

Our mosaics are Voronoi-Dirichlet tessellations obtained from monosize hard discs assemblies. Discs are set on an air cushion table (Lemaître *et al* 1990); they rearrange permanently because of the air flow through the table and small local defects of the table, and after a short thermalization time, we get a homogeneous assembly, which may be thought of as a particle gas. We explore the ensemble by taking successive snapshots of the structure (figure 1) which, although in statistical equilibrium, moves permanently. The tessellation is derived by tracing the mediator line between two neighbour discs (figure 2): each disc is then the centre of a convex polygon made of

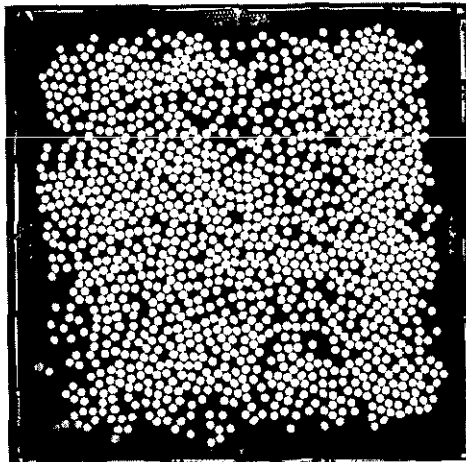


Figure 1. Experimental system: equal disc packing on an air table.

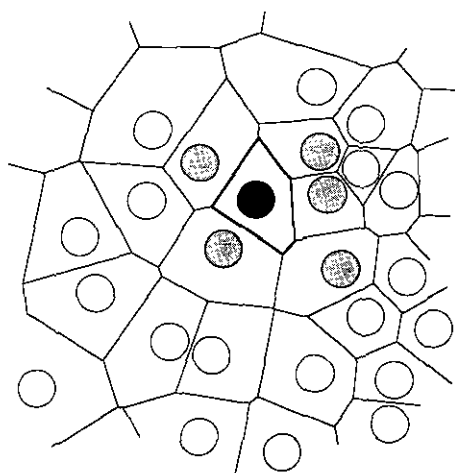


Figure 2. Voronoi tessellation: grey discs are near neighbours of the central black disc, which is represented by a Voronoi polygon with $n=5$ sides. For this central disc, $nm(n) = 5m(5) = 32$ (Lemaître *et al* 1992a).

such mediator lines and the polygon contains completely the particle. All quantities of interest, number of edges of the polygon, number of edges of the near neighbours, perimeters, lengths and areas are derived by using an image treatment analysis.

For our cells, it was shown (Lemaître *et al* 1992a) that the Lewis law *does not hold* even at rather small coverage ($C \geq 20\%$). The average area A_n is not a monotonously increasing function of n , but shows a minimum for $n \approx 5-6$ which is more pronounced for compact systems (figure 3). Steric exclusion is responsible for such behaviour as a n -polygon cannot have an area less than that of the regular n -polygon circumscribing the disc: triangles and quadrilaterals need more room than pentagons or hexagons, whence the minimum close to $n = 5-6$; $n = 6$ corresponds to the regular arrangement around the centre disc. For $n > 6$, the area increases again as the smallest distance must increase to allow the possibility for new neighbours. When n is large ($n = 9-10$), the central disc plays a less important role and as in previous experiments, A_n grows linearly with n .

To support our results, we have performed another analysis on numerical assemblies of hard discs built using the random sequential adsorption (RSA) procedure (Feder 1980, Feder and Giaever 1980): the centre of a disc is chosen at random in a given area and if it does not overlap an already deposited disc, it is definitely deposited and fixed. This algorithm is very different from the experimental particle gas as no reorganization is possible. Nevertheless, steric exclusion is again the determinant factor. In RSA mosaics, the Lewis law is violated but in a less spectacular way and at higher concentrations. In both cases, a correct approximation is given by expression (2); the linear term corresponds to the large n behaviour and the last term is the simplest, but not unique, possibility to get an extremum. It fits well our experimental data.

We must emphasize the peculiar characteristics of our mosaics: first, steric exclusion plays a fundamental role, which is not the case in the usual examples where small cells are always possible (see for example the foams by Aboav 1980). Second, the number of cells remains constant in time: we are in the presence of a non-evolving process, probably in thermodynamical equilibrium. The impossibility of destroying or

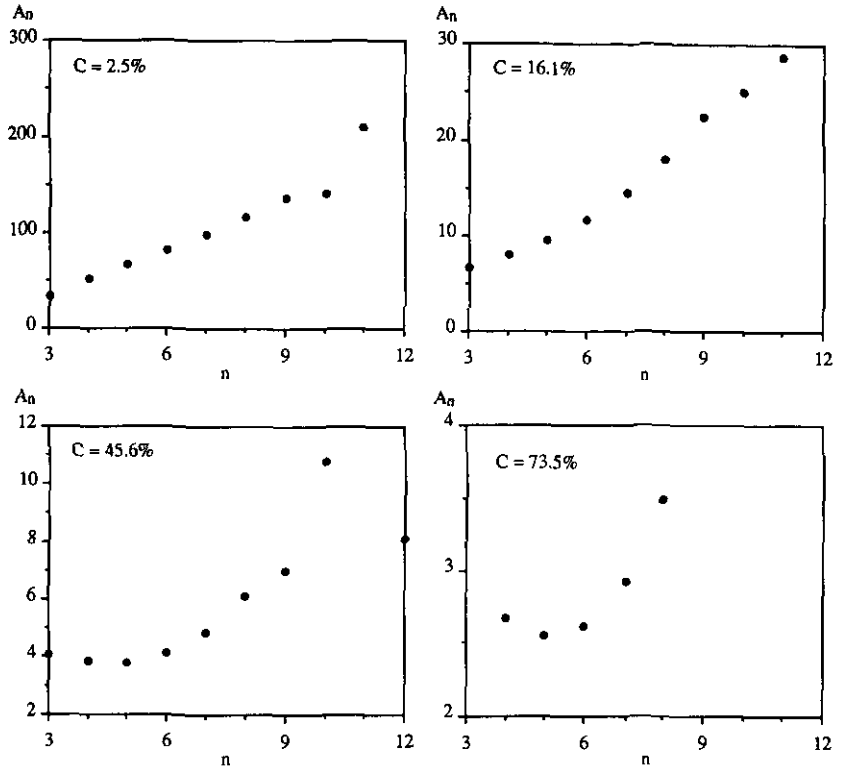


Figure 3. Plot of the average area A_n versus n at four concentrations: $C = 2.5\%$, $C = 16\%$, $C = 45.5\%$ and $C = 73.5\%$.

creating cells is probably not as important as was sometimes claimed in the literature: it has recently been shown that the Lewis law is violated too during the coalescence process of breath figures (Steyer *et al* 1990). In this nice experiment, the number of cells decreases but the total quantity of matter is preserved.

3. MAXENT principle

We first recall how the distribution p_n of the edges can be derived from entropy requirements, then show how it applies in our hard core systems.

3.1. Rivier-Lissowski approach

Rivier and Lissowski (1982) have associated with the probability distribution p_n an entropy

$$S = -\sum_n p_n \ln p_n. \quad (3)$$

The choice of this form relies on a hidden statistical hypothesis, namely the assignment of equal *a priori* weights to each value of n . It is then natural to determine the p_n by assuming that S is maximum provided all known conservation laws or constraints are taken into account (MAXENT principle).

We have the two straightforward conservation laws

$$\sum_n p_n = 1 \quad (\text{normalization}) \tag{4a}$$

$$\sum_n n p_n = 6 \quad (\text{the average number of edges is 6}). \tag{4b}$$

This last identity is a consequence of the Euler theorem when three and only three lines occur at the same vertex, which is here the generic situation (it is the rule in tessellations). In our case, the six-fold axis is especially important as it corresponds to the ordered array and to the maximum number of close contacts. Further on, we have a constraint on the total area

$$\sum_n A_n p_n = A_0 \quad (\text{fixed average area}). \tag{5}$$

Other constraints probably exist, for example related to the short-range correlations and to the Aboav law (Aboav 1980), but no simple formulation for them is known. Assuming that such an additional constraint may be written in a similar way,

$$\sum_n f_n p_n = f_0 \tag{6}$$

where f_n is some function depending on the geometry or dynamics of the mosaics, Rivier and Lissowski have shown that the least biased distribution of the polygons has the form

$$p_n = K^{-1} \exp(-\lambda n - \mu A_n - \nu f_n) \tag{7}$$

where K is a normalization constant and λ, μ, ν are the Lagrange multipliers issued from conditions (4)-(6). Maximization of entropy with three constraints is possible only when at least four types of polygons are present. If we have only pentagons, hexagons and heptagons, partially ordered zones exist and the entropy is not a maximum. Actually, octagons ($n=8$) are always present, even weakly.

If the Lewis law is satisfied, condition (5) is automatically fulfilled as a consequence of (4b) and the parameter μ may be set equal to zero. This is the most common situation, and unfortunately it is not a simplification: as the probability p_n is not a monotonic decreasing function of n for n small, a supplementary hidden condition (6) must exist and one fundamental problem is then to find it.

If the Lewis law *does not hold* and if the conditions (4)-(5) alone are sufficient to get a correct fit for the p_n , the possible hidden condition (6) becomes irrelevant since it is a consequence of conditions (4)-(5), in particular of the law (5) which replaces the Lewis law. We shall rely below on that idea.

3.2. Application to hard core systems

Coming back to our own mosaics, the Lewis law is replaced by expression (2) for A_n which implies the constraint

$$\left\langle \frac{1}{n} \right\rangle = \sum_n \frac{1}{n} p_n. \tag{8}$$

Let us assume that no further constraint exists. Then the probability for an n -polygon reads

$$p_n = K^{-1} \exp\left(-\lambda n - \frac{\nu}{n}\right) \tag{9}$$

where K , λ , ν are determined from (4a), (4b) and (8). The explicit determination of these parameters is not necessary to get p_n or related quantities such as the entropy (equation (3)) or the deviation to the hexagonal configuration

$$\mu_2 = \langle n^2 \rangle - \langle n \rangle^2 \quad (10)$$

both quantities being measures of the dispersion of the law p_n . Technical points and expressions in term of two (related) parameters are given in the appendix.

4. Results and discussion

We have represented all the quantities introduced above in terms of the probability of presence of hexagons, i.e. in term of p_6 . This parameter plays a central role in our analysis because the average number of neighbours is six and p_6 is (in general) the largest probability; moreover, in our specific case (monosize discs) it is a measure of the importance of six-fold symmetry. Another possibility would be to use as a parameter, global quantities such as S or μ_2 but they are less sensitive, precisely because they are averages. Such measurements were reported in a companion paper (Lemaître et al 1992b).

In figure 4 we have plotted μ_2 as a function of p_6 for our hard core experimental data, and as derived from the MAXENT principle with the constraint (8) implied by the expression (2) for A_n in the case $n = 4$ to 10. The agreement is then fairly good. The same has been performed for the entropy, with identical conclusions but we shall not consider it here. Similarly, we have plotted in figures 5a and 5b the ratios p_4/p_6 , p_5/p_6 , p_7/p_6 and p_8/p_6 . Again, experimental and theoretical results agree well for hard core tessellations.

The above analysis relies on the use of the law (2) instead of the Lewis law. Equivalently, one could make no hypothesis on the average sizes of the polygons, and introduce instead an additional geometric constraint (6) with the Ansatz $f_n = 1/n$. With

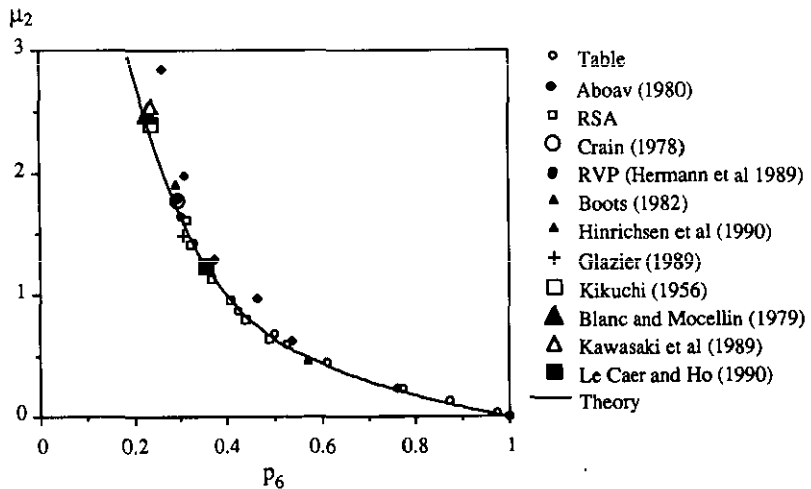


Figure 4. Variance μ_2 as a function of the percentage p_6 of hexagons for air table and RSA assemblies as compared to the theoretical expression (with $n = 4-10$ and $f_n = 1/n$). Representative points for other mosaics in the literature are indicated. They are roughly on the same curve, Aboav foams (Aboav 1980) excepted.

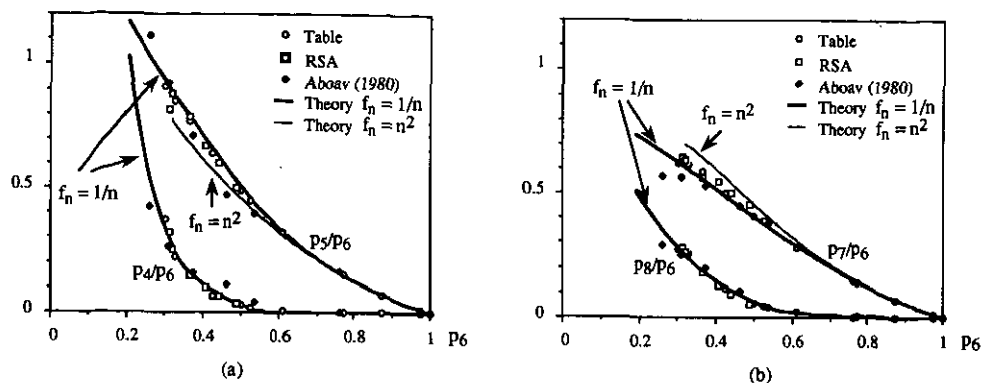


Figure 5. Plot of p_n/p_6 as a function of p_6 for air table and RSA assemblies compared to the theoretical variations for $f_n = 1/n$. (a) Plot of p_4/p_6 and p_5/p_6 . (b) Plot of p_7/p_6 and p_8/p_6 . The corresponding ratios for Aboav foams are given for comparison. Also are shown theoretical variations of p_5/p_6 and p_7/p_6 for $f_n = n^2$.

this viewpoint, we can try to fit the results existing in the literature with a law of the form (9). This was done in figures 4 and 5. It is worthwhile noticing that, once the nature (8) of the constraint is known (but not necessarily the numerical value), then all p_n are uniquely determined in terms of the single parameter p_6 —at the order of approximation which was fixed before. The plot of μ_2 versus p_6 is in some sense universal. This may explain why RSA and air table assemblies behave in the same way (Lemaître *et al* 1992b) and why the representative point for RVP polygons tessellation is also on the same curve, which is rather natural as they can be thought of as a low density limit for hard core systems (Lemaître *et al* 1992a, Hermann *et al* 1989). Data found in the literature for various bidimensional structures fit the curve too. This strengthens the idea that some universal features exist, at least for most mosaics. There is however an important exception, which is related to the foams generated by Aboav (1980) and analysed at different stages of the coalescence process: at long times, large n -cells are present. Another hidden law, ‘stronger’ than the $1/n$ constraint, probably exists, which should account for the wider spread in the distribution.

A question then arises, which it would be interesting to answer. Why does $f_n = 1/n$ work so well and even for systems where the Lewis law holds, like RVP polygons?

Another possibility remains that the quantities studied are not very sensitive to the choice of f_n . We have performed several trials: power law ($f_n = n^\lambda$ with negative and positive exponents), logarithm law ($f_n = \ln n$ or $f_n = \ln(n-2)$, which is Rivier’s guess (Rivier 1985)) or exponential law ($f_n = \exp(\pm n)$). In most cases, the plot of μ_2 is in good agreement with the experimental data. This may be explained by the common shape (convex or concave monotonous curves) of all functions f_n , and by the corresponding slow change in the exponent δ (see appendix) for all these laws; moreover, in the calculation of the variance μ_2 , compensations probably exist. With the quantities p_4/p_6 , $p_5/p_6 \dots$, it is really possible to distinguish between the constraints and the best fit of experimental data is obtained with $f_n = 1/n$: for example, as shown in figure 5, a law such as $f_n = n^2$ gives, for p_5 and p_7 variations, more symmetry than observed experimentally. More fundamentally, is the choice $f_n = 1/n$ related to the $1/n$ expansion in the Aboav law for nearest neighbours which seems up to now to be universal, even if the slope itself is not always close to 5 (Steyer *et al* 1990, Peshkin *et al* 1991)?

5. Conclusion

We are able to produce experimentally with our discs on the air table, mosaics which are representative of an ensemble of froths in statistical equilibrium. We obtain distributions and properties for this ensemble, notably the distribution p_n of the number of sides for each cell. We have shown that a maximum entropy principle gives a good account of the distribution p_n of the sides and of related quantities, provided the average $\langle 1/n \rangle$ is fixed. The fit remains good in many situations described in the literature, even though the Lewis law may hold. The constraint on $f_n = 1/n$ is probably a deeper condition than expected.

A more detailed study should be undertaken, to see whether other classes of constraints may exist, as seems to be the case for Aboav foams.

Acknowledgments

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Appendix

The technical aim consists of replacing parameters λ and ν in (8) by variables easier to handle. The method holds for any constraint f_n . Starting from $p_n = K^{-1} \exp(-\lambda n - \nu f_n)$, we first rewrite (4b) as

$$\sum_n (n-6) \exp[-\lambda(n-6) - \nu(f_n - f_6)] = 0 \quad (\text{A1})$$

where the central role of $n=6$ is clearly put in evidence. Then, the contribution of pentagons and heptagons is made more 'symmetric' by multiplying both sides of (A1) by

$$\exp[-\nu(2f_6 - f_5 - f_7)/2]$$

so that $n=5$ and $n=7$ contribute with inverse terms $e^\lambda e^{-\nu(f_5 - f_7)/2} = Y$ and $e^{-\lambda} e^{\nu(f_5 - f_7)/2} = Y^{-1}$ respectively. Substituting Y in λ and ν , we get

$$\sum_n (n-6) Y^{6-n} e^{-\nu \rho_n / 2} = 0 \quad \text{with} \quad \rho_n = (n-6)(f_5 - f_7) + 2f_n - (f_5 + f_7) \quad (\text{A2})$$

and by construction $\rho_5 = \rho_7 = 0$. Now, as octagons usually occur before quadrilaterals, we particularize $n=8$ by setting $Z = e^{-\nu \rho_8 / 2}$ and rewrite condition (A1) in its final form as

$$\sum_n (n-6) Y^{6-n} Z^{\rho_n / \rho_8} = 0. \quad (\text{A3})$$

With this substitution, all quantities are rewritten in terms of Y and Z (as calculated from A3). We have,

$$\begin{aligned} p_n &= [Y^{6-n} Z^{\rho_n / \rho_8}] / \Delta \\ \mu_2 &= \left[\sum_n (n-6)^2 Y^{6-n} Z^{\rho_n / \rho_8} \right] / \Delta \\ \Delta &= \sum_n Y^{6-n} Z^{\rho_n / \rho_8} \end{aligned} \quad (\text{A4})$$

where Δ is the normalization factor. Given Y , we get Z through (A3) then deduce all relative frequencies, and related quantities. As an example, for $f_n = 1/n$, the exponents are respectively $\rho_4/\rho_8 = 2$, $\rho_6/\rho_8 = -4/9$, $\rho_9/\rho_8 = 64/27$, ... The negative value for $n = 6$ is in agreement with the existence of hexagons at any concentration, while other polygons appear successively: first $n = 5$ and 7, then $n = 8$, and $n = 4$ a little later. This constation may be extended to any concave (or convex) function f_n .

As an example, let us write explicitly the solution when only $n = 4-9$ polygons are represented. Equation (A3) is rewritten

$$2Y^2Z^\alpha + Y - \frac{1}{Y} - 2\frac{Z}{Y^2} - 3\frac{Z^\gamma}{Y^3} = 0 \quad \alpha = \rho_4/\rho_8, \gamma = \rho_9/\rho_8$$

and a solution exists for $Y > 1$ ($Z = 0$ if $Y = 1$). Then

$$\begin{aligned} p_4 &= Y^2 Z^{\alpha+\delta} / \Delta' & p_5 &= YZ^\delta / \Delta' & p_6 &= 1/\Delta' \\ p_7 &= Z^\delta / Y\Delta' & p_8 &= Z^{\delta+1} / Y^2\Delta' & p_9 &= Z^{\gamma+\delta} / Y^3\Delta' \\ \mu_2 &= Z^\delta [Y + Y^{-1} + 4ZY^{-2} + 4Y^2Z^\alpha + 9Z^\gamma Y^{-3}] / \Delta' \end{aligned}$$

with $\Delta' = \Delta Z^\delta = 1 + Z^\delta [Y + Y^{-1} + ZY^{-2} + Y^2Z^\alpha + Z^\gamma Y^{-3}]$ and $\delta = |\rho_6/\rho_8$.

A better approximation consists in taking p_{10} into account. The corresponding approximation is shown in figures 4, 5a and 5b.

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