Eur. Phys. J. E 7, 123–127 (2002)
DOI 10.1140/epje/i200101168

The European Physical Journal E

EDP Sciences

Uniqueness, stability and Hessian eigenvalues for two-dimensional bubble clusters

D. Weaire[1], S.J. Cox[1,a], and F. Graner[2,b]

[1] Department of Physics, Trinity College, Dublin 2, Ireland
[2] Laboratoire de Spectrométrie Physique, Boîte Postale 87, F-38402 St. Martin d'Hères Cedex, France

Received 8 November 2001

Abstract. A recent conjecture on two-dimensional foams suggested that for fixed topology with given bubble areas there is a unique state of stable equilibrium. We present counter-examples, consisting of a ring of bubbles around a central one, which refute this conjecture. The discussion centres on a novel form of instability which causes symmetric clusters to become distorted. The stability of these bubble clusters is examined in terms of the Hessian of the energy.

PACS. 82.70.Rr Aerosols and foams – 46.32.+x Static buckling and instability

1 Introduction

In the course of a fresh approach to the description of the structure of a foam and its rheological properties, [1] advanced the following conjecture: A dry two-dimensional foam of specified topology and bubble sizes should have a unique equilibrated structure corresponding to a unique local minimum of energy. Structures related by exact symmetries (translation, rotation or reflection) are excluded.

This conjecture is here refuted by counter-example. We shall describe structures that are metastable states corresponding to local energy minima; they can (and will) have different values of energy. Note therefore that we do not discuss the global energy minimum, or ground state, with either free or fixed topology.

We must consider two possible boundary conditions; firstly a fixed-boundary condition, where we may choose a closed loop in the plane and fill it with bubbles. The counter-example in this case is trivial, and is described briefly in Appendix A. More interesting is the free-boundary case. In the next section we give examples where two or more stable equilibrated structures exist with different bubble *shapes*, but with the same *areas* and *topology*, for this free-boundary case. Note that we seek an example other than the degenerate ones typified by a chain of three bubbles, in which different shapes with the same energy are obtained depending upon, for example, whether the bubbles' centres are co-linear or not.

These examples lead to the consideration of a family of 2D clusters of cells, which we have simulated using the Surface Evolver [2]. In Section 3 we explore the details of these clusters and in Section 4 we examine their stability, primarily by calculating Hessian eigenvalues and identifying those which are associated with incipient instability.

2 Non-unique geometry with free boundary conditions

We seek a free bubble cluster which has the property that alternative minima exist for given topology and bubble areas. The underlying idea which we have used is that a chain of bubbles under compression should exhibit symmetry-breaking instabilities, leading to multiple minima. It is most convenient to arrange such a chain in a ring around a single central bubble whose area can be gradually reduced to achieve the desired compression.

Figure 1a shows such a configuration as simulated with the Surface Evolver [2], for the case of ten bubbles with equal areas. More details of this method are given below. In fact this symmetric configuration is simple enough to be found analytically.

The obvious equilibrium configuration shown in Figure 1a has ten-fold rotational symmetry, but as the central area is reduced it exhibits the expected instability in the form of a symmetry-breaking transition in which the central bubble becomes elongated, shown in Figure 1b. Note that the topology is unaffected by this transition, provided that it is not pursued too far. Also, the minimum shown is one of a several which have similar energy, corresponding to distortion in different directions; another example is shown in Figure 1c.

The conclusion is therefore that the conjecture fails, and not just for singular special configurations. It may

[a] e-mail: simon.cox@tcd.ie
[b] CNRS UMR 5588 & Université Grenoble I.

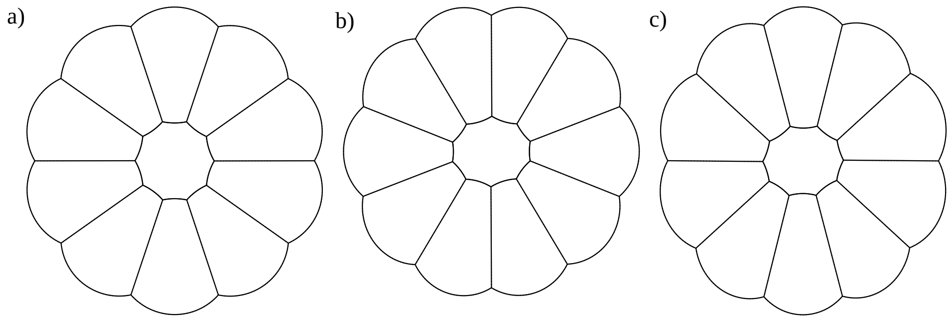

Fig. 1. Different configurations for a two-dimensional bubble cluster with ten "petals" of unit area around a central bubble. a) With the central area at $A_c = 0.7$, the symmetric, circular configuration is stable. b) Putting $A_c = 0.65$ gives a stable elliptical cluster instead. However, there are many possibilities for the configuration which results from the instability; another example is shown in c). Panel c) cannot be obtained from b) by either rotation or reflection.

be wondered how it arose in the first place. The conjecture seemed reasonable because computer simulations of foams, typically with one hundred cells [3,4], have been examined in the past to see whether they exhibited multiple minima when subjected to random perturbations, but such minima were never found. It seems that typical foam samples under periodic boundary conditions do not readily exhibit more than one minimum, but this could be well worth revisiting now. It should be possible to find rare examples of multiple minima.

Additional details of our calculations on these unusual configurations of free clusters are presented below. We describe in greater detail the onset of instability (Sect. 3) and analyse the instability in terms of the energy Hessian (Sect. 4).

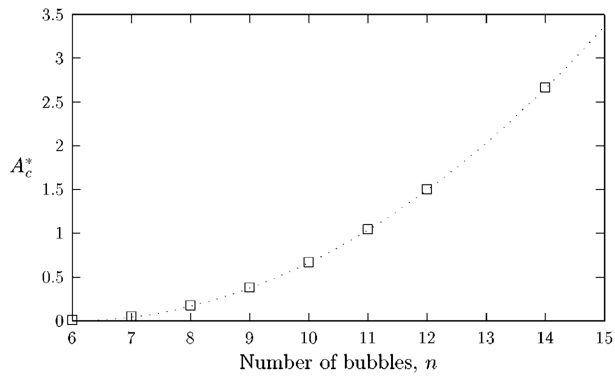

Fig. 2. The critical area of the central bubble at which the instability occurs is plotted against the number n of bubbles in the ring. Also shown is the power law fit, given by $A_c^* = 0.0415(n-6)^2$. For these data the bubble area is $A = 1$.

3 Surface Evolver calculations

We have made extensive use of the Surface Evolver [2], a software package which can find minimal energy configurations, subject to certain constraints. It has been used elsewhere in the study of instabilities of bubble clusters, for example by [5].

For the two-dimensional case described here, consisting of n ring-bubbles, or "petals", surrounding a central bubble, we create an initial configuration consisting of $2n$ vertices joined by straight lines, with defined bubble topology, and then use the Evolver, with quadratic mode and four levels of refinement, to minimise the edge length subject to the given bubble areas.

In our calculations the free-boundary buckling instability occurs whenever the ring contains more than six equal sized petals (of area A). It is not immediately clear why the instability should only show itself for $n > 6$. We start from an initial configuration in which the central bubble is large enough that the buckling will not occur. Then we use the following procedure: the area of the central bubble is reduced by a small amount, and then the new minimum energy structure is found. If the system is still rotationally symmetric (we describe below a way of measuring this symmetry) we perturb it by making small random changes to the positions of the vertices. (Without such perturbations, the symmetric state may persist because the numerical calculation is stuck at a saddle point.) The structure is next evolved to its minimum energy. If this leads to buckling then we have reached the critical bubble area at which the symmetric minimum configuration becomes unstable. Otherwise we repeat the procedure and further reduce the area of the central bubble.

In Figure 2 we show the critical area of the central bubble, A_c^*, at which an n-sided ring (*i.e.* with n petals) is unstable, as a function of n. This is for fixed ring-bubble area $A = 1$. The results are fitted extremely well by

$$A_c^* = 0.0415(n-6)^2 A. \tag{1}$$

Thus the instability is found for $n > 6$ only. It seems that the case $n = 6$ plays a special role here, on the margin of stability. In attempting to explain this, we note that the instability is found at precisely the minimal energy of the cluster as a function of central area, as shown in Figure 3. Such a minimum is found only for $n > 6$; thus the cluster is only able to reduce its energy by buckling for $n > 6$. After buckling, as A_c is further decreased, the energy of the deformed cluster remains constant as it becomes more elliptical. It is interesting to note that we might have expected the case $n = 6$ to be stable, since a hexagonal

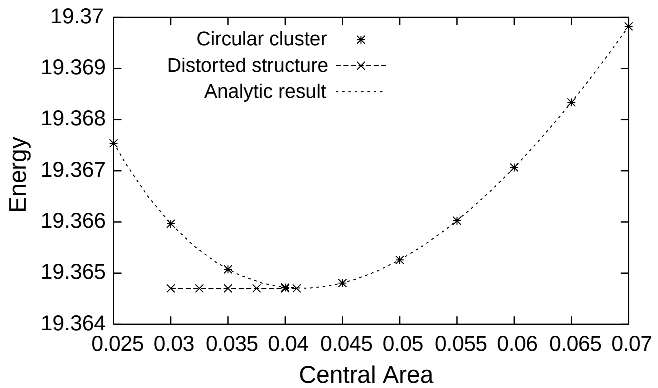

Fig. 3. The variation in energy of a cluster with seven petals ($n = 7$) as the area of the central bubble is decreased. Surface Evolver calculations show excellent agreement with the analytic result for the symmetric cluster. Below the critical point at $A_c^* \approx 0.04$, the energy of the distorted cluster is constant, while the energy of the metastable circular cluster increases steeply. Surface tension is equal to one.

bubble in a cluster of constant total area can change its area without changing the total energy. The energy curve shown in Figure 3 exhibits qualitatively similar behaviour to the energy of a buckling regular honeycomb [6]. Our analysis, based on the above ideas and the method given in [1], shows that a minimum in energy is attained only for $n > 6$, at a value of central area given by

$$A_c^{\min} = A\left(\frac{1}{3}+\frac{\sqrt{3}}{2\pi}\right)^{-1}\left[\frac{n}{2\pi}\frac{\sin(\pi/6-\pi/n)}{\sin(\pi/n)}+1-\frac{n}{6}\right] \quad (2)$$

with which the fit in (1) shows excellent agreement. As A_c is decreased below this value, the perimeter of the central bubble remains constant, forcing the symmetry to break.

Note that the value of A_c^* is easily estimated by using the "target" diagram of Figure 4 to calculate areas and perimeters, leading to the formula

$$A_c^* = \frac{1}{8\pi}(n-2\pi)^2 A. \quad (3)$$

This is quite close to the empirical formula (1): the exponent 2 is the same, the offset is 2π rather than 6 because of the circularity, and the prefix $(8\pi)^{-1} = 0.0398$ is very close to the empirical 0.0415.

As a measure of the magnitude of the distortion due to the buckling instability, we shall use an eccentricity parameter defined as follows. Given the positions of each vertex (x_i, y_i), with origin at the centre of the ring, we calculate the 2×2 moment of inertia matrix

$$\begin{pmatrix} \sum_i x_i^2 & \sum_i x_i y_i \\ \sum_i x_i y_i & \sum_i y_i^2 \end{pmatrix}.$$

We diagonalise this matrix to find the principal moments λ_1 and λ_2. The eccentricity is then defined to be the normalised difference: $(\lambda_2 - \lambda_1)/\sqrt{\lambda_1^2 + \lambda_2^2}$.

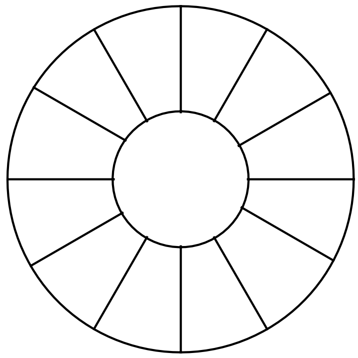

Fig. 4. This simple target model of a cluster (in this case for $n = 12$) can be used to estimate the critical area at which the minimum energy occurs. The annulus is divided into n petals of area A, and the cluster has energy $E = nR + 2nA/R$, where R is the width of the annulus. E is minimised when $R = \sqrt{2A}$, which gives the critical central area at which this minimum is attained.

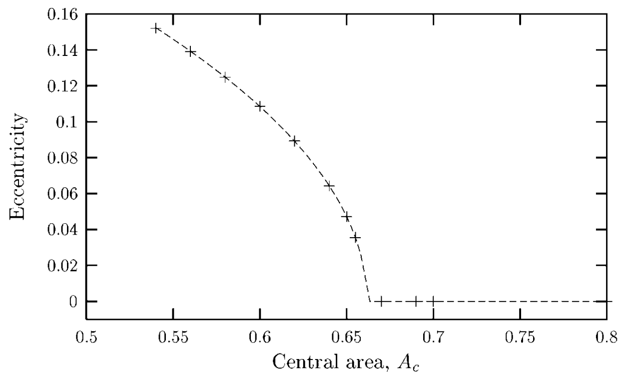

Fig. 5. A measure of the eccentricity of the system, as the critical bubble area is varied, using the difference of the principal moments of inertia. The results shown are for $n = 10$ and bubble area $A = 1$, with the points denoting the numerical results. As A_c is decreased, the configuration remains symmetric until the critical point $A_c^* \approx 0.661$ when the eccentricity increases with the square root of A_c (dashed line), in the classic manner of a supercritical bifurcation.

The results for the eccentricity of a 10-bubble ring are shown in Figure 5. The instability shows the typical square-root shape of such a bifurcation and this provides a confirmation of the critical point when the data are fitted to such a square root. It is not possible to pursue this curve to lower values of A_c indefinitely, because topological change occurs when the length of a side of the central bubble shrinks to zero.

The analogy with a compressed chain of bubbles is very suggestive. It indicates that there will be higher modes of buckling; following the elliptical elongation described above, there will be a triangular mode, then a square mode, and so on. We shall remark further upon these modes of instability in the next section. In future work we intend to provide an experimental demonstration of the instability, using the techniques described by [7].

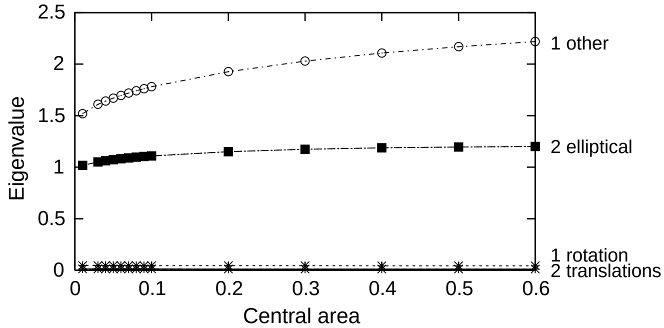

Fig. 6. The lowest six eigenvalues for a cluster consisting of six bubbles surrounding a central one ($n = 6$). Each eigenvalue (1), or pair of eigenvalues (2) is labelled on the right with the kind of distortion to which it corresponds. No eigenvalues descend to zero, so the cluster is stable for all values of the central area A_c.

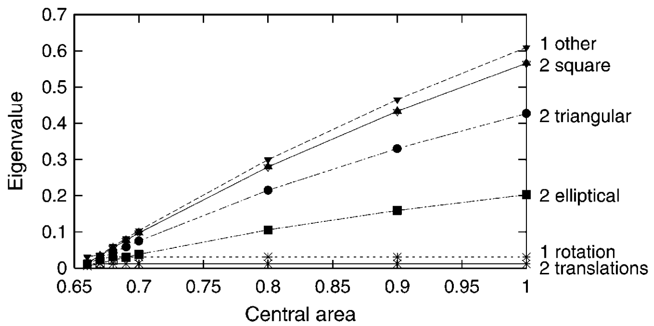

Fig. 7. The lowest ten eigenvalues in the case $n = 10$, for the cluster illustrated in Figure 1a. As for the case $n = 6$ (Fig. 6) there are three small constant eigenvalues (representing translations and a rotation) but the next seven eigenvalues all descend to zero as the central area is decreased (they exist in pairs, except for the highest one). This defines the critical point at which the cluster becomes unstable, $A_c^* \approx 0.65$.

4 Calculation of Hessian eigenvalues

The Surface Evolver program contains a facility for the calculation of the Hessian matrix and its eigenvalues. This is described by [8] and has been used by [9], for instance, to investigate the distortion associated with two non-coalescing droplets.

The Hessian is defined as the matrix of second-order partial derivatives of the energy with respect to the coordinates of the vertices (including those generated when refining the edges). Figures 6 and 7 present eigenvalues for two cases of interest: a ring with six petals and one with ten. It is immediately apparent that, for the case $n = 10$, which was previously identified as exhibiting instability when the area of the central cell was reduced to a critical value, many eigenvalues tend to zero at or close to this critical point. However, for $n = 6$, which exhibits no such instability, the eigenvalues remain positive. In each case there are three small, constant eigenvalues; these correspond to two translations and a rotation.

In the $n > 6$ cases one of the eigenvalues actually reaches zero and provokes the kind of distortion described earlier. In total there are $n-3$ eigenvalues that reach zero at, or close to, the critical point. The significance of the other $n - 4$ decreasing eigenvalues can be made clear by recognising that the relevant degrees of freedom are essentially the motions of the individual cells as a whole. If we think of the bubbles as interacting points, then we would expect the system to exhibit many "soft modes" tending to instability at much the same point. Because of this multiplicity of unstable modes, there is a corresponding multiplicity of distorted structures in equilibrium, within the unstable regime. Thus the energy landscape is much richer than that implied by the initial bifurcation of stable structures due to the first vanishing eigenvalue.

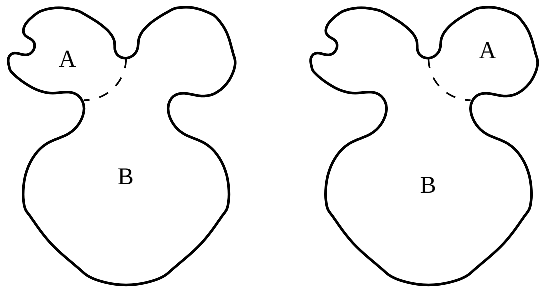

Fig. 8. In the fixed-boundary case we choose the boundary shape above to demonstrate the required counter-example. Bubble A can go in either of the two lobes, but in each case the topology is the same while the bubble shapes are different.

5 Conclusion

Although the initial impact of this work has been negative, since it was explicitly developed in order to refute the conjecture of [1], it now offers an interesting object of study in the instability of bubble clusters. This type of instability is new, and takes its place alongside others which are well known in the study of foams [10]. Similar clusters have been studied already, usually for equal sized bubbles; the present work points in a hitherto unsuspected direction and raises fresh questions regarding the simple relationships which we have found here. Moreover, we would also expect similar instabilities to occur in three-dimensions. It may well provide a useful model system for the study of bifurcation, energy landscapes and other aspects of nonlinear systems. Its advantages include a simple model and simulation procedure, an equally tractable experimental realisation, and rich possibilities for multiple minima when the procedure used here is taken further.

The authors wish to thank F. Morgan for advice and N. Kern, A. Kraynik and F. Vaz for useful discussions. SJC thanks C. Pittet, N. Pittet and G. Bradley for assistance with the Surface Evolver. SJC was supported by a Marie Curie fellowship and DW acknowledges financial assistance from the Ireland-France Exchange Scheme. FG thanks TCD for hospitality.

Appendix A. Non-unique geometry with fixed-boundary conditions

We describe briefly a counter-example to the conjecture that for given topology and a fixed boundary, the bubble geometry is unique. This is much easier than the free-boundary case, discussed in Section 2: indeed it is quite trivial —so much so that it does not require computation to provide a convincing demonstration. We are free to choose a boundary and then attempt to insert bubbles which can be arranged in configurations that differ in terms of geometry but not topology. We fill the region shown in Figure 8 with two bubbles, A and B, which have different areas. Then there are two possible shapes for A and B, although the topology remains unchanged.

References

1. F. Graner, Y. Jiang, E. Janiaud, C. Flament C., Phys. Rev. E **63**, 011402 (2001).
2. K. Brakke, Exp. Math. **1**, 141 (1992).
3. D. Weaire, J.P. Kermode, J. Wejchert, Phil. Mag. B **53**, L101 (1986).
4. J.P. Kermode, D. Weaire, Comput. Phys. Commun. **60**, 75 (1990).
5. S.J. Cox, D. Weaire, M.F. Vaz, submitted to Eur. Phys. J. E (2002).
6. S. Hutzler, D. Weaire, J. Phys. Condens. Matter **9**, L323 (1997).
7. M.F. Vaz, M.A. Fortes, J. Phys. Condens. Matter **13**, 1395 (2001).
8. K. Brakke, Philos. Trans. R. Soc. A **354**, 2143 (1996).
9. G. Bradley, D. Weaire, Comput. Sci. Eng. Sept/Oct, 16 (2001).
10. D. Weaire, S.Hutzler, *The Physics of Foams* (Clarendon Press, Oxford, 1999).