Elastic properties of an inhomogeneously diluted isotropic medium

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We have investigated the elastic properties of an inhomogeneously diluted isotropic medium described by means of a triangular network whose nearest-neighbor nodes interact through a central-force Hamiltonian, and its constitutents are removed with a probability that decreases with their distance to a given point. This model interpolates between the case of homogeneously distributed voids (percolation) and that of voids concentrated at the central zone of the system. The percolation transition in the inhomogeneous case is analyzed, and the results are interpreted on simple grounds.

The mechanical properties of disordered media is a subject of great current interest.[1] In particular, the effects of dilution have been intensively investigated on homogeneously diluted systems.[2–7] In this paper we shall investigate a situation in which matter is removed randomly but not homogeneously from the system; in particular, we shall assume that the constituents of the system are removed with a probability that decreases with their distance to a given point (radial inhomogeneity). This may be the situation in some cases of corrosion or wear, where the material suffers a damage which diminishes as a function of the distance to the zone where damage was originated. On the other hand, the percolation transition in this case might show interesting peculiarities.

Note that in all the studies of interacting percolation carried out up to now,[8] the assumed correlation between neighbors do also lead to homogeneously diluted media (in this case the media can be considered as being homogeneous at a scale larger than for the system with no correlations), whereas in this paper we shall consider correlations which are inherently inhomogeneous. Our model interpolates between those corresponding to voids concentrated at the central zone of the sample[5,6,9] and those for the case of homogeneously distributed voids. The numerical results are very satisfactorily fitted by means of a continuum model that accounts for the inhomogeneity of the dilution. On the other hand, the system does undergo a percolation transition which takes place at a fraction of removed matter $(1-p)$ which increases as the degree of inhomogeneity increases; the critical exponents seem also to be different from those of the homogeneous case. A more detailed analysis of the results reveals that this dependence of the critical properties on the inhomogeneity might only be apparent; in fact, if p is referred to the region of the sample that might be considered as being radially homogeneous, the critical parameters are very similar to those obtained in the homogeneous case.[3]

The system whose properties we shall be discussing consists of a triangular network made of identical Hookean springs; the corresponding Hamiltonian is

$$H=\tfrac{1}{2}\sum_{\langle i,j\rangle} k_{ij}[(\mathbf{u}_i-\mathbf{u}_j)\cdot\hat{\mathbf{r}}_{ij}]^2 , \tag{1}$$

where the sum runs over all nearest-neighbor nodes of the triangular network, $\mathbf{u}_i$ is the displacement vector at site i and $\hat{\mathbf{r}}_{ij}$ is the unit vector between sites i and j. The force constants k_{ij} will be taken either equal to 1 or 0, according to the procedure outlined below. This system has been previously used to investigate elasticity percolation, and its critical properties are relatively well known,[3] although controversial results[7] have been published recently. Numerical simulations were carried out on hexagons of side L (all length magnitudes will be hereafter expressed in units of bond length).

In this study we remove bonds with probabilities that decrease with their distances to the center of the hexagonal samples. In order to eliminate a fraction $(1-p)$ of bonds, we remove a particular one in the following way. Each bond i is characterized by the middle point of the hexagonal band where it lies, that is $(h-1/2)$, where $h=1,L$; then, a probability

$$P_i(h)=\{\exp[a(h-1/2-q)]+1\}^{-1} \tag{2}$$

is assigned to it. This probability density resembles the Fermi-Dirac probability distribution, where a and q in Eq. (2) play roles similar to those of the inverse of the absolute temperature and the chemical potential, respectively. In the case of fermions at finite temperatures, the chemical potential is calculated to give the total number

of particles. This procedure would pose important practical difficulties in the present case; thus, the probability distribution of Eq. (2) has been used as follows. First we order at random the set of bonds corresponding to each hexagon. Then we take $q=1$ and assign random numbers $\mathcal{R}_i$ to all bonds in the network; all bonds having $\mathcal{R}_i < P_i(h)$, for $i=1,n_p$ (n_p being the number of unbroken bonds corresponding to the fraction p) are subsequently removed. If the fraction of broken bonds is less than the actual value of $(1-p)$, we proceed with the next value of q. The process is repeated until the fraction of removed bonds equals $(1-p)$. The parameter a determines the shape of the distribution. In this context we shall remark that the product aL must be kept constant in order to have, for the different sample sizes, distributions of broken bonds that are invariant upon scale transformations. Two limiting cases are described by the present model: when $aL=0$ the distribution corresponds to the case of homogeneous (but random) bond elimination and when $aL\to\infty$ voids are concentrated at the center of the sample (in this case a hexagonal ring results).

To develop a continuum model suitable to handle a medium such as the one considered here, we first need to write the equilibrium equations for the case in which λ and μ are not constants but radial functions, $\lambda(r)$ and $\mu(r)$. The density of elastic energy for an isotropic medium in 2D is given by

$$E=\frac{\lambda}{2}(\partial_x u_x+\partial_y u_y)^2 +\mu[(\partial_x u_x)^2+\tfrac{1}{2}(\partial_x u_y+\partial_y u_x)^2+(\partial_y u_y)^2] , \quad (3)$$

where $\partial_{x,y}$ stand for the partial derivatives with respect to x or y, respectively, and $\mathbf{u}=(u_x,u_y)$ is the displacement field. Under isotropic dilation (the case considered here) we can write $u_x=xF(r)$ and $u_y=yF(r)$. Then, the equilibrium equation is

$$(\lambda+2\mu)(3F'+rF'')+2(\lambda'+\mu')(F+rF')-\lambda' rF'=0 , \quad (4)$$

where the prime stands for the radial derivative.

In the homogeneously diluted case, the results obtained with the Hamiltonian given by Eq. (1) can be very accurately fitted by[6]

$$\frac{\lambda}{\lambda_0}=\frac{\mu}{\mu_0}=3p-2, \quad \text{for } p\geq 2/3 . \quad (5)$$

This approximation is valid up to a value of p very close to the percolation threshold, p_c. We now proceed by using a local approximation in which Eq. (5) is assumed to hold for each value of r,

$$\lambda=\lambda[p(r)], \quad \mu=\mu[p(r)] , \quad (6)$$

where $[1-p(r)]$ is the fraction of voids at r. This assumption gives very satisfactory results away from the percolation threshold (see below) and is in line with the local interpretation of the percolation transition discussed at the end of this paper.

To speed up the calculations, instead of using the function $p(r)$, i.e., the local fraction of remaining matter, we fit them by means of the following analytical expression

$$p(r)=\frac{\exp[\alpha(r-\beta)]}{1-\exp[\alpha(r-\beta)]} , \quad (7)$$

where α and β are functions of aL (i.e., the degree of inhomogeneity) and the total fraction of remaining bonds, p.

As regards the boundary conditions, several points are worth to comment. We fix the displacements, C, at the outer boundary, $u_r(r_{\text{out}})=C$. On the other hand, below a given total fraction of remaining bonds, we can define an inner radius r_{in}, for which $p(r)\leq 0.66$ when $r\leq r_{\text{in}}$; as the percolation threshold has already been reached in this region, then, concerning its elastic properties, the inner region can be treated as a circular hole and, thus, $\mu(r)=\lambda(r)=0$ for $r\leq r_{\text{in}}$. The second boundary condition is then obtained by imposing that no transversal forces are transmitted through $r=r_{\text{in}}$, that is, at the inner border the radial component of the stress tensor verifies that $\sigma_{rr}(r_{\text{in}})=0$; this leads to

$$\left.\frac{F(r)}{F'(r)}\right|_{r=r_{\text{in}}}=-\tfrac{3}{4}r_{\text{in}} . \quad (8)$$

Then considering the inner and outer boundary conditions above and introducing Eqs. (5)–(7) into the differential equation, Eq. (4), the solution to the function $F(r)$, which gives account of the radial inhomogeneity, is found by standard numerical techniques. The bulk modulus is then directly obtained from the total elastic energy.

In order to calculate the bulk modulus of the diluted medium we applied a uniform dilation at the boundary of the hexagonal samples. Then the interior nodes were allowed to relax until the equilibrium equations were satisfied; the iteration process was stopped when the maximum force on the interior nodes was less than 0.001 times the initial force on the boundary nodes (between 2000 and 8000 iterations were required). Simulations were carried out on hexagons of sides $L=10$, 15, 30, and 45, containing nodes in the range 331–6211. In order to smooth out statistical fluctuations, the calculations were performed for a number of realizations which varied with the size of the hexagon (around 30 for the smaller size and 15 for the larger one). The critical properties of the percolation transition were investigated by means of the generalized phenomenological renormalization method:[10] From four hexagonal samples such that their sizes L_1, L_2, L_3, and L_4 were related by $L_1/L_2=L_3/L_4$, the percolation threshold p_c and the ratio $\delta=f/\nu_e$ (where f is the elasticity percolation exponent and ν_e is the correlation length exponent), can be obtained.

Figure 1 shows the normalized bulk modulus [$\bar{B}=B(p)/B_0$, where $B_0=B(p=1)$] of the diluted medium as a function of unbroken bonds, p, for three values of aL. Despite that these results correspond to a finite sample ($L=45$) and that extrapolation to infinite systems is not straightforward, it seems apparent that the bulk modulus vanishes, and at values of p which are clearly smaller than the one corresponding to the homogeneous case, i.e., $p\simeq 0.65$,[3,4,7] for which the results are also

shown in Fig. 1. On the other hand, the bulk moduli, near percolation, are bounded by that corresponding to the homogeneous case (lower bound) and that for a hexagonal ring (upper bound). In the latter case the bulk modulus is given by[5,9]

$$\bar{B}(p)=p/(3-2p)\ , \tag{9}$$

and the results are also shown in Fig. 1. Thus, the macroscopic behavior of the present inhomogeneous model interpolates between that of the homogeneous case and that of hexagonal rings, describing the properties of systems having a nonuniform distribution of voids. We also note that for values of p near unity, the bulk moduli for the inhomogeneous case are smaller than that for the homogeneous case. This is a consequence of the considerable amount of disconnected bonds in the inner region of the samples, which do not contribute to the elastic energy. This effect increases with the degree of inhomogeneity (see Fig. 1).

The results obtained by means of the continuum model described previously compared to those given by simulations appear in the inset of Fig. 1. The remarkable agreement supports the local approximation used to obtain the Lamé coefficients of the inhomogeneous medium, Eq. (6).

As discussed above, the behavior of the bulk modulus in the inhomogeneous case suggests that these systems do also show a percolation transition. The question is whether the critical properties are or not different from those found in homogeneously diluted media. In Fig. 2 we present the results of the phenomenological renormalization procedure outlined above, for $aL=4$. It is noted a clear intersection between the curves corresponding to the two sets of sizes used here (10/30 and 45/15). This intersection gives values for p_c and δ, 0.27 ± 0.05 and 0.85 ± 0.10, respectively, which are markedly different from those most widely quoted for the homogeneous case, i.e., 0.65 and 1.35, respectively.[3] These results indicate that the radial inhomogeneity considered in this work does in fact affect the critical properties of the percolation transition.

The analysis of the percolation transition discussed above is rather unclear, as it is very unlikely that an inherently inhomogeneous medium could be characterized by a single correlation length, as in the perfectly homogeneous case. To overcome this difficulty we define two regions in the inhomogeneously diluted system, an inner region with an average p below the standard percolation threshold, and a surface region which we assume to be radially homogeneous and where standard percolation theory holds. Note that it is rather difficult to find the exact placement of the boundary between those two regions, which should strongly depend upon the degree of inhomogeneity (aL). Nonetheless, to go further into this argument, we take the largest value of aL here considered and define the surface region as the outer hexagonal band, which is clearly homogeneous. Then, we define p_s as the fraction of unbroken bonds in the surface band, and plot the results of Fig. 1 as a function of p_s; this is done in Fig. 3. The bulk modulus renormalized in this way does behave very similarly to that for the homogeneous case. An estimate of the critical parameters through a procedure similar to that used above (although the errors involved in this estimation are much higher than in

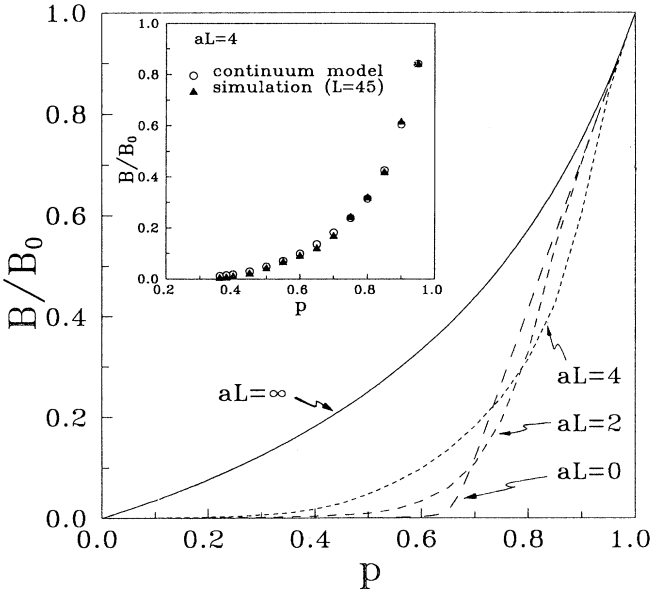

FIG. 1. Normalized bulk modulus as a function of p for a hexagon of side $L=45$, where the bonds have been removed following the probability distribution shown in Eq. (2) for two different cases: $aL=2$ and $aL=4$. Results for the homogeneous case ($aL=0$) and hexagonal rings [Eq. (3)] are also shown. The inset shows the normalized bulk modulus as a function of p, obtained by means of the continuum model described in the text and by simulation, the latter for the case $aL=4$.

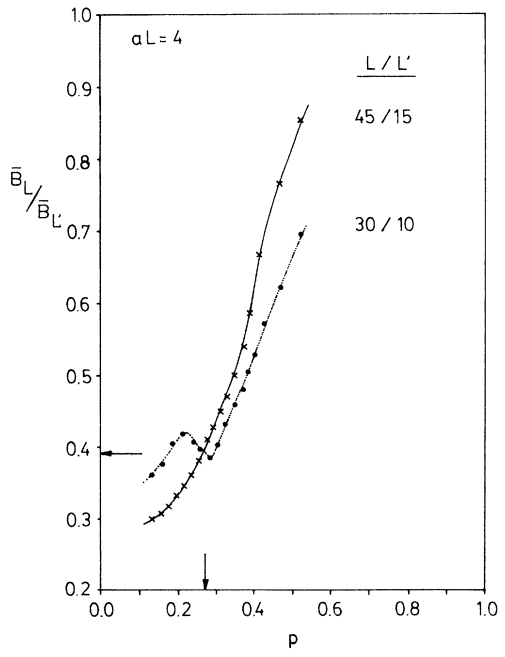

FIG. 2. Finite-size scaling estimation of the critical parameters p_c and f/ν_e corresponding to the case $aL=4$.

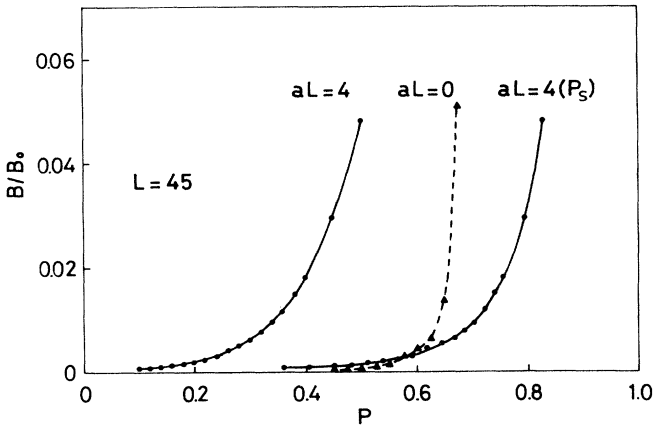

FIG. 3. Normalized bulk modulus as a function of p. The bulk modulus corresponding to the inhomogeneous case ($aL=4$) has been plotted as a function of the total fraction of bonds and as a function of the fraction of surface bonds, p_s (see text). The bulk modulus corresponding to the homogeneous case ($aL=0$) is also depicted (dashed line). The side of the hexagon is $L=45$.

the previous case) gave 0.69 for the percolation threshold and 1.1 for δ, which are much closer to those of the most quoted elasticity percolation results.[3] The agreement is rather remarkable and somewhat unexpected, considering the rather small width of the surface band. We find that a *local* application of standard percolation theory works rather well for our inhomogeneous distribution of missing bonds. However, close to the percolation threshold, p_c, the correlation length diverges, and the system should show strong nonlocal features which we do not observe in our simulations. We believe that our findings can be partially ascribed to the extreme narrowness of the critical region in elastic percolation, which, in turn, is associated with large critical exponents, in particular, for the correlation length. If this explanation holds, it means that similar results should be found for other systems with different correlations between missing bonds. We also note that the validity of this local interpretation of the percolation transition in the inhomogeneous medium is further supported by the agreement between the continuum model and simulations mentioned above (inset in Fig. 1).

The above results suggest that the macroscopic properties of inhomogeneous systems, as far as the percolation transition is concerned, are controlled by the surface region. As remarked above, this region is rather elusive and its precise definition is outside the scope of this paper, as much more extensive numerical simulations might be required. We would only like to add that as aL is decreased its width will increase and, eventually, becomes of the order of the correlation length; at this point the whole system would behave as being homogeneous.

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