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Precision Calculation of Elasticity for Percolation

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Monte Carlo transfer matrix evaluation of the elastic constants at the percolation threshold of the random-bond honeycomb lattice, with widths of up to 96 and lengths of about two million lattice constants (roughly 200 hours CDC Cyber 205 vector computer time) gave a critical exponent $T = 3.96 \pm 0.04$ with a logarithmic correction term. This exponent agrees well with the scaling hypothesis $T = t + 2\nu = 3.97$, relating T to the two-dimensional conductivity exponent.

KEY WORDS: Elasticity; percolation; conductivity; critical exponents.

1. INTRODUCTION

The elasticity of random networks was originally[1] thought to be proportional to the electrical conductivity of the corresponding random resistor network. It is widely believed by now that the elasticity vanishes at its percolation threshold with a critical exponent T much larger than the exponent t of the conductivity. With the help of an efficient program run for roughly 200 h on a CDC Cyber 205 vector computer, we tried to determine accurately this new elastic exponent T, in order to test possible scaling relations like $T = 1 + 2\nu = 3.67$ or $T = t + 2\nu = 3.97$ in two dimensions.[2,3] A short account of our work was given at the Percolation 1985 conference, Cologne University, June 1985.

We used the same randomly diluted honeycomb lattice as Bergman,[4] the same model, the same parameters, and roughly the same Monte Carlo transfer matrix algorithm. We also refer to that paper for earlier literature. Thus the elastic constants C_{11} and μ were calculated as a function of strip

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width $L = 96, 72, 48, 36,...$ for strips of length above 10^6. Both length and width are much larger than in Ref. 4 and allow us to conclude that the log–log plot of Ref. 4, if extended to $L = 96$, would show clear signs of curvature. Thus corrections to scaling are important, which affect the estimate also for the leading critical exponent T. Moreover, we also investigated the infinite network away from the percolation threshold.

2. THE HONEYCOMB RANDOM ELASTIC BOND NETWORK

If a lattice is diluted, that means if some of the sites of the lattice, or some of the bonds between them, are omitted, its resistance against shear and stretching is reduced. If the dilution is strong, then there is no longer an infinite network of sites present that are connected by interaction bonds. Then, even an infinitely small force can destroy the lattice and stretch it infinitely. The minimum concentration of sites or bonds needed to have such an infinite network present is called the percolation threshold, p_c.

However, even if such an infinite network is present the elastic resistance might still vanish. Even without any dilution, the square or simple cubic lattice can be sheared strongly by an infinitely small force, if the interactions between the lattice sites depend only on the distance between the sites and are restricted to nearest-neighbor pairs. For a realistic description of the elastic properties of disordered solids it is therefore desirable to take into account bond-bending in addition to bond-stretching forces.

That means: If the distance b between two neighbors is changed by δb away from its equilibrium value of the undiluted lattice, a force $k\,\delta b$ tries to restore the bond length to its original value, and the energy is increased by $k(\delta b)^2/2$. And if the angle ϕ between a pair of adjacent bonds is changed away from its equilibrium value by an amount $\delta\phi$, the energy is increased by $m(\delta\phi)^2/2$. We work only with nearest-neighbor forces and set the equilibrium distance between such neighbors equal to unity. Then the ratio k/m is dimensionless and will play an important role in our simulation. Also, because of this simplification, the dilution itself does not shift the equilibrium positions of the lattice sites; external forces are needed to produce small changes away from the original lattice structure. Furthermore we assume all lattice sites to be occupied, but only a random fraction of the bonds between nearest neighbors is active (bond percolation).

We apply the transfer matrix technique to systems generated randomly by a Monte Carlo method. The complexity of this transfer matrix increases drastically with the number of nearest neighbors in the lattice; this matrix, and not the production of the random structure, consumes most of the computer time. Therefore our work is restricted to two dimensions (which also has the advantage that p_c is known exactly), and we take that lattice

with the lowest number, 3, of nearest neighbors—the honeycomb lattice. The universality principle suggests that the critical exponent T to be calculated is the same for all two-dimensional randomly diluted lattices. In three dimensions, however, a different exponent is expected, and even higher dimensionalities would be of interest, as well as nonrandom distributions of bonds or sites. Nevertheless, the present work deals only with the random bond-diluted honeycomb lattice.

3. TECHNICAL ASPECTS OF THE SIMULATION

The simulations were carried out on a Control Data Cyber 205 vector computer at Ruhr University (Bochum, West Germany). Since a large amount of machine time was to be used, a rather careful optimization of the program for this machine has been performed.

In Table I we give the CPU time, depending on system size and optimization level. For comparison, column 1 gives execution times on a high-performance scalar machine, the Control Data Cyber 170-855. We see that an approximate factor 3 in speed is gained by moving to the Cyber 205 in scalar mode, i.e., not employing any vector instructions on this vector machine. This unusually large gain is due to the rather large complexity of the program, involving many scalar variables. The large file of 256 registers on the Cyber 205 is sufficient to hold all scalar variables, and thus a large number of central memory load/store operations is avoided in comparison with the 170-855.

In a first step we tried out the vectorizing FORTRAN compiler of the Cyber 205. Not a single change to the original[4] scalar version of the code was made. For strips of width $L = 48$, a factor of almost 10 was gained

Table I. Computer Time per Column[a]

L	CY 170-855, scalar only	CY 205, scalar	CY 205, autovector	CY 205, handvector	CY 205, sparse
12	0.10	0.03	0.01	0.009	0.004
24	0.72	0.19	0.04	0.033	0.010
48	5.2	1.38	0.17	0.14	0.03
96	(35)	9.8	9.8[b]	0.70	0.08
192	(250)	(70)	(70)[b]	3.8	(.25)

[a] Computed in seconds, for Transfer Matrix Calculation of Strips of width L, using various computers and algorithms. The numbers in parentheses are estimates, not measurements;
[b] Cases where automatic vectorization was inoperative (array too long).

compared to the scalar Cyber 205 speed. For larger systems the size of the matrix to be manipulated (about $8L^2$ words of storage) exceeds 64*K*. Unfortunately the automatic vectorizer does not recognize that only small parts of the matrix, and never the complete matrix, are worked upon in any given loop. Since the maximum allowed vector length on the Cyber 205 is 65536 elements, the vectorizer is no longer operative, even if "unsafe vectorization" is selected. Thus we had to vectorize the program "by hand."

The fourth column of Table I gives execution times for a completely hand-vectorized version of the program (about one day of work by JGZ). It is seen that vectorization by hand is slightly more efficient than automatic vectorization for those sizes where the latter works. Of course, hand vectorization may be used for all sizes within the relevant region, $L = 16384$ being the theoretical limit. For our large systems, this hand-vectorized code is about 20 times faster than the scalar version on the Cyber 205 and a factor of 65 faster than the program on the Cyber 170-855.

For occupancy probabilities p near $p_c = 0.6527$ (and even more so for smaller p) the transfer matrix is rather sparse, with about 10% of its elements nonzero for larger L. This sparsity allows us to save some CPU time with nontrivial techniques described in the case of conductivity calculations.[5] The very same technique applied in the present case gives the execution times in the last column of Table I. For 10% nonzero elements in the matrix, about a factor of 10 is gained. Thus, for our largest system, the overall speed increase in comparison to the original scalar program on the Cyber 170-855 reaches a factor near 1000. We do not believe that the present type of computation could be made to run appreciably faster by any further optimization like hand-coding in assembly language. Thus our final version of the program still is written in Cyber 205 FORTRAN, with heavy use of special calls, however.

Within the course of the calculation, elements of the transfer matrix may become approximately zero. Because of numerical rounding errors, a true zero cannot be reliably distinguished from a sufficiently small but finite number. If some matrix element vanishes, significant parts of the calculation may be skipped.[5] It is customary to select some level of accuracy ε, which is used as a threshold value below which all numbers are considered to be zero. In Table II we present some results of a set of simulations carried out by employing identically the same set of (pseudo)-random numbers but for different values of ε. We see that for sufficiently small ε the results become independent of ε. We used 64-bit floating point numbers; the first entry in Table II raises some doubt if the calculation could have been carried out successfully with 32-bit words, having a precision of about 6.5 digits only. Use of such half-precision variables on the Cyber 205 would result in a speed-up of about a factor 1.5 for larger L.

Table II. Effect of Rounding Errors[a]

ε	C_{11}	μ	t
10^{-6}	0.00888225	0.00253660	43
10^{-8}	0.00889437	0.00256671	46
10^{-10}	0.00889437	0.00256671	47
10^{-12}	0.00889437	0.00256671	47
10^{-14}	0.00889437	0.00256671	48
10^{-16}	0.00889437	0.00256671	48
0	0.00889437	0.00256671	48

[a] Strips are of size 24×5000 at p_c. The first column gives ε, the quantity below which all matrix elements are regarded as zero. The last column gives the computer time in seconds.

In order to avoid further discussion of rounding errors we refrained from employing the 32-bit floating point option; all further calculations were performed at $\varepsilon = 10^{-14}$.

4. ELASTIC MODULI AT THRESHOLD

The elastic moduli of a given random bond network depend upon two constants, the microscopic bond bending and bond stretching constants, m and k. Alternatively, the elastic moduli κ and μ of the undiluted infinite system may be used to specify the elastic properties. There we have the unique relations[4]

$$\kappa = k/3.4641 \qquad \mu = 3.4641 \text{ km}/(k + 6m)$$

Obviously, one of the two constants may be chosen arbitrarily to set the scale (unit of measurement), and only one nontrivial constant remains to be chosen. According to Kantor and Webman[2] the elastic behavior of the infinite system at p_c should depend only upon m. Therefore, the choice of constants should not matter at all in this case.

Unfortunately, computer simulations have to be carried out with finite systems. For small strip widths L we see from Table III that the elastic constants C_{11} and μ depend strongly on the ratio k/m. However, the variation is smaller the larger L is, and thus for infinite L the elastic properties might well become independent of k/m. For example, if k/m jumps from 2.28 to 22.8, then μ increases by nearly a factor 2 for $L = 12$ but by only 5% for $L = 96$. The smaller k/m is, the larger L must be chosen in order to reach the asymptotic independence from k/m. However, the ratio C_{11}/μ of elastic constants varies already for small L much weaker

Table III. Elastic Constants at p_c[a]

L	k/m	0.0027	0.228	2.28	22.8	228	2280
12		0.0000079(2)	0.00403(10)	0.0173(4)	0.0348(1)	0.0405(11)	0.0413(12)
24		0.0000045(1)	0.00163(3)	0.00507(11)	0.00746(4)	0.0086(3)	0.0087(3)
48		0.0000022(1)	0.00048(2)	0.00105(5)	0.001354(9)	0.00142(6)	0.00142(6)
96		0.00000108(5)	0.000116(10)	0.000196(18)	0.0002219(19)		
12		0.0000048(1)	0.00162(3)	0.0059(1)	0.01067(3)	0.0124(3)	0.0126(3)
24		0.00000260(5)	0.00059(1)	0.00163(4)	0.00225(1)	0.00262(7)	0.00264(7)
48		0.00000117(4)	0.000158(5)	0.00032(1)	0.000411(3)	0.00042(2)	0.00042(2)
96		0.0000055(2)	0.000038(2)	0.000063(3)	0.0000660(5)		
12		1.64	2.48	2.93	3.26	3.26	3.27
24		1.72	2.75	3.12	3.32	3.29	3.29
48		1.86	3.05	3.28	3.29	3.35	3.35
96		1.99	3.05	3.11	3.36		

[a] Strips of size $L \times 25000$ and various ratios k/m, using $m = 0.365$. The top part gives C_{11}, the center gives μ, and the bottom lines give the ratio C_{11}/μ. The statistical errors in the last decimals are given by the numbers in parentheses.

Table IV. Main Results: Elastic constants at Threshold[a]

L	$N/10000$	C_{11}	μ	C_{11}/μ	t
4	2250	0.2463(4)	0.07480	3.29	$\frac{1}{2}$
6	1300	0.1294(3)	0.04006(10)	3.23	$\frac{1}{2}$
8	5000	0.0773(1)	0.02396(4)	3.23	3
12	2000	0.03483(11)	0.01067(3)	3.26	2
16	2000	0.01878(7)	0.00576(2)	3.26	3
24	2000	0.00746(4)	0.00225(1)	3.32	6
36	1810	0.00279(2)	0.000843(6)	3.31	9
48	2525	0.001354(9)	0.0004113(27)	3.29	19
72	1850	0.000473(5)	0.000142(2)	3.33	27
96	3104	0.0002219(19)	0.0006596(54)	3.36	67

[a] For $L \times N$ strips. The last column gives the Cyber 205 computer time in hours. Errors are marked as in Table III. $k = 8.3138$, $m = 0.3646$, $k/m = 22.8$, and $p = 0.65271$.

with k/m, as Table III shows. From now on we take $k/m = 22.8$, the same value as in the preliminary study.[4]

Our calculations for L up to 96 at a bond occupancy probability $p = p_c = 0.6527$, where for the first time an infinite network appears, are summarized in Table IV. Calculations for $L > 96$ would be desirable and would have been possible with the available memory. However, in order to obtain results of 1% accuracy for $L = 144$, about 330 h would be required on the Cyber 205. We do not feel that the present investigations warrant this significant investment. Already now, the total CPU time to obtain the results of this paper was about 200 h, or nearly 10^{14} arithmetic operations.

5. CORRECTIONS TO SCALING ANALYSIS

The results of Table IV, in contrast to those of the preliminary study,[4] are accurate enough to indicate that they do not follow a straight line in a log–log plot versus L. In other words, no simple power law

$$C_{11} \propto L^{-T/\nu} \tag{1}$$

without correction terms is valid over the intermediate range of L investigated here. In a first transparent attempt to find some regular behavior, we plot in Fig. 1, the average of the apparent exponents T/ν for C_{11} and μ versus $L^{-1/2}$. These apparent exponents were determined as the slope between two consecutive points on the log–log plot; the exponent $-\frac{1}{2}$ for L was chosen because in this way we obtain a line that looks straight. We see clearly that the apparent exponent is a monotonically increasing

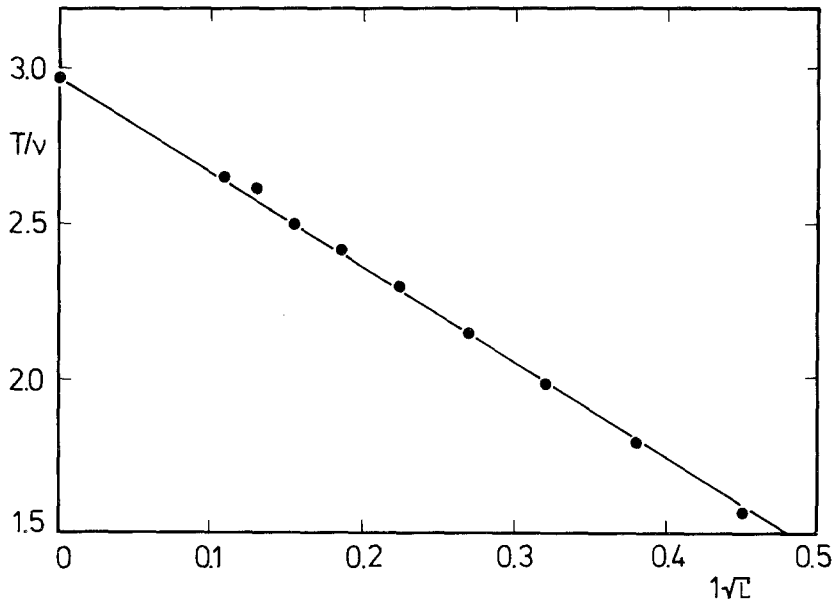

Fig. 1. Variation of effective exponent with strip width. The intercept is the thermodynamic limit.

function of strip width and needs to be extrapolated to infinite systems, corresponding to the intercept in our Fig. 1. The way we plotted Fig. 1 corresponds to the assumption that only one correction-to-scaling term is present

$$C_{11} \propto L^{-T/\nu}(\text{const} + L^{-\omega}) \tag{2}$$

with $\omega = \frac{1}{2}$. The extrapolation to infinite systems points to T/ν near 3, or T near 4, with the well-known[6] two-dimensional correlation length exponent $\nu = \frac{4}{3}$. On the other hand, for small L the effective exponent is appreciably smaller and compatible with the estimate $T = 3.5$ from Ref. 4. Thus this earlier estimate needs to be revised upward since now, perhaps for the first time in elastic percolation properties, corrections to scaling can be taken into account quantitatively.

A more quantitative investigation, however, shows that (2) is not adequate. The χ^2 test, which compared the deviations from the fitted expression with the statistical error bars for each point, gave values of order 10 whereas a good fit should give values not much larger than unity. Thus we next tried a more general ansatz with two correction terms

$$C_{11} \propto L^{-T/\nu}(1 + bL^{-\omega} + c/L) \tag{3}$$

This attempt yielded fits which became better the smaller ω was, and thus suggest a logarithmic variation corresponding to $\omega = 0$. However, a fit with only such a logarithmic term,

$$C_{11} \propto L^{-t/\nu}[\text{const.} + 1/\log(bL)] \tag{4}$$

did not turn out to be good, as was to be expected from Fig. 1.

Finally we tried

$$C_{11} \propto L^{-T/\nu}[1 + a/\ln(bL) + c/L] \tag{5}$$

and found excellent fits with unique minima in the χ^2 tests as function of the parameters. Our best fits ($\chi^2 < 1$) were obtained with $a = -3.69$, $b = 2.2$, and $c = 2.92$; the fact that all these coefficients are of order unity gives further credence to their reliability. The good fit in Fig. 1 then has to be explained as an accident due to the opposing signs of the first and the second correction terms, i.e., due to the fact that a/c in (5) is negative. Also for

$$C_{11} \propto L^{-T/\nu}[1 + a/\ln\ln(bL) + c/L] \tag{6}$$

we found good fits.

Figs 2, 3, and 4 show our χ^2 contours corresponding to (3), (5), and (6), with an unsatisfactorily stretched valley for Fig. 2 corresponding to (3), and relatively sharp minima for Figs. 3 and 4 corresponding to (5) and (6). It did not matter much if the smallest L values were omitted from the

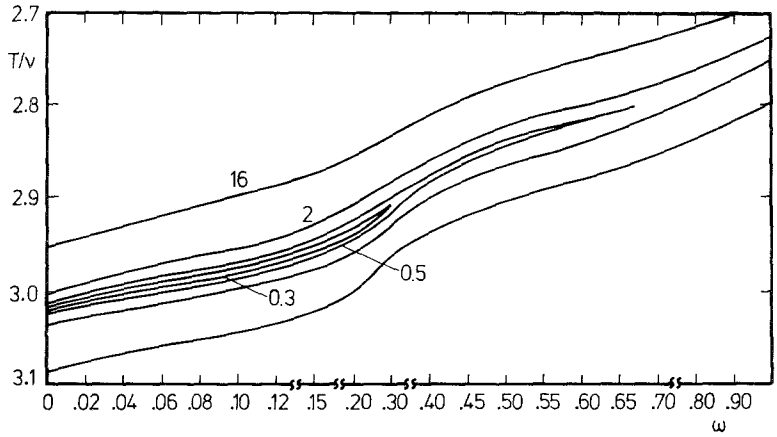

Fig. 2. Contour plot of χ^2 (average deviation from fit, normalized by statistical error) in the T/ν versus ω plane for (3).

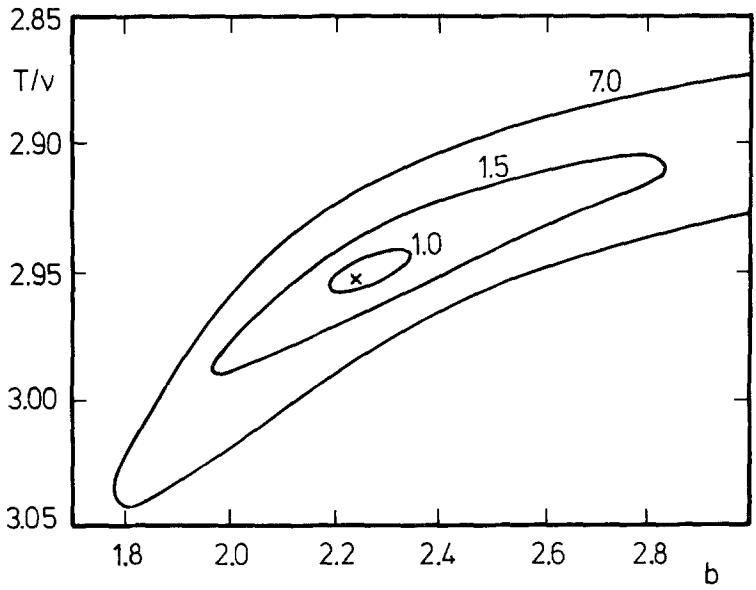

Fig. 3. Contour plot as in Fig. 2, but in the T/v versus b plane for (5).

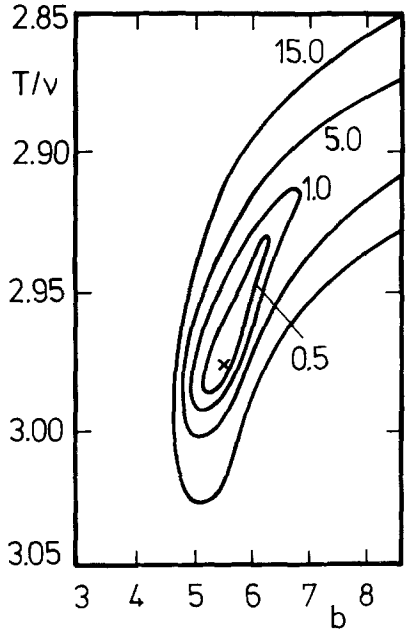

Fig. 4. Contour plot as in Fig. 2, but in the T/v versus b plane for (6).

fits, or if μ instead of C_{11} was used for the fits. The crucial quantity, of course, is the leading exponent T/ν, not the correction term. Both Figs. 3 and 4, as well as the simpler Fig. 1, support the estimate

$$T/\nu = 2.97 \pm 0.03 \qquad \text{or} \qquad T = 3.96 \pm 0.04 \tag{7}$$

five times more accurate than the estimate published in Ref. 4.

Obviously, if simple relations like (1) and (2) are not correct, there is no reason to believe that two correction terms as in (5) and (6) are sufficient. If reliable data for much larger L values were available more terms would be needed to fit them. It would then be possible that the unexpected logarithmic term in (5) and (6) would be replaced by a more conventional power law. However, the consistency of our various estimates for the leading exponent T suggests that estimate (7) would not be proven wrong from such calculations for larger L.

The estimate (7) is now clearly larger than $1 + 2\nu = 3.67$, whereas the preliminary estimate,[4] 3.5 ± 0.2, was lower. This result is satisfactory because $1 + 2\nu$ is supposed[2] to be a lower bound for T. It is highly unlikely now that this inequality is actually an equality. Instead, our results are in excellent agreement with the speculation[3] $T = t + 2\nu = 3.97$ in two dimensions. (We use the conductivity exponent $t = 1.3$ from Ref. 7; but even with the lower t from Ref. 8, we find agreement within the error bars.) Thus, perhaps the elasticity puzzle is solved, and in the spirit of de Gennes[1] the elasticity exponent is related to the conductivity exponent at the percolation threshold for this model.

6. BEHAVIOR ABOVE THRESHOLD

While critical exponents like T, or fractal dimensions like T/ν are fashionable for theorists, experimentors[9] often measure elastic properties for the infinite network far above the percolation threshold. Our computer program also gives such results, but in contrast to critical exponents like T one should not expect the behavior away from the critical point to be universal, i.e., to be independent of the lattice structure and other microscopic details. For a fixed p one has to extrapolate the measured elastic constants to $L = \infty$. Figure 5 shows the variation of this extrapolated value with p for $k/m = 43.1$. We choose the microscopic elastic constants appropriate for pure gold films and thus have gigapascals as units in Fig. 5. We challenge laboratory experiments to be more accurate than these computer experiments.

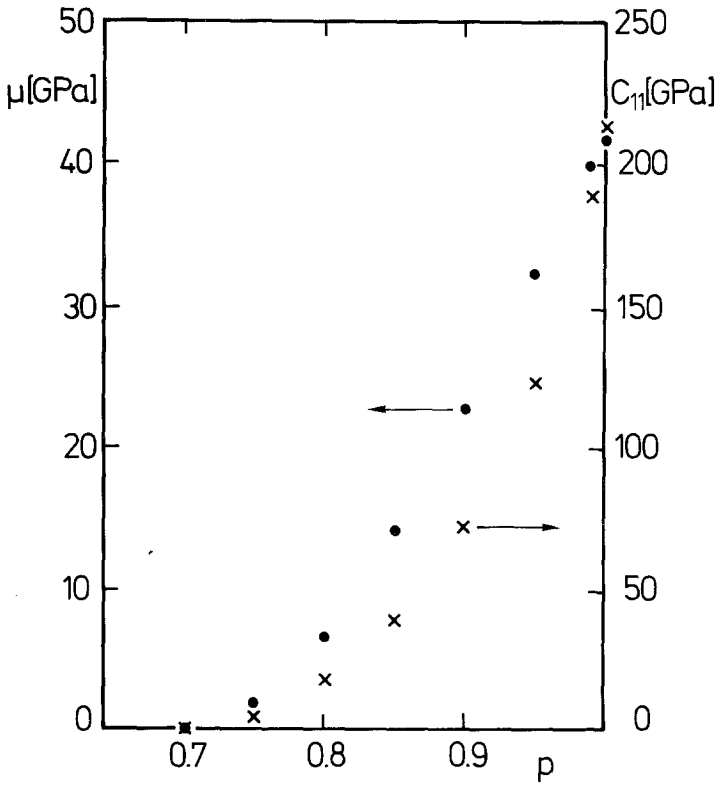

Fig. 5. Variation of elastic constants with p above threshold.

SUMMARY

By increasing the computational efficiency and effort by some orders of magnitude, we were able to find and analyze corrections to scaling in the elastic properties of a two-dimensional model for a disordered solid. We found the critical exponent T so the leading term will be close to 4 and to the value predicted by a recent scaling law.

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