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Electrical conductivity of finite-size percolation networks

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Abstract. Calculating, by a Monte Carlo technique, the conductivities of small, two-dimensional, square, bond-percolation networks (4×4 to 50×50) at a limited number of probability values, from the critical region to full conductivity, we have been able to show, by an original interpolation technique, that in the critical region the conductivity function does indeed obey a universal, Fisher-type, finite-size scaling function. We further show that this technique permits us to deduce values of the critical exponents for both the conductivity and the correlation length, even from calculations on relatively small networks.

1. Introduction

The study of size effects in percolation problems is of interest for two reasons.

(1) Such systems are met in nature and show smeared properties in the critical region, in contrast with systems with an infinite number of elements where the critical behaviour is clearly evident. Generally, the softening of the critical behaviour in the former case results from the expected statistical fluctuations in finite systems.

(2) By extrapolating data obtained from small systems, we would hope to get accurate predictions for larger ones. Different versions of size renormalisation have been developed (Roussenq *et al* 1975, Sur *et al* 1976, Derrida and Vannimenus 1980).

It is particularly important to establish this technique for the conductance of resistive percolation networks, since calculation times for the solution of even moderate-size networks can be quite long, even where large, fast computers are available.

We have chosen to treat the problem of two-dimensional, square, bond-percolation lattices with free boundaries—defining as a lattice of size '$N\times N$' one having $(N-1)$ rows of N nodes each, and consequently N rows of N vertical bonds each and $(N-1)^2$ horizontal bonds, the vertical rows meeting at common test nodes at the top and bottom. (Figure 1 provides an illustration for $N=3$.) If we assume bonds of unit resistance, the resulting lattices have, when all bonds are present, unit conductance (independent of N). Networks based on this lattice have the property of being self-dual; this latter property leads to the exact critical percolation probability $p_c=\frac{1}{2}$.

We shall describe below: in § 2, the results of our Monte Carlo conductance calculations for lattices 4×4 to 50×50; the general analytic properties of the conductance function $G_N(p)$ of such a lattice (§ 3); the predictions of Fisher's finite-size scaling theory (§ 4); the original interpolation scheme which we have developed, and which

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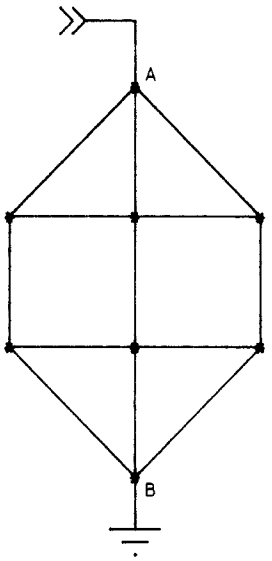

Figure 1. Schematic diagram of the conductance lattice for $N = 3$. The connection of bonds to nodes A and B is equivalent to connecting the topmost and lowest rows of vertical bonds to limiting plane electrodes. It is readily verified, that for an ideal lattice ($p = 1$), and bonds of unit resistance, the overall conductance is unity. In a typical given realisation ($p < 1$), some of the bonds will be missing.

permits us to infer the entire conductance function from Monte Carlo calculations of the conductivity at a limited set of probability values (§ 5); and, in § 6, the resultant calculation of the critical exponents, t and ν, respectively for the conductivity and correlation length.

2. Monte Carlo conductance calculations

We calculate, using the method described in an earlier paper (Blanc *et al* 1980), the resistance of a random, bond lattice.

For a given $N \times N$ lattice, defined as above, setting an *a priori* probability p, we generate the vertical and horizontal bonds of the lattice by comparing p with random numbers between 0 and 1 generated by a new, efficient algorithm (Kirkpatrick and Stoll 1981). We first simplify the network, by means of another algorithm which eliminates all tree-like 'dead' arms, so that the resulting network, all the nodes of which are connected by active bonds of unit resistance, is made up of the conductive 'backbone' and possibly also isolated loops. The top row of active vertical bonds is assumed to be connected to a source of unit potential (node A in figure 1), and the lowest row of vertical bonds is grounded (at B). Because of the possible existence of floating loops, which our search algorithm does not distinguish from portions of the backbone, we have also found it convenient to tie to each node of the network a resistance of $10^6\ \Omega$, connecting that node to a separate 0.5 V source. The existence of these additional high resistances does not affect, to the accuracy of our solution, the conductance of our network, but serves to stabilise the potentials of any floating loops.

We then proceed to solve, for each active node, Kirchhoff's equations $V_i = \Sigma_j g_{ij} V_j / \Sigma_j g_{ij}$ where the g_{ij} represent the conductances lying the neighbouring potentials V_j to the node i. Since, for any but the smallest values of N, the number of active nodes of our network leads to a number of equations unmanageable for simultaneous solution, we solve the system by an iterative over-relaxation method (Webman *et al* 1975). After each iteration, we calculate the conductance by summing the dissipated energy:

$$G = \sum_{i<j} (V_i - V_j)^2 \qquad \text{(for all active nodes and values } i<j\text{)}. \tag{1}$$

This has the advantage of second-order accuracy for first-order errors in the V_i. We terminate the iteration when the difference between successive conductance calculations is less than 4×10^{-5}†.

To obtain the conductance function $G_N(p)$, we have averaged, for given p, the conductances of a very large number of realisations of lattices, ranging from 20000 for $N = 4$ to 96 for $N = 50$. Data were obtained for $N = 4$, 5, 6, 7, 8, 10, 15, 20, 30, 40, 50 and for 22 values of p—of these latter, ten were chosen to be clustered around p_c (the higher N, the tighter the clustering), and the rest nearly evenly spaced to span the range remaining to $p = 1$. Figure 2 displays a typical set of such curves.

It is perhaps also worth mentioning that, because of the self-dual nature of the lattices, at $p = p_c$ conducting and non-conducting configurations occur with equal probability. More generally, we obtain, for each value of p and N, a histogram for the conductances of individual realisations, whose mean value is $G_N(p)$. The histogram contains a δ function at zero conductance, corresponding to all non-conducting configurations, and a smeared distribution of the non-zero conductances, which becomes narrower and closer to zero (at $p = p_c$) as N increases. We may expect finite-size scaling to apply to this distribution also.

3. Analytical properties of the conductance function $G_N(p)$

The conductance function $G_N(p)$ is a polynomial of order $k (= N^2 + (N-1)^2)$—k being the total number of bonds in the $N \times N$ lattice—with $G_N(p) = \Sigma_{j=0}^{k} C_j p^j (1-p)^{k-j}$ where the coefficient C_j corresponds to the sum of the conductances of all possible configurations of the $N \times N$ lattice having j bonds present and $(k-j)$ broken bonds. Accordingly, it is easily verified that all $C_{j<N} = 0$ and that the first term of the polynomial is $1p^N(1-p)^{k-N}$. It is, of course, relatively trivial to calculate

$$G_1(p) = p \tag{2}$$

and

$$G_2(p) = 1p^2q^3 + \tfrac{11}{3}p^3q^2 + \tfrac{17}{5}p^4q + 1p^5 \tag{3}$$

(where $q = 1-p$), since the $N = 2$ lattice involves only 2^5 configurations. We have

† In the case of p near p_c where a significant fraction of realised lattices are not conducting, we have found that the convergence to zero tends to be very slow. Since, both from our own observations and from the extensive percolation literature, it is apparent that the conductive backbone is then always characterised by multiple loops joined by a few critical bonds, we have found that the calculations could be greatly speeded up by recognising that any lattice for which the conductance drops below that of a 'monofilament' resistor three times the length of the lattice is, to an extremely high probability, non-conducting.

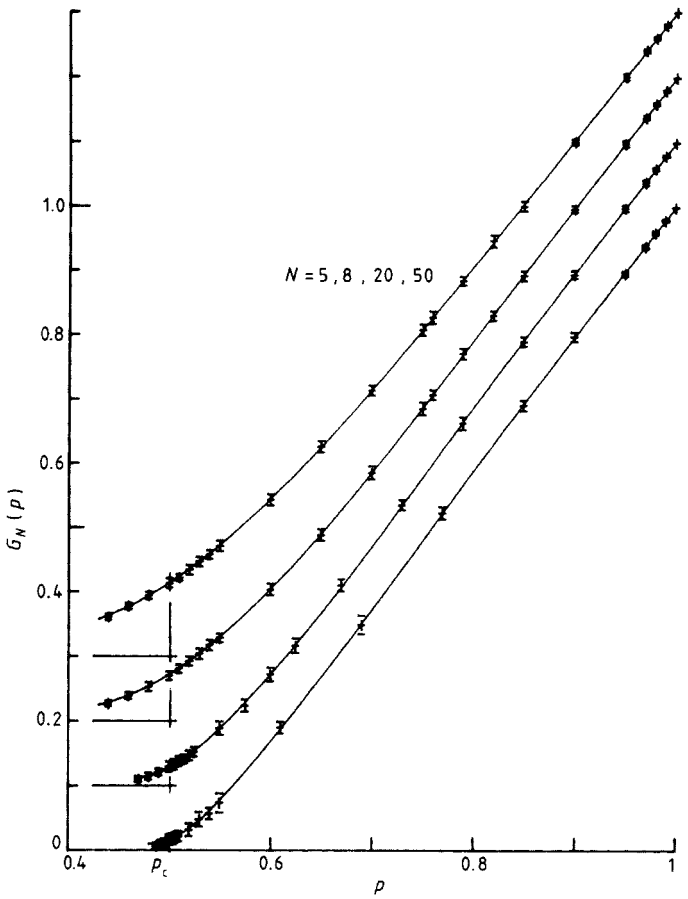

Figure 2. Monte Carlo results of $G_N(p)$ against p for four different values of N. The full curves are calculated by means of the interpolation functions described in the text. Note that, for clarity between the different data, the vertical scales have been displaced for the three upper curves, with the location of the p axis indicated in each case.

also calculated, for purposes of testing our interpolation techniques, $G_3(p)$, which already involves 2^{13} configurations:

$$G_3(p) = 1p^3q^{10} + 12p^4q^9 + 63.333\,33p^5q^8 + 189.109\,09p^6q^7 + 348.208\,01p^7q^6 + 408.725\,81p^8q^5 + 318.414\,23p^9q^4 + 166.027\,66p^{10}q^3 + 56.130\,16p^{11}q^2 + 11.181\,59p^{12}q + 1p^{13}. \quad (4)$$

Even with computer assistance, however, $G_4(p)$ with 2^{25} variations is virtually beyond the limit of reasonable attempts.

Aside from the previously stated fact that $G_N(1) = 1$, it is also possible to show, by an effective-medium approach, that for large lattices the slope at $p = 1$ equals 2. This slope has been previously (Ottavi *et al* 1978) called the 'vulnerability' of the lattice, and found to be closely related to the coordination number of various lattices. By considering all configurations with one missing bond, we have calculated the exact vulnerabilities for all lattices 2×2 to 10×10, which we tabulate below.

Table 1. Exact vulnerabilities of small square lattices.

N	$\alpha(N)$	N	$\alpha(N)$	N	$\alpha(N)$
2	1.600 000 00	5	1.963 777 90	8	2.012 332 56
3	1.818 414 32	6	1.989 450 31	9	2.017 336 10
4	1.915 659 18	7	2.003 904 06	10	2.020 303 62

We have found that the slopes, just tabulated above, are extremely well approximated by the function

$$\alpha_1(N) = 2 - 0.701807/N + 5.56973/N^2 - 6.19944/N^3 + 2.13434/N^4. \tag{5}$$

Given the further fact that the 10×10 lattice consists already of 181 bonds, it seems a most reasonable generalisation to assume that the above equation will continue to be a good representation of the slope for all $N > 10$.

In summary we see, as illustrated in figures 2 and 3, that the function $G_N(p)$ starts off unity at $p = 1$, descends linearly with slope two, goes through an inflection and then becomes very small at $p = p_c$, but that, for all finite N, the transition is smeared

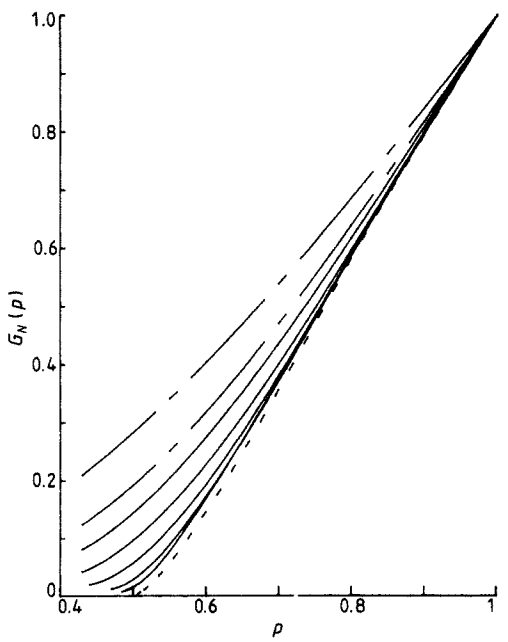

Figure 3. Summary of the experimental results for $G_N(p)$. The intermittent curves (unequal dashes) are exact calculations for $N = 2$, 3. The full curves are interpolation functions calculated from numerical Monte Carlo data as shown in figure 2, for $N = 4$, 6, 10, 20, 50. The broken curve represents an extrapolation for $N \to \infty$, discussed in the text, obtained at constant p from the family of interpolation curves. The present paper is principally concerned with the smearing of the critical behaviour around the exact threshold $p_c = \frac{1}{2}$, and to a lesser extent with the 'vulnerability' (slope at $p = 1$) of the conductance functions $G_N(p)$.

out and there exists a small, finite probability that conductivity will occur even for $p < p_c$. We shall keep these general properties in mind in the development of our interpolation method below.

4. Finite-size scaling on $G_N(p)$

The smearing observed on the set of numerical curves (figure 1) is a general characteristic of the critical transitions in finite systems. While in the true asymptotic limit, critical properties display, at the critical point, non-analytic behaviour with critical exponents, for finite systems there exists a limited region around the critical point where the discontinuity is 'smeared'. This softening can be understood in terms of the divergence of a characteristic length, the 'correlation length', ξ, as the critical point is approached—$\xi(p) \propto |\varepsilon|^{-\nu}$ (where $\varepsilon = p - p_c$). In the case of the percolation problem, this length is associated with the average size of clusters. So long as the correlation length, ξ, is small with respect to the linear dimensions of a finite system, the system will display the expected critical behaviour. However, as the critical point is approached, ξ eventually becomes comparable to the size of the system and rounding occurs, because a finite fraction of configurations remains conducting for all p. The operative universal variable thus becomes the ratio of the linear dimension to the correlation length, in our case $N/\xi \propto N\varepsilon^{\nu}$. We can therefore write, in the spirit of finite-size scaling (Fisher 1971, Roussenq *et al* 1975, Sur *et al* 1976), the conductance variation

$$G_N(p) = N^{-x} X(z) \tag{6}$$

where the homogeneous function $X(z)$ of the modified universal variable $z = \varepsilon N^{1/\nu}$ describes the rounding effect near p_c for finite N. In the thermodynamic limit

$$G_\infty(p) \propto \varepsilon^{t}. \tag{7}$$

We must consequently have a behaviour $X(z) \propto z^{t}$ for $z \to \infty$, and therefore the exponent x of the prefactor of equation (6) must be such as to ensure independence of N, for large N, i.e.

$$x = t/\nu. \tag{8}$$

Recalling, in addition, that $G_N(p)$ is an analytic function of p for all finite N, we conclude that in the 'smeared' region we must have a Taylor series development

$$X(z) = X(0) + zX'(0) + z^2 X''(0)/2 + \ldots \tag{9}$$

i.e.

$$G_N(p) = N^{-x} X(0) + N^{-x+y}\varepsilon X'(0) + N^{-x+2y}\varepsilon^2 X''(0)/2 + \ldots \tag{10}$$

where we have defined for notational convenience $y = 1/\nu$.

We therefore come to the new conclusion that the variation with N of the coefficients in the development of $G_N(p)$ in powers of ε, around $p = p_c$ should permit us to obtain both critical exponents t and ν, from an overdetermined problem.

In order to do this, however, we must be able to obtain for each value of N a sufficiently accurate approximation for $G_N(p)$, so that we can compute not only $G_N(p_c)$, but equally $G'_N(p_c)$ and $G''_N(p_c)$. The interpolation technique which we will presently describe allows us to do just that, from the various values of $G_N(p)$ calculated by the Monte Carlo method.

5. The interpolation method

After observing the general features disclosed by the conductance points displayed in figure 1, we have somewhat arbitrarily chosen to divide the curves into three regions: (i) $p \leqslant 0.57$, (ii) $0.57 < p \leqslant 0.84$, and (iii) $0.84 < p \leqslant 1$; the point $p = 0.57$ was chosen as being outside the critical region around p_c, while the point $p = 0.84$ was selected so as to be in the region where the curves $G_N(p)$ begin to display some curvature. We then do a simultaneous least-squares fit of the entire set of 22 data points to a cubic arc for region (i), another cubic arc for region (ii) and a parabolic arc for region (iii). The least-squares fit is carried out, however, under the constraints: (a) that at the boundary between regions (i) and (ii), the interpolating function, its first and second derivatives should be continuous, (b) that at the boundary between regions (ii) and (iii), the function and its first derivative should be continuous, and (c) that at $p = 1$, the parabolic arc should not only pass through the correct value of unity but that it should equally have the proper slope, predicted from equation (5). These various constraints have the effect not only of reducing the number of free parameters to four, but also of producing an interpolating function with a second derivative which is a continuous function throughout regions (i) and (ii). We have placed this particular condition because we wish to be able to ascribe some significance to the curvature of the interpolation function at $p = p_c$.

We have tested the interpolation method by carrying out this procedure on values calculated from the exact, known functions $G_2(p)$ and $G_3(p)$ at the 22 values of p used for Monte Carlo calculations for lattices $N = 4$ to 10. Upon recalculating the conductance values from the interpolation function, we find that for both $N = 2$ and $N = 3$ they never deviate from the exact values by more than 6×10^{-4}, and typically 2×10^{-4}, and that, at p_c, the function values agree to 0.05%, the first derivatives to 0.3%, and the second derivatives to 3.3% or better.

When we recall that $G_3(p)$ is in fact a polynomial of order 13 in p, this kind of agreement is indeed satisfying.

6. Critical exponents and other results

The continuous curves through the Monte Carlo points of figure 2 are in each case computed from the corresponding interpolation function. It should be noted that in all cases they pass well within the corresponding statistical error bars.

We further display, in figure 3, a more complete set of interpolation curves for $G_N(p)$. We show, in the same figure, the exact functions $G_2(p)$ and $G_3(p)$ (from equations (3) and (4)), while the broken line represents an extrapolation, discussed below, for $N \to \infty$ in an attempt to visualise the curve $G_\infty(p)$, and to complete the family of curves.

Finally, in figure 4, we present a log–log plot, against lattice size N, of the coefficients

$$A(N) = G_N(p_c), \qquad A_1(N) = G'_N(p_c), \qquad A_2(N) = G''_N(p_c), \tag{11}$$

as deduced from our interpolation functions for each value of N. In equation (10), we have predicted that these coefficients should vary respectively as N^{-x}, N^{-x+y}, and N^{-x+2y}. Consequently, in figure 4, the slopes of the three resulting straight lines must be fitted by these two parameters, x and y. We have found values of these parameters which best fit our data, in a weighted least-squares sense. (The values of $A_2(N)$ are

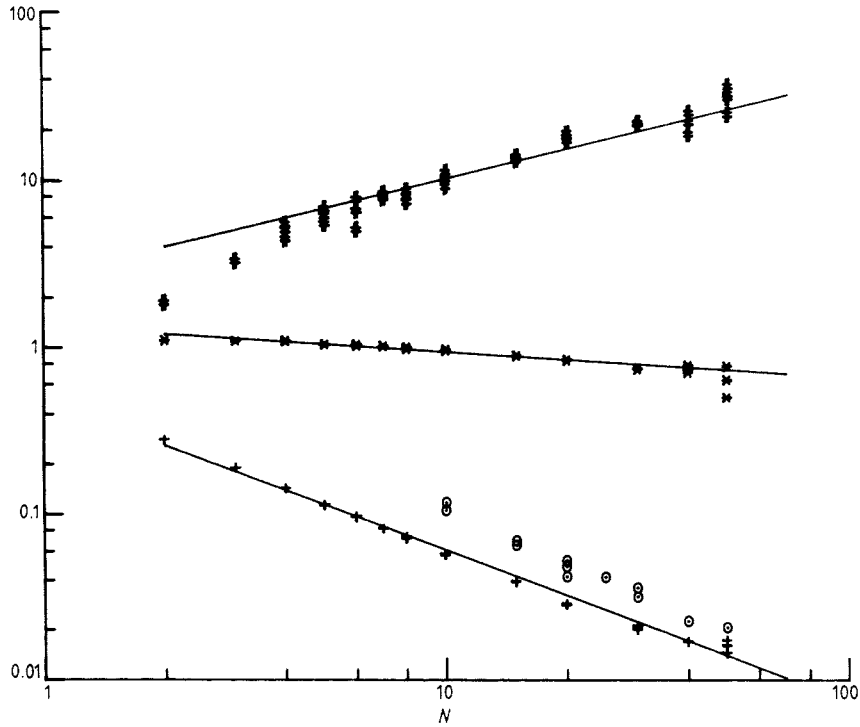

Figure 4. Logarithmic plot (at $p_c = \frac{1}{2}$) of the value of the conductance $G_N(p_c)$, and of its first two derivatives with respect to p, against lattice size N. The two critical exponents $t = 1.22 \pm 0.08$ and $\nu = 1.35 \pm 0.06$ (for the conductivity and correlation length) are obtained, in an overdetermined way, from a weighted, linear, least-squares fit of the functions, illustrated by the straight lines through the data. The open circles represent less reliable preliminary data, shown for comparison purposes only. ⋕, $A_2(N) = G''_N(p_c)$; *, $A_1(N) = G'_N(p_c)$; +, $A(N) = G_N(p_c)$.

given only $\frac{1}{4}$ the weights of the $A(N)$ and $A_1(N)$, in recognition of the much greater uncertainty associated with the curvature values.) We have also omitted in this fit all values for the smaller lattices $N = 2$, 3, 4, which are, however, shown in the figure. The straight lines appearing on figure 4 are the results of our fit, corresponding to

$$x = t/\nu = 0.91 \pm 0.03, \qquad y = 1/\nu = 0.74 \pm 0.03,$$

whence

$$t = 1.22 \pm 0.08, \qquad \nu = 1.35 \pm 0.06.$$

We can compare these with the current preferred values (Stinchcombe and Watson 1976, Den Nijs 1979, Reynolds *et al* 1980, Straley 1980)

$$t = 1.13 \pm 0.09 \qquad \text{and} \qquad \nu = 1.34 \pm 0.02.$$

The open circles in figure 4 represent results from some preliminary Monte Carlo calculations performed with poorer statistics and less stringent convergence criteria than those discussed in § 2 above. We present them to indicate that even under those conditions, one could have inferred a reasonable value of $x = t/\nu$, and at the same time to emphasise the need for stringent convergence in obtaining lattice-conductance

solutions. (The values are larger than the present ones because of the poor convergence to $G_N = 0$ of some of the realisations near p_c.)

It is also very interesting to observe how close the results on lattices with N as low as 2, 3 and 4 lie to the best-fit lines, particularly for the function $A(N)$ and the first derivative $A_1(N)$. The deviation, at low N, of the second derivative $A_2(N)$ is not unexpected, since there is a greater contribution to the curvature of $G_N(p)$ from configurations with many broken bonds to which the smaller lattices are more sensitive.

To obtain an idea of the shape of $G_\infty(p)$ in the limit $N \to \infty$, we have used as an extrapolation scheme, at each of about 100 values of p_i in the range $0.5 < p < 1$, a least-squares fit for the values of $G_N(p_i)$ obtained, at constant p, from our interpolation functions to the function $a_i + b_i/N^x$. This gives the correct result $G_\infty(p_c) = 0$ in accordance with equation (10), as well as $G_\infty(1) = 1$. That extrapolation, plotted as the broken curve in figure 3, gives approximately the correct shape for the conductivity of infinite systems. A power-law fit near $p_c = 0.5$ gives a crude value of exponent 1.5, not inconsistent with our results. Let us emphasise, however, that our extrapolation scheme is only an empirical and illustrative one for p above p_c.

In conclusion, we have established, as surmised above, that good values of the critical exponents t and ν can be obtained using our method even on relatively small lattices. We plan to report at a later date on similar results in the three-dimensional case, as well as on lattices with anisotropic percolation.

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