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1989 J. Phys. A: Math. Gen. 22 L891

(http://iopscience.iop.org/0305-4470/22/18/008)

J. Phys. A: Math. Gen. **22** (1989) L891-L894. Printed in the UK

LETTER TO THE EDITOR

Elastic property of the self-avoiding random walk

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Received 16 June 1989

Abstract. We have calculated the end-to-end elastic susceptibility for the bond-bending model on the self-avoiding random walk. Our numerical result shows clearly that the central force term is irrelevant when the bond-bending term is present. Our result also indicates that when the elastic constant of the bond-bending term is set equal to infinity the elastic network is governed by the conductivity exponent of the random resistor network.

The elastic network has been the subject of recent studies [1-6]. The simplest model is the central force model [1], where each bond in the cluster is associated with a spring of spring constant k_{cen}. Since its rigidity threshold p_{cen} is higher than the percolation threshold, a more realistic model has been investigated, i.e. the bond-bending model [2]. This model can be defined as the central force model plus a bond-bending term where each nearest-neighbour pair of bonds is associated with another spring of spring constant k_{bb}. For the bond-bending model, the scaling analysis of Kantor and Webman [2] gives the lower bound for the bulk modulus exponent f which is $d\nu+1=3.67$ in two dimensions, where ν is the correlation length exponent. The early numerical simulations by Feng *et al* [6] and Bergman [7] yield the estimates $f=3.3\pm0.5$ and $f=3.5\pm0.2$ respectively. The real space renormalisation group study [8] gives $f=3.5$-3.75. The most recent and the most accurate simulation is by Zabolitsky *et al* [9] and gives $f=3.96\pm0.04$ in two dimensions. This leads to the conjecture [6, 10-12]

$$f=2\nu+t \tag{1}$$

where t is the conductivity exponent for the random resistor network. This agrees with $f=3.96\pm0.04$ very well if we take $\nu=4/3$ and $t=1.30$†. In the resistor network, one can define resistive susceptibility χ_{re} [14] as

$$\chi_{re}=\left[\sum_i R_{ij}\nu_{ij}\right]_{av}\simeq|\Delta p|^{-\phi_{re}-\gamma} \tag{2}$$

where R_{ij} is the resistance between site i and j, $[\cdot]_{av}$ denotes the configurational average, and ϕ_{re} is the critical exponent which describes the way in which two-point resistance scales with the distance. From a node-link picture [15] or a scaling analysis [14], we have the relation

$$t=(d-2)\nu+\phi_{re}. \tag{3}$$

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† Several authors [13] all give $t\simeq1.30$ in two dimensions.

0305-4470/89/180891+04$02.50

Similarily, we expect that $f=(d-2)\nu+\phi_{el}$ for the elastic network, where ϕ_{el} is a crossover exponent. From a node-link picture [16], ϕ_{el} is identified to be the crossover exponent describing the way that two-point elastic susceptibility χ_{el} scales with the distance. Here χ_{el} is defined as

$$\chi_{el}=\left[\sum_i \chi_{ij}\nu_{ij}\right]_{av}\simeq|\Delta_p|^{-\phi_{el}-\gamma} \tag{4}$$

where χ_{ij}^{-1} is the effective elastic constant between site i and j.

One can define another crossover exponent ϕ_{sr} as [4]:

$$\chi_{sr}=\left[\sum_b \chi_{b,b'}\nu_{b,b'}\right]_{av}\simeq|\Delta p|^{-\phi_{sr}-\gamma} \tag{5}$$

where $\chi_{b,b'}=\theta/\tau$ is the splay elastic susceptibility [4], b is the bond index, θ is the angular displacement between bonds b and b', and τ is the torque on bonds b and b' needed to maintain equilibrium.

The dimensional argument suggests that $\phi_{el}=2\nu+\phi_{sr}$. This agrees with the mean-field value [16] $\phi_{el}=2$ and $\phi_{sr}=1$. A series-expansion calculation [17] up to p^{13} of ϕ_{el} on a honeycomb lattice, which should give a result of ϕ_{el} around 3.96 if we assume equations (1) and (3) to be exact, does not agree with numerical simulations presumably because the series is not long enough to extrapolate the exponent. The series calculation [18] on the lattice animal, however, supports $\phi_{el}=2\nu+\phi_{sr}$. It has been shown [18] that $\phi_{sr}=\phi_{re}$ for the lattice animal. For percolation, it has also been shown [19] that $\phi_{sr}=\phi_{re}$. In this letter, in order to study the scaling of the elastic susceptibility as we vary k_{bb} and k_{cen}, we have calculated the end-to-end elastic susceptibility, as defined in (4), of the self-avoiding walk on a square lattice χ_{saw}. We assume that each step of the walk is represented by a bond. For a chain of length n, we have [2]:

$$\chi_{saw}(n)=S^2(n)/k_{bb}+L(n)/k_{cen} \tag{6}$$

where

$$S^2(n)=\sum_{i=1}^{n}[(\hat{F}\times\hat{z})\cdot(\boldsymbol{R}_i-\boldsymbol{R}_n)]^2 \tag{7}$$

and

$$L(n)=\sum_{i=1}^{n}[\hat{F}\cdot(\boldsymbol{R}_i-\boldsymbol{R}_{i+1})]^2 \tag{8}$$

Here $\boldsymbol{R}_i$ is the position vector of site i and $\hat{F}=(\boldsymbol{R}_1-\boldsymbol{R}_n)/|\boldsymbol{R}_1-\boldsymbol{R}_n|$. Therefore, we can obtain χ_{saw} as a function of k_{bb} and k_{cen}. The series we obtain is:

$$\chi_{saw}=\sum C(n)\chi_{saw}(n)K^n=\chi_1/k_{bb}+\chi_2/k_{cen} \tag{9}$$

where $C(n)\simeq n^{-\theta_{saw}}\lambda^n$ is the number of the self-avoiding walks, with $\theta_{saw}=43/32$ [20] and $\lambda^{-1}=2.6381\pm0.0002$ [21] on the square lattice. For $S^2(n)$ and $L(n)$, we assume that they obey the following scaling forms:

$$\sum_{\gamma_n} S^2(\gamma_n)/C(n)\simeq n^{\phi_b} \tag{10}$$

$$\sum_{\gamma_n} L(\gamma_n)/C(n)\simeq n^{\phi_{cen}} \tag{11}$$

Table 1. The coefficients of the series on the square lattice.

n	$\chi_1(n)$	$\chi_2(n)$
1	0.00	4.00
2	4.00	8.00
3	35.20	44.80
4	176.00	179.20
5	858.87	654.66
6	3 600.62	2 196.25
7	14 558.13	7 209.08
8	54 325.81	22 639.17
9	198 880.90	70 413.40
10	693 229.94	213 149.76
11	2385 497.48	641 656.91
12	7942 414.17	1896 912.01
13	26 202 969.61	5 587 306.25
14	84 420 461.12	16 244 077.99
15	270 133 898.69	47 108 059.47
16	849 039 685.23	135 269 106.90
17	2654 560 821.62	387 722 652.48
18	8 183 952 957.33	1 102 718 656.00
19	25 126 058 026.74	3 132 043 249.68
20	76 274 713 761.93	8 840 184 979.61
21	230 765 610 361.48	24 925 873 135.11

where ϕ_b and ϕ_{cen} are two critical exponents and γ_n denotes all the n-step self-avoiding walks. The series of the splay elastic susceptibility is readily shown to be the same as χ_2 for a chain, from which we have $\phi_{sr} = \phi_{cen}$. We have calculated χ_{saw} on a square lattice up to p^{21}. The calculation was done on a Masscomp 5700 (which is about three times slower than a VAX 8650) and took about 18 h of CPU time. The series coefficients are listed in table 1. We analysed the series using a Padé approximant and a differential Padé approximant [22]. We obtained $\phi_b = 2.493 \pm 0.008$ and $\phi_{cen} = 0.992 \pm 0.010$. Since $\phi_{re} = 1$ for the self-avoiding walk, our result suggests that $\phi_b = 2\nu + \phi_{re}$ and $\phi_{cen} = \phi_{re}$ with $\nu = 3/4$ [20, 23]. From this analysis, we clearly see that in (9) the central force term is irrelevant when the bond-bending term is present. This is the crucial argument in order to show $\phi_{sr} = \phi_{re}$ for percolation in two dimensions. We also notice that in the limit that k_{bb} goes to infinity, the elastic network is governed by the conductivity exponent of the resistor network. A series expansion calculation [19] for percolation on a honeycomb lattice has also indicated this point. We do not yet know how to map the bond-bending model in which k_{bb} is set equal to infinity onto the resistor network.

In summary, we have calculated the end-to-end elastic susceptibility for the self-avoiding walk. Our numerical result confirms that the central force term is irrelevant when the bond-bending term is present. Our result supports $\phi_{el} = 2\nu + \phi_{sr}$, $\phi_{sr} = \phi_{re}$, and in turn $f = 2\nu + t$. Our result also indicates that in the limit the k_{bb} goes to infinity, the elastic network is governed by the conductivity exponent of the resistor network.

I would like to thank Dr R Kozack for a careful reading of this manuscript. I also thank the NIH for support under grant no 4-60357.

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