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LETTER TO THE EDITOR

Renormalisation of the 'true' self-avoiding walk

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Abstract. It is shown that the renormalisation of the 'true' self-avoiding walk of Amit *et al* at its upper critical dimensionality two involves at least *two* (possibly three) coupling constants. Fixed points to first order in $\varepsilon = 2-D$ are identified and the asymptotic behaviour at $D = 2$ is discussed.

Amit *et al* (1982, to be referred to as I) have recently observed that the common use of the expression 'self-avoiding walk' as synonymous with the problem of polymer statistics in a good solvent is misleading. The statistical problem of a traveller who steps randomly, but tries to avoid places he has already visited, appears as a natural interpretation of the expression 'self-avoiding walk' (SAW): it was shown in I that this problem (called the 'true' SAW) belongs to a different universality class from that of the polymer problem (for which see, e.g., de Gennes 1979), and in particular that its upper critical dimensionality—above which it essentially behaves like an ordinary, not self-avoiding, walk—is two, whereas it is four for the polymer problem.

A heuristic renormalisation scheme was set up in I and led to the prediction that the average square end-to-end distance $\langle R_N^2\rangle$ for a 'true' SAW in two dimensions behaves asymptotically for $N\to\infty$ in the following way:

$$\langle R_N^2\rangle \propto N|\ln N|^{\zeta} \tag{1}$$

where the exponent $\zeta = 0.4$. This prediction was checked against computer simulations: the results were acceptable when the self-avoidance parameter g was rather small; it failed, however, in the limit $g\to\infty$ where ζ appeared to approach one.

It must be remarked that the renormalisation procedure of I was heuristic in the sense that it was assumed that the renormalisation of the single coupling constant g and of the diffusion parameter $\mathcal{D}$ of the random walk was sufficient to remove all infinities in the perturbation theory as the dimensionality D of the space approached the upper critical dimension $D_c = 2$.

We wish to point out in this letter that this assumption is incorrect and that the renormalisation of the 'true' SAW involves at least *two* (possibly three) coupling constants. As a consequence the prediction $\zeta = 0.4$ in (1) is incorrect. The asymptotic behaviour depends on some details of the model. If only two coupling constants (g_1, g_2) are involved and the starting point of the renormalisation group is chosen to be $(g_1, 0)$ with $g_1 > 0$, then the asymptotic behaviour corresponds to $\zeta = 1$ and is reached the faster, the larger the initial value of g_1 (we are neglecting the effects of terms of higher order in the coupling constants). This can explain the results of the simulations of I in the $g \to \infty$ limit. One obtains on the other hand that the present theory agrees quite well with the data of I for smaller values of g. We have so far been unable to rule out the possible appearance of a third coupling constant g_3 in the renormalisation of the theory. We remark, however, that although its presence will eventually modify the asymptotic behaviour, its effects are likely to be very small for the path lengths investigated in I. We report here only the results of a one-loop calculation. Fuller results and proofs will be reported elsewhere.

The 'true' SAW in a D-dimensional continuum is defined as in I by the equations

$$\mathrm{d}\boldsymbol{R}(t)/\mathrm{d}t = -g_1 \nabla \rho(R(t), t) + \boldsymbol{\eta}(t), \tag{2}$$

$$\partial \rho(\boldsymbol{r}, t)/\partial t = \delta(\boldsymbol{r} - \boldsymbol{R}(t)), \tag{3}$$

where $\boldsymbol{\eta}(t)$ is a Gaussian noise which satisfies

$$\langle \boldsymbol{\eta}(t)\rangle = 0, \qquad \langle \eta_i(t)\eta_j(t')\rangle = 2\mathscr{D}\delta_{ij}\delta(t-t'). \tag{4}$$

$\mathscr{D} > 0$ is the diffusion and $g_1 > 0$ is the coupling constant of the process. The perturbation procedure outlined in I can be then reproduced by a diagrammatic technique.

Let us consider the Laplace transform with respect to time and the Fourier transform with respect to space of the end-to-end distance probability distribution function (denoted $\Delta(\mu, \boldsymbol{p})$ in I):

$$G(\mu, p) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\mu t} \int \mathrm{d}^D r\, \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}} \langle \delta(r - R(t))\rangle. \tag{5}$$

The quantity $G(\mu, \boldsymbol{p})$ can be then computed by the following rules.

(i) For n-loop order, draw all diagrams containing one directed continuous line and up to n broken lines joining points on the continuous one.

(ii) Associate a wavenumber $\boldsymbol{p}$ to each segment of the continuous line and a wavenumber $\boldsymbol{q}$ to each broken line, satisfying conservation at each vertex; the wavenumber $\boldsymbol{q}$ is assumed to run *opposite* to the direction of the continuous line (figure 1).

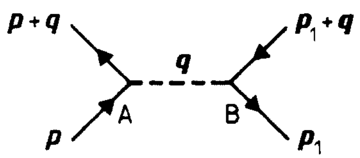

Figure 1. The basic vertex. The point A is assumed to come *earlier* than B along the directed line.

(iii) Associate a factor $(\mu + \mathscr{D}p^2)^{-1}$ to each continuous segment with wavenumber p.

(iv) Associate a factor $g_1(\boldsymbol{p}_1 \cdot \boldsymbol{q})$ to each dotted line with wavenumber $\boldsymbol{q}$, where $\boldsymbol{p}_1$ is the wavenumber of the *latest* outgoing continuous segment.

(v) Integrate over all free wavenumbers, dividing by $(2\pi)^D$ for each integration.

It is possible to justify these diagrammatic rules by means of a Martin *et al* (1973) field theoretical approach: the derivation will be reported elsewhere. It is, however, easy to check that it reproduces the results of I.

The building blocks of the diagram technique are:

(a) the self-energy Σ; it is obvious that it is proportional to its wavenumber argument $\boldsymbol{p}$, hence to p^2;

(b) the dressed vertex Γ (figure 2). It is obviously proportional to $\boldsymbol{p}_1$; hence it may be written

$$\Gamma(p, q, p_1) = (\boldsymbol{p}_1 \cdot \boldsymbol{q})\Gamma_1 + (\boldsymbol{p}_1 \cdot (\boldsymbol{p}_1 + \boldsymbol{q}))\Gamma_2 + (\boldsymbol{p}_1 \cdot \boldsymbol{p})\Gamma_3. \tag{6}$$

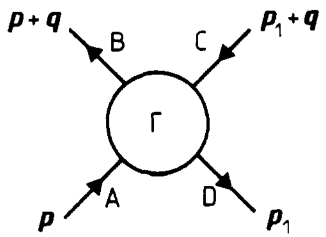

Figure 2. The dressed vertex Γ. The line joining A and B is assumed to come *earlier* than that joining C and D along the directed line.

Power counting immediately shows that $\partial\Sigma/\partial p^2$ and Γ_1, Γ_2, Γ_3 are dimensionless at $D = 2$. The upper critical dimension is therefore 2, where the theory can be renormalised by introducing:

(a) a diffusion constant renormalisation factor Z via

$$\mathscr{D} = Z\mathscr{D}_{\mathrm{R}}; \tag{7}$$

(we shall set $\mathscr{D}_{\mathrm{R}} = 1$ for convenience) and

(b) *three* renormalised coupling constants $u_1\kappa^{\varepsilon}$, $u_2\kappa^{\varepsilon}$, $u_3\kappa^{\varepsilon}$ (where κ is the renormalisation wavenumber), which take care of the primitive divergences of Γ_1, Γ_2, Γ_3 respectively.

The results of a one-loop calculation at $D = 2$ via dimensional regularisation and minimal subtraction (cf Amit 1979, §§ 9–10) are

$$Z = 1 + \varepsilon^{-1}(-u_1 + u_3), \tag{8}$$

$$K_D g_1 = \kappa^{\varepsilon}[u_1 + \varepsilon^{-1}(\tfrac{5}{2}u_1^2 + \tfrac{1}{2}u_2^2 - 2u_1u_2 - 3u_1u_3)], \tag{9}$$

$$K_D g_2 = \kappa^{\varepsilon}[u_2 + \varepsilon^{-1}(-u_1^2 - u_2^2 + 3u_1u_2 + u_1u_3 - 3u_2u_3)], \tag{10}$$

$$K_D g_3 = \kappa^{\varepsilon}[u_3 + \varepsilon^{-1}(-\tfrac{5}{2}u_3^2 + 2u_1u_3 - u_2u_3)]. \tag{11}$$

K_D indicates as usual the factor $2^{1-D}\pi^{-D/2}/\Gamma(D/2)$. Remark that if $g_3 = 0$, then $u_3 = 0$, at least to one-loop order. It is uncertain whether this property remains at higher orders. If we assume this to be the case, we obtain the following flow equations for u_1, u_2 in the $u_3 = 0$ plane:

$$\mathrm{d}u_1/\mathrm{d}\tau = W_1 = -\varepsilon u_1 + \tfrac{5}{2}u_1^2 + \tfrac{1}{2}u_2^2 - 2u_1u_2, \tag{12}$$

$$\mathrm{d}u_2/\mathrm{d}\tau = W_2 = -\varepsilon u_2 - u_1^2 - u_2^2 + 3u_1u_2, \tag{13}$$

where $\tau = \ln(\kappa'/\kappa)$ is the logarithm of the scale parameter. Equations (12), (13) have as a stable fixed point for $\varepsilon > 0$: $u_1 = u_2 = \varepsilon$, with a corresponding critical exponent:

$$\eta = W_i(\partial \ln Z/\partial u_i) = \varepsilon + \mathrm{O}(\varepsilon^2). \tag{14}$$

The exponent η is related to the asymptotic behaviour of $\langle R^2(t)\rangle$ as a function of the length t of the walk:

$$\langle R^2(t)\rangle \propto t^{1+\eta}. \tag{15}$$

The prediction (14) disagrees therefore with the interesting conjecture of Pietronero (1982), which gives for $0 \leqslant \varepsilon < 1$:

$$\eta = \varepsilon/(1-\varepsilon). \tag{16}$$

If $g_3 \neq 0$ the situation is more complicated. There are six fixed points of order ε (the one given above is double). If $u_3 > 0$ there is runaway, if $u_3 < 0$ the stable fixed point appears to be $u_1 = u_2 = 0$, $u_3 = -2\varepsilon/5$, to which corresponds $\eta = 2\varepsilon/5$. This fixed point is probably relevant for some problems of the random walk in a random environment.

At $\varepsilon = 2 - D = 0$ we may remark the following: starting from $u_1 = u_1^0$, $u_2 = u_3 = 0$, the flow equations yield a trajectory which tends to lie along the $u_1 = u_2$ line. The analysis of Amit (1979, §§ 9–6), then allows one to compute the asymptotic value of ζ (equation (1)), which equals one. This appears to be in contradiction with the results of the simulations of I. If, however, we consider the behaviour of the quantity

$$Y = \langle R_N^2\rangle/N \tag{17}$$

as a function of the number of steps N, we see that the results of the present calculation are compatible with the numerical results of I. We have in fact

$$Y \propto \exp\left(-\int_0^{\tau_0} \mathrm{d}\tau\, u_1(\tau)\right), \tag{18}$$

where $(u_1(\tau), u_2(\tau))$ is the solution of (12), (13) which satisfies $(u_1(0), u_2(0)) = (u_1^0, 0)$, and $\tau_0 = -\frac{1}{2}\ln(\langle R_N^2\rangle/a^2)$, where a is an elementary length which plays the role of a lattice constant. We have plotted in figure 3 Y as a function of $\ln_2 N$ as computed from the present theory, against the data of I. The coupling constant $g_1 = u_1^0 = 1$. The non-universal quantity a is chosen in such a way that the curve passes through the data point at $\ln_2 N = 8.5$. The broken line is computed from the theory of I.

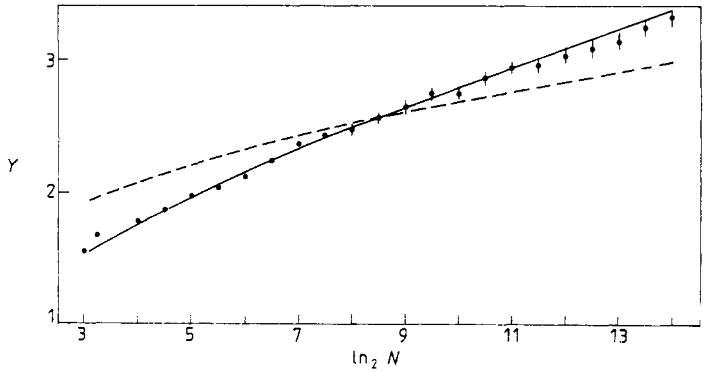

Figure 3. Y (equation (17)) against $\ln_2 N$ (N is the number of steps) for $g_1 = 1$. The data are from I. Full line: present theory. Broken line: theory of I.

When u_1^0 grows larger, higher-order terms will come into play. It is easy to see, however, that the solutions of the flow equations (12), (13) for $\varepsilon = 0$ satisfy the scaling relation, valid for all $\lambda > 0$:

$$(u_1(\tau), u_2(\tau)) = \lambda (u_1(\lambda\tau), u_2(\lambda\tau)). \tag{19}$$

The ratio u_2/u_1 and the exponent ζ will therefore settle to their asymptotic value of one with values of $|\tau|$ which are inversely proportional to u_1^0. This may explain the behaviour of the simulation data of I for the $g \to \infty$ limit, which were more compatible with $\zeta = 1.0$ than with $\zeta = 0.4$.

We have shown in conclusion that a diagrammatic expansion of the 'true' SAW can be renormalised by means of familiar techniques around its upper critical dimensionality two.

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