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LETTER TO THE EDITOR

Walks, trails and polymers with loops

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Abstract. Lattice models interpolating between free and self-avoiding random walks are investigated. Generating functions are constructed for k-tolerant walks, various trail problems, etc. For trail problems the effective field theory describing the global behaviour is analysed in the vicinity of the upper critical dimension $d_c = 4$. Their asymptotic large-scale behaviours are the same as those of the self-avoiding walk. Arguments are presented to support the same conclusion for much more general classes of walks including k-tolerant walks. One of the models exhibits a new tricritical point of order $\varepsilon^{1/2}$ if the fugacity for crossing is increased.

Very recently, there has been renewed interest in the effect of loop formation on the statistical properties of polymers (Malakis 1976, Chen 1981a,b,c, Wheeler and Pfeuty 1981, Family 1982, Rys and Hefrich 1982, Gujrati 1983, Petschek *et al* 1983). The question is: Is the large scale behaviour of the single polymer (or the self-avoiding walk) affected by the presence of rings, doubly occupied bonds, etc.? Most of the earlier work suggests a negative answer to this question‡. These results have been reached by exact enumeration for trails (Malakis 1976), by a renormalisation group approach (Oono 1979) and exact enumeration (Oyama and Shiokawa 1983) for k-tolerant walks, and by a real space renormalisation method for polymers with loops (Family 1982).

In the present letter, we initiate a more systematic approach by suggesting new methods to construct generating functions for generalised lattice polymer models. These functions are then transformed into continuum field theories, and analysed via momentum space renormalisation group and the ε-expansion. General conclusions we can draw are in agreement with previous results where they have already existed; allowing finitely multiple occupancies of bonds and/or vertices does not change the large scale behaviour of the self-avoiding walk. It seems that the free random walk behaviour is recovered only without any constraint on the walk.

First, we define models to be investigated. The *k-tolerant walk* (Malakis 1976) is a random walk which may return to the same lattice site at most k times. In particular the l-tolerant walk is the self-avoiding walk (figure 1). The *v-vertex trail* is a walk which may return to the same lattice site at most v times without passing through any bond more than once. Thus loops are formed, but the excluded volume is not ignored (as a polymer with fused loops. The ∞-vertex trail problem is the standard trail

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‡ One may say that the 'true' self-avoiding walk of Amit *et al* (1983) is an exception, but in this case the modification of the self-avoiding walk is far more drastic than the introduction of rings, etc. The authors are grateful to the referee who brought our attention to the true self-avoiding walk.

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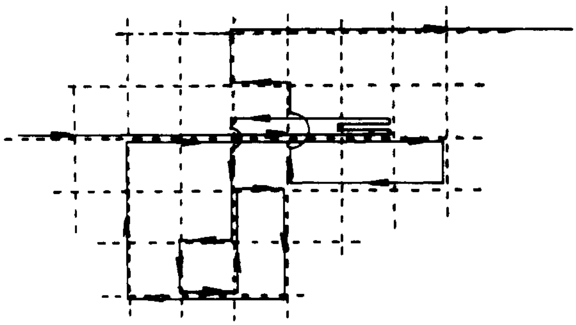

Figure 1. A typical k-tolerant walk with $k = 5$ or higher.

problem. We call the graph on the lattice made by the trajectory of the walk the silhouette of the walk (Domb 1960). In other words, the shadow is an equivalence class of walks obtained when we ignore the chronological order of elements (bonds and vertices) appearing in trajectories (see figure 2).

We start our study by looking at the silhouettes of ∞-vertex trails which mimic polymers with loops (the silhouettes of ∞-vertex closed trails mimic the lattice animal with vertices of even degrees only).

$$G_{0R}(w) = \lim_{n\to 0} \langle S_0' S_R' \rangle, \tag{1}$$

where w is the fugacity of monomers, S_i^α ($\alpha = 1, \ldots, n$) are n replicas of Ising-like spin variables, and $\langle\ \rangle$ is the equilibrium ensemble average defined by the Hamiltonian

$$-\mathscr{H}(w) = \tanh^{-1} w \sum_{\substack{\langle i,j\rangle \\ \alpha}} S_i^\alpha S_j^\alpha \tag{2}$$

with the summation over all the nearest-neighbour pairs and replicas. We impose the following trace rules:

$$\mathrm{Tr}(S_i^\alpha)^{2k} = 1, \qquad \mathrm{Tr}(S_i^\alpha)^{2k-1} = 0 \qquad \text{for } k = 1, 2, \ldots, \tag{3}$$

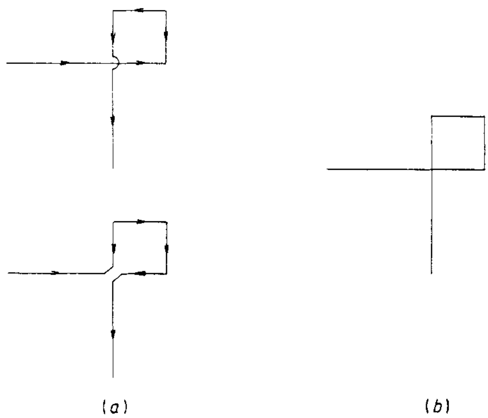

Figure 2. (a) Two different trails with one 2-vertex. (b) The common silhouette of the trails in (a).

and

$$\mathrm{Tr}(S_i^\alpha)^{2k}(S_i^\beta)^{2l}=\delta^{\alpha\beta} \qquad \text{for } k, l=1,2,\ldots. \tag{4}$$

All other traces of monomials vanish. It is important to realise that the trace or the integral is a linear map from the set of all the polynomials to real numbers completely defined by the values on monomials, and that we may freely invent this map as long as the rule is not inconsistent with the algebraic structure of the variables. The requirement (4) introduces an interaction among different replicas which exclude each other completely. Therefore, any monomial will give a vanishing trace if it includes more than one replica.

Using the standard Gaussian transformation, we can express the generating function as the following functional integral:

$$G_{0R}=\lim_{n\to 0}\int \prod_{i,\alpha} \mathrm{d}\varphi_i^\alpha \varphi^1(\mathbf{0})\varphi^1(\boldsymbol{R}) \exp\left[-\int \mathrm{d}^d r \mathscr{L}[\varphi(\boldsymbol{r})]\right]. \tag{5}$$

If we expand $\mathscr{L}[\phi]$ in terms of fields and their gradients and keep only relevant terms near four dimensions, we obtain

$$\mathscr{L}[\varphi]=\frac{m^2}{2}\sum_\alpha(\varphi^\alpha)^2+\frac{1}{2}\sum_\alpha|\nabla\varphi^\alpha|^2+u\Big(\sum_\alpha(\varphi^\alpha)^2\Big)^2-\frac{u}{3}\sum_\alpha(\varphi^\alpha)^4, \tag{6}$$

where m and u are known functions of w and the lattice coordination number, and a trivial rescaling of fields has been performed.

Thus the Lagrangian (6) is exactly that of the cubic model (see, e.g., Aharony 1976 and references therein). In the limit $n\to 0$, there is a second-order phase transition which is in the isotropic O(n) universality class (Aharony 1976, Newman and Riedel 1982). Therefore the silhouettes of ∞-vertex trails or the polymers with loops are in the same universality class as that of linear polymers (de Gennes 1972); the formation of loops is irrelevant to the scaling behaviour as long as we assign identical weights to all the patterns. Increasing the fugacity which controls the number of crossings we expect a collapsed phase with $\nu=1/d$. The new tricritical point between these two regimes is of $\mathrm{o}(\varepsilon^{1/2})$; the corresponding fixed point was discussed in the context of the random bond Ising model (Khmel'nitzkii 1975, Fishman and Aharony 1978)†.

To study the true trail problem, we must be able to discriminate between trajectories with the same silhouette. For the ∞-vertex trail model, we have not been able to find a closed Hamiltonian. We therefore limit our study to the two-vertex trails. Note that this is identical to the ∞-vertex trails on the square lattice or on the diamond lattice. To study the two-vertex trails, we consider a replicated version of the XY model. On each lattice site we define $2n$ variables $S_i^{\alpha+}$, S_i^α with the following trace rules:

$$\mathrm{Tr}(S_i^{\alpha+})^k=\mathrm{Tr}(S_i^\alpha)^k=0 \qquad k=1,2,\ldots. \tag{7a}$$

$$\mathrm{Tr}\, S_i^{\alpha+}S_i^\beta=\mathrm{Tr}(S_i^{\alpha+}S_i^\alpha)(S_i^{\beta+}S_i^\beta)=\delta^{\alpha\beta} \tag{7b}$$

$$\mathrm{Tr}(S_i^{\alpha+}S_i^\alpha)^k=0 \qquad \text{for } k=3,4,\ldots. \tag{7c}$$

The value of the trace on other monomials is zero. The constraint (7c) is required to remove all vertices of third or higher order. The Hamiltonian is

$$-\mathscr{H}=z\sum_{\substack{\langle i,j\rangle\\ \alpha}} S_i^{\alpha+}S_j^\alpha+\mathrm{cc}-z^2\sum_{\substack{\langle i,j\rangle\\ \alpha}} S_i^{\alpha+}S_i^\alpha S_j^{+\alpha}S_j^\alpha \tag{8}$$

† We are grateful to Aharony and Fishman for bringing this to our attention.

where z is the monomer fugacity. The second term is necessary to cancel dimers arising from the expansion of the first term. The generating function is then

$$G_{0\boldsymbol{R}}(z)=\lim_{n\to 0}\langle S_0^1 S_{\boldsymbol{R}}^1\rangle=\lim_{n\to 0}\mathrm{Tr}\, S_0^{1+}S_{\boldsymbol{R}}^1\,\mathrm{e}^{-\mathcal{H}}$$
$$=\lim_{n\to 0}\mathrm{Tr}\, S_0^{1+}S_{\boldsymbol{R}}^1\prod_{\substack{\langle i,j\rangle\\ \alpha}}[1+z(S_i^{\alpha+}S_i^{\alpha}+\mathrm{cc})]. \tag{9}$$

To transform this to a field theory, we have to introduce three types of fields $\phi_i^{\alpha+}$, ϕ_i^{α}, and a real field ψ_i^{α} conjugate to $S_i^{\alpha+}$, S_i^{α} and $S_i^{\alpha+}S_i^{\alpha}$, respectively. The resulting field theory (details will be published elsewhere) contains not only linear and cubic terms (with imaginary couplings) but interaction terms like $\mathrm{i}\psi\phi^+\phi$ which couples two types of fields. The linear term in ψ is eliminated by a shift of the origin. Comparison of the coefficients of the quadratic term shows that the ϕ field become massless while ψ is still massive and can be ingegrated out from the partition function completely. The resultant effective theory of ϕ is an isotropic O($2n$) theory with a cubic symmetry breaking term $\Sigma_\alpha\,(\phi^{\alpha+}\phi^{\alpha})^2$. Again, this term is irrelevant near four-dimension, so that the two-vertex trail is in the same universality class as the self-avoiding walk. In this case, however, the transiton is second order for any loop fugacity in contrast to the silhouette problem discussed above. The argument above can be extended to other v-vertex trails with appropriate introduction of more field variables.

In order to consider k-tolerant walks we generalise the approach used above. Again, we define $2n$ variables $\bar{x}_i^{\alpha}$ and x_i^{α} ($\alpha=1,\ldots,n$) at each site. Each trajectory of the walker going from the origin to $\boldsymbol{R}$ is uniquely represented by the *free product* of the form $\bar{x}_0^1x_0^1\ldots\bar{x}_i^1x_i^1\bar{x}_j^1x_j^1\ldots\bar{x}_{\boldsymbol{R}}^1x_{\boldsymbol{R}}^1$, where each adjacent pair $x_i^1\bar{x}_j^1$ is associated to the arrow from i to j. (Here, the free product implies that we make words from $\bar{x}_i^1$ and x_i^1 without any reduction rule.) Since we have n replicas, we can use any other replica to do the same as above. We use the replica trick to eliminate all the disconnected graphs as usual, so that we do not regard any free product with mixed replica indices to have graphic representation on the lattice. Thus the set $\mathcal{F}$ of all the free products of $\bar{x}_i^{\alpha}$, x_j^{β} is much bigger than its subset $\mathcal{S}$ of free products with graphic representations. The trace rule is as follows. Tr is zero on $\mathcal{F}\backslash\mathcal{S}$. Tr on $\mathcal{S}$ depends on the model. For the k-tolerant walk, Tr is zero on free products which contains l factors of $(\bar{x}_i^{\alpha}x_i^{\alpha})$ for $l>k$, since more than k visits to the same site are not allowed. Otherwise Tr is one on $\mathcal{S}$. Since we are on a finite lattice, this trace rule ensures that the subset of $\mathcal{S}$ on which Tr is non-zero is a finite set†. This is important to justify several interchanges of order of operations in the following (we take the thermodynamic limit at the final stage). We regard Tr to be a linear map, i.e., for any f and $g\in\mathcal{S}$ Tr $(\alpha f+\beta g)=\alpha$ Tr $f+\beta$ Tr g, where $\alpha,\beta\in R$. The generating function for the k-tolerant walks may simply be expressed as

$$G_{0\boldsymbol{R}}(R)=\lim_{n\to 0}\mathrm{Tr}[x_0' sP_s(\{x,\bar{x}\})x_{\boldsymbol{R}}'] \tag{10}$$

with $z=w/s$ (here, again we must respect the order of variables) and

$$P_s(\{x,\bar{x}\})=s^{-1}\left\{1+\sum_{l=1}^{V(k+1)}\left(\frac{w}{s}\right)^l\left[\sum_{\substack{\langle i,j\rangle\\ \alpha}}(x_i^{\alpha}\bar{x}_j^{\alpha}+x_j^{\alpha}\bar{x}_i^{\alpha})\right]^l\right\}, \tag{11}$$

† The formalism works only for finite k. The order of thermodynamic limit and the $k\to\infty$ limit are not interchangeable.

where V is the number of lattice points. Note that the products of x and $\bar{x}$ variables are calculated as free products.

$$\operatorname{Tr} P_s(\{x, \bar{x}\}) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st} \operatorname{Tr} \exp\Big\{ wt \sum_{\substack{\langle i,j \rangle \\ \alpha}} (x_i^\alpha \bar{x}_j^\alpha + x_j \bar{x}_i^\alpha) \Big\}. \tag{12}$$

The next step is to Gaussian transform this to a field theory of $\bar{\phi}_i$ and ϕ_i^α.

We have

$$\operatorname{Tr} P_s(\{x, \bar{x}\}) = \int \prod_{\substack{i \\ \alpha}} \mathrm{d}\bar{\varphi}_i^\alpha \, \mathrm{d}\varphi_i^\alpha \exp\Big(-\frac{1}{2w} \sum_{\substack{i,j \\ \alpha}} \bar{\varphi}_i^\alpha (A^{-1})_{ij} \varphi_i^\alpha \Big) \Phi, \tag{13}$$

where A is the matrix for the quadratic form in { } of (12) and

$$\Phi = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st} \operatorname{Tr} \exp[\sqrt{t} \sum_{i,\alpha} (x_i^\alpha \bar{\varphi}_i^\alpha + \bar{x}_i^\alpha \varphi_i^\alpha)]. \tag{13a}$$

Here note that sequences (words) in $\mathscr{F}\backslash\mathscr{S}$ produced by the expansion of the exponential factor give no contribution to Φ, since Tr vanishes. Our trace rule guarantees that Φ is a finite order polynomial of $|\phi_i^\alpha|^2$. Since all the values of Tr are non-negative, all the coefficients of Φ are non-negative. Moreover, Φ is bounded from above (even in the thermodynamic limit) by $\exp(\Sigma_{i,\alpha} |\varphi_i^\alpha|^2/4s)$. Therefore, if s is sufficiently large, the resulting field theory is stable.

If we expand the obtained effective Lagrangian as before we get almost the same form as for the silhouette of the ∞-vertex trail. Hence, again from the general statement against symmetry breaking of the isotopic fixed point for the $n \to 0$ limit, we conclude that the k-tolerant walk is also in the same universality class as the 1-tolerant walk = self-avoiding walk.

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