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LETTER TO THE EDITOR

A new mapping between self-avoiding walks and the $n \to 0$ limit

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Abstract. It is shown that by considering a new mapping between self-avoiding walks and the $n \to 0$ limit of the n-component classical spin system with the constraint that each spin has a fixed length $\sqrt{n}$ ($S^2 = n$), one can study a grand canonical ensemble of self-avoiding walks of all lengths, including those with *zero* lengths. It is shown that this new mapping is also *not isomorphic*. Moreover, the mapping is *physically meaningful* only for $H \leq \sqrt{2}$: higher values of H in the magnetic system *do not* produce a meaningful analogy with self-avoiding walks. The correlation functions for self-avoiding walks can be shown to be different from those proposed by other authors.

It is well known by now from the work of de Gennes (1972) and of des Cloizeaux (1975) that the $n \to 0$ limit of the n-component classical spin system provides a description of self-avoiding random walks (SAWs). In order to establish the above analogy, it is convenient to assume (Sarma 1979, de Gennes 1979) that the length of each spin is *constrained* to be $\sqrt{n}$: $S^2 = n$. It has been argued (Sarma 1979, de Gennes 1979) that the activities for a bond and for an end-point of a SAW are given by K and H respectively, where K and H are the ferromagnetic coupling constant and the magnetic field respectively (see (1) below). It has also been argued (des Cloizeaux 1975, Schäfer and Witten 1977) that the susceptibility χ and the specific heat C of the magnetic system as $n \to 0$ describe the long-wavelength limits of the end–end correlation function and the monomer–monomer correlation function respectively for SAWs. However, it has recently been pointed out (Gujrati 1981a, b, to be referred to jointly as I) that the above correspondence requires two important *modifications*. The first modification is to realise that for the magnetic system on a *lattice*, the bond and the end-point activities of the corresponding system of SAWs as $n \to 0$ are given by $\kappa = K/z$ and $\eta = H/\sqrt{z}$ respectively, where $z = 1 + H^2/2$, and not by K and H respectively as argued by other authors (Sarma 1979, de Gennes 1979). (It is not clear what happens to this modification if one considers a magnetic system in a continuous space.) The other modification, which is quite *independent* of the first modification, is to realise that the 'chemical potentials' controlling the number of bonds and the number of SAWs are $\ln \kappa$ and $\ln \eta$ respectively (I, Wheeler and Pfeuty 1981a). The second modification assures (see I) that the system of SAWs satisfies the proper *convexity* properties, even though the magnetic system need not as $n \to 0$ (Gujrati and Griffiths 1981, Wheeler and Pfeuty 1981a). The correspondence between SAWs and the $n \to 0$ limit of the magnetic system is *not* isomorphic (see I). Various correlation functions for SAWs are also shown in I to

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be very different in form from those proposed by other authors (des Cloizeaux 1975, Schäfer and Witten 1977).

The grand canonical ensemble of SAWs considered in I unfortunately does *not* allow any SAW of *zero* length, i.e. a single-site SAW (see Gujrati (1981b) for the reason leading to the exclusion of zero-length SAWs). As usual, a SAW is considered as an ideal representation of a linear polymer chain with length l and with $s = l + 1$ monomers. Thus, a single-site SAW or a zero-length SAW can be thought of as a single monomer. Therefore, if one is interested in studying the polymerisation of monomers into linear polymers (SAWs) (Flory 1953), one would like to consider a grand canonical ensemble of SAWs which would also allow any number of SAWs of zero lengths. Our aim in the present Letter is to obtain a correspondence between the $n \to 0$ limit of the magnetic system with constrained spins and the grand canonical ensemble of SAWs of *all* lengths (including zero lengths). This is achieved by considering a different mapping from the one used in I. We will establish that the new correspondence is also *not* isomorphic. The activities $\bar{\kappa}$ and $\bar{\eta}$ (we shall use a bar to denote quantities in the new mapping to distinguish from the quantities without bar used in I) controlling the total length of SAWs and their number respectively are given by $K/\bar{z}$ and $H/\sqrt{\bar{z}}$, where $\bar{z} = 1 - H^2/2$. Therefore, the new correspondence between SAWs and the $n \to 0$ limit of the magnetic system is *physically meaningful* only for $H \leqslant \sqrt{2}$: for $H \geqslant \sqrt{2}$, $\bar{\kappa}$ and $\bar{\eta}$ become negative and have no physical meaning as activities. We calculate various quantities characterising SAWs and relate them to quantities characterising the magnetic system as $n \to 0$. We also point out that the system of SAWs satisfies proper convexity properties, even though the magnetic system lacks such properties for $n < 1$. Moreover, the correlation functions for SAWs are shown to be very different from the expressions suggested by other authors (des Cloizeaux 1975, Schäfer and Witten 1977). After the work was completed, we found out that Wheeler and Pfeuty (1981b) have also made similar attempts. However, their correspondence is based on plausibility arguments and is very different from the correspondence given below.

We start with the effective Hamiltonian given by

$$\mathcal{H} = \sum_{\langle ij \rangle} K \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \sum_i H S_i^{(1)} \tag{1}$$

where K is the ferromagnetic coupling constant and H is the external magnetic field in the one-direction. The sum over $\langle ij \rangle$ is over distinct nearest-neighbour pairs. We have absorbed a factor of $-1/kT$ in $\mathcal{H}$. The length of each spin is constrained to be $\sqrt{n}$: $\forall i$, $\boldsymbol{S}_i^2 = n$. It has been shown in I that the partition function $Z_n(K, H)$ has the following limit as $n \to 0$:

$$Z_0(K, H) = z^N + \sum_{p>1} \sum_{l>p} H^{2p} K^l z^{N-s} U_{p,l} \tag{2}$$

where $z = 1 + H^2/2$, $s = p + l$ and $U_{p,l}$ is the number of ways of drawing p non-intersecting SAWs of total length l on the lattice of total sites N, such that there are *no* SAWs of zero length.

We now introduce the following two activities: $\bar{\eta}^2$ is the activity for a SAW and $\bar{\kappa}$ is the activity for a bond (or step) of a SAW. We define the following grand canonical partition function for SAWs of *all* lengths, including those of zero length:

$$\bar{Z}(\bar{\kappa}, \bar{\eta}) = 1 + \sum_{c \geqslant 1} \sum_{l \geqslant 0} \bar{\eta}^{2c} \bar{\kappa}^l \bar{U}_{c,l} \tag{3}$$

where $\bar{U}_{c,l}$ is the number of ways of drawing c non-intersecting SAWs of total length l on the lattice with N sites, such that there may be any number of SAWs of *zero length*. To establish a correspondence between (2) and (3), we rewrite (2) as follows:

$$Z_0(K, H) = \sum_{p\geqslant 0} \sum_{l\geqslant p} H^{2p} K^l z^{N-s} U_{p,l} \tag{4}$$

where $U_{0,0} = 1$ and $U_{0,l} = 0$ for all $l \geqslant 1$. Let us also rewrite $z = \bar{z} + H^2$ where

$$\bar{z} = 1 - H^2/2 \tag{5}$$

and expand $(\bar{z} + H^2)^{N-s}$. This enables us to rewrite (4) as follows:

$$\begin{aligned} Z_0(K, H) &= \bar{z}^N \sum_{p\geqslant 0} \sum_{l\geqslant p} \sum_{u\geqslant 0} \left(\frac{H^2}{\bar{z}}\right)^{(u+p)} \left(\frac{K}{\bar{z}}\right)^l \binom{N-s}{u} U_{p,l} \\ &= \bar{z}^N \sum_{c\geqslant 0} \sum_{l\geqslant 0} \left(\frac{H^2}{\bar{z}}\right)^c \left(\frac{K}{\bar{z}}\right)^l \bar{U}_{c,l} \end{aligned} \tag{6}$$

with $c = p + u$ and

$$\bar{U}_{c,l} = \binom{N-s}{u} U_{p,l}.$$

A comparison of (3) and (6) shows that

$$Z_0(K, H) = \bar{z}^N \bar{Z}(\bar{\kappa}, \bar{\eta}) \tag{7}$$

provided we have

$$\bar{\kappa} = K/\bar{z}, \qquad \bar{\eta} = H/\sqrt{\bar{z}}. \tag{8}$$

The correspondence (7) and (8) is different from the one given in I. We note from (5) and (8) that the correspondence between SAWs and the magnetic system ($n \to 0$) is physically meaningful if and only if $H \leqslant \sqrt{2}$ so that the activities $\bar{\kappa}$ and $\bar{\eta}$ are non-negative. For $H > \sqrt{2}$, both $\bar{\kappa}$ and $\bar{\eta}$ become negative and *cannot* be treated as activities in (3): there is *no* correspondence between $Z_0(K, H)$ and $\bar{Z}(\bar{\kappa}, \bar{\eta})$ for $H > \sqrt{2}$. We also observe from (5) and (8) that

$$\forall K > 0, \quad \bar{\kappa} \to \infty \quad \text{and } \bar{\eta} \to \infty \quad \text{as } H \to \sqrt{2}^-,$$

where $\sqrt{2}^-$ means $\sqrt{2} - \delta$, $\delta > 0$. Thus, the correspondence between SAWs and the magnetic system ($n \to 0$) is again *not* isomorphic, a conclusion similar to the one drawn in I.

We now proceed to calculate various thermodynamic quantities characterising SAWs. It is easily seen that the chain density, i.e. the density of SAWs ϕ_c and the bond density ϕ_l are given in the thermodynamic limit $N \to \infty$ by

$$\begin{aligned} \phi_c &= \lim_{N\to\infty} \left(\frac{\bar{\eta}}{2N} \frac{\partial \bar{W}}{\partial \bar{\eta}}\right) = \tfrac{1}{2} H \bar{z} m + \tfrac{1}{2} H^2 (1 - K\varepsilon), \\ \phi_l &= \lim_{N\to\infty} \left(\frac{\bar{\kappa}}{N} \frac{\partial \bar{W}}{\partial \bar{\kappa}}\right) = K\varepsilon, \end{aligned} \tag{9}$$

where $\bar{W} = \ln \bar{Z}(\bar{\kappa}, \bar{\eta})$, and where

$$m = \lim_{N\to\infty} \left(\frac{1}{N} \frac{\partial W_0}{\partial H}\right), \qquad \varepsilon = \lim_{N\to\infty} \left(\frac{1}{N} \frac{\partial W_0}{\partial K}\right) \tag{10}$$

with $W_0 = \ln Z_0(K, H)$. Here m is the magnetisation per particle and ε is the energy per particle of the magnetic system as $n \to 0$. It should be evident that the bond density ϕ_l must be the same whether one considers $\bar{Z}(\bar{\kappa}, \bar{\eta})$ or $\hat{Z}(\kappa, \eta)$ introduced in I, since the inclusion of SAWs of zero lengths in $\bar{Z}(\bar{\kappa}, \bar{\eta})$ does not change the total length of SAWs. However, ϕ_c includes the contribution of zero-length SAWs that are absent in $\hat{Z}(\kappa, \eta)$ (see I).

It is easily seen that if one makes the substitutions $z_i \to \bar{z}_i$, $\kappa_{ij} \to \bar{\kappa}_{ij}$, $\eta_i \to \bar{\eta}_i$ and $\hat{Z}(\{\kappa_{ij}\}, \{\eta_i\}) \to \bar{Z}(\{\bar{\kappa}_{ij}\}, \{\bar{\eta}_i\})$, where $\bar{z}_i = 1 - H_i^2/2$, $\bar{\kappa}_{ij} = K_{ij}/(\bar{z}_i\bar{z}_j)^{1/2}$, $\bar{\eta} = H_i/(\bar{z}_i)^{1/2}$ and where we are considering the inhomogeneous magnetic system (1) with $K \to K_{ij}$ and $H \to H_i$, then one can follow the analysis given in Gujrati (1981b) and calculate various correlation functions (cf equations (31) and (51), Gujrati 1981b). However, because of the presence of SAWs of zero length, the actual analysis is involved and will be presented elsewhere. Here, it will suffice to note that these correlation functions are indeed very different from those proposed by other authors (des Cloizeaux 1975, Schäfer and Witten 1977), just as was the case in I. However, from the structure of (3), we conclude that the system of SAWs *satisfies* usual convexity conditions with respect to $\ln \bar{\eta}$ and $\ln \bar{\kappa}$. Moreover, it can also be shown, as in I, that the long-wavelength limits $\bar{\chi}$ of the end–end correlation function and $\bar{C}$ of the nonomer–monomer correlation function satisfy the condition

$$\bar{\chi} \geqslant 0, \qquad \bar{C} \geqslant 0,$$

even though the susceptibility χ and the specific heat C of the magnetic system may become negative for $n \to 0$.

Let us briefly summarise our results. We have shown that a correspondence between SAWs of *all* lengths and the $n \to 0$ limit of the magnetic system can be established by a new mapping. However, the mapping is *not isomorphic*. Moreover, the correspondence is physically meaningful if and only if $H \leqslant \sqrt{2}$. The free energy $\bar{W}$ of SAWs is shown to differ from the magnetic free energy W_0 as $n \to 0$. We have calculated various quantities characterising SAWs. We have also shown that $\bar{W}$ *satisfies* proper convexity properties, even though the magnetic system need not as $n \to 0$.

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