# FIELD THEORY OF SELF-AVOIDING RANDOM CHAINS

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We present a new lattice model whose partition function is equal to the sum over all self-avoiding closed random chains of $m$ colors. The fluctuating variables are pure phases similar to an $XY$ model and, contrary to previous proposals, no awkward $n \to 0$ limits are involved. The model can be transformed to a real $O(m)$ invariant field theory, which shows that the critical indices are $O(m)$ like. There exists a simple relation to $O(m)$ spin models which serves to estimate the critical temperatures.

Self-avoiding random chains play an important role in polymer physics [1]. It is therefore desirable to possess a simple model which permits a complete study of the statistical mechanics of such chains. Guided by the knowledge that classical planar spin models are dually equivalent to non-backtracking oriented random chains [2] and that a model involving an $n$-dimensional spin vector $S_a$ of length $S_a^2 = n$ contains, in the strong coupling expansion and the limit $n \to 0$, all configurations of a single self-avoiding random chain [3,4], it has been suggested [5] that the partition function

$$Z = \prod_x \int \mathrm{d}\Omega(x) \exp\left(\sum_{a=1}^{m} \beta_a \sum_{x,i} S_a(x) S_a(x+i)\right), \tag{1}$$

with

$$\sum_{a=1}^{n} S_a^2 = n \to 0, \tag{2}$$

should be used to study grand canonical ensembles of self-avoiding polymer chains with $m$ colors. The measure of integration $\mathrm{d}\Omega$ covers the surface of the $n$-dimensional sphere and is normalized to unity, and the vectors $i$ run over all $\frac{1}{2}q$ positively oriented next neighbors. The parameters $\beta_a$ are the Boltzmann factors $\exp(-\epsilon_a/T) \equiv \exp(-\beta_a^{\mathrm{pol}})$ where $\epsilon_a$ is the energy per link of the polymer chain.

Unfortunately, this model does not really fulfill its purpose. When performing a low $\beta_a$ (i.e. low $T$) expansion, the partition functions contain contributions of the form

$$\int \mathrm{d}\Omega(x) \int \mathrm{d}\Omega(x+i) \frac{1}{2} \sum_a \beta_a^2 S_a^2(x) S_a^2(x+i) = \tfrac{1}{2} m \sum_a \beta_a^2 . \tag{3}$$

These correspond to chains running back and forth on the same link, which a self-avoiding chain cannot do. In addition, when allowing for a break-up of chains by adding to the exponent in (1) an external field term $\Sigma_{x,a} h_a(x) S_a(x)$ with a Boltzmann factor $h_a = \exp(-\epsilon_a^{\mathrm{br}}/T)$, there are terms $\frac{1}{2} \Sigma_a h_a^2$ which correspond to spurious "zero-link" objects [6,7].

The purpose of this note is to remedy such difficulties by setting up a new model which has the additional merit of being much simpler than (1).

If $\{L\}$ denotes all self-avoiding closed random chain configurations we want to calculate,

$$Z = \sum_{\{L\}} \exp[-(\epsilon/T)l] = \sum_{\{L\}} \beta^l , \tag{4}$$

where $l$ denotes the total number of link vectors $\boldsymbol{i}$ occupied by the chains. We may assign to each link vector $\boldsymbol{i}$ an occupation number $n_i(\boldsymbol{x})$ whose value can be zero or one. The property of being self-avoiding means that whenever one looks at all occupation numbers around each site $\boldsymbol{x}$, the numbers $n_i$ have to be either all zero, or two of them can be unity which means that

$$\sum_{i=1}^{q/2} n_i(\boldsymbol{x}-\boldsymbol{i}) + n_i(\boldsymbol{x}) = 0 \quad \text{or} \quad 2 .$$

This constraint can be written as follows:

$$\prod_{\boldsymbol{x}} \sum_{z(\boldsymbol{x})=0,2} \delta_{\Sigma_i n_i(\boldsymbol{x}-\boldsymbol{i})+n_i(\boldsymbol{x}),z(\boldsymbol{x})} = \prod_{\boldsymbol{x}} \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta(\boldsymbol{x})}{2\pi} \sum_{z(\boldsymbol{x})=0,2} \exp\left[\mathrm{i} \sum_{\boldsymbol{x}} \left( \theta(\boldsymbol{x}) \sum_i [n_i(\boldsymbol{x}-\boldsymbol{i}) + n_i(\boldsymbol{x})] - z(\boldsymbol{x}) \right)\right]$$

$$= \prod_{\boldsymbol{x}} \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta(\boldsymbol{x})}{2\pi} \sum_{z(\boldsymbol{x})=0,2} \exp\left(-\mathrm{i} \sum_{\boldsymbol{x}} \theta(\boldsymbol{x}) z(\boldsymbol{x})\right) \exp\left(\mathrm{i} \sum_{\boldsymbol{x},i} [\theta(\boldsymbol{x}) + \theta(\boldsymbol{x}+\boldsymbol{i})] n_i(\boldsymbol{x})\right) . \tag{5}$$

Introducing the complex pure phase variables $U(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}\theta(\boldsymbol{x})}$, this becomes

$$\prod_{\boldsymbol{x}} \left( \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta(\boldsymbol{x})}{2\pi} \{1 + [U^*(\boldsymbol{x})]^2\} \right) \prod_{\boldsymbol{x},i} [U(\boldsymbol{x})U(\boldsymbol{x}+\boldsymbol{i})]^{n_i(\boldsymbol{x})} \tag{6}$$

Multiplying this with the Boltzmann factor $\beta^{n_i(\boldsymbol{x})}$ and summing over all $n_i(\boldsymbol{x})$ gives the partition function

$$Z = \prod_{\boldsymbol{x}} \left( \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta(\boldsymbol{x})}{2\pi} \{1 + [U^*(\boldsymbol{x})]^2\} \right) \prod_{\boldsymbol{x},i} [1 + \beta U(\boldsymbol{x}) U(\boldsymbol{x}+\boldsymbol{i})] . \tag{7}$$

It can easily be checked that an expansion in powers of $\beta$ does indeed reproduce all self-avoiding chains. The factor $1 + (U^*)^2$ in the measure of integration makes sure that each site is either empty or touched by two occupied links, while the factors $U(\boldsymbol{x})U(\boldsymbol{x}+\boldsymbol{i})$ guarantee the connectedness of the chain. Notice that $Z$ is real since it is invariant under the exchange $U \to U^*$, although it does not have a conventional Boltzmann form.

The calculation of the thermodynamic properties is most convenient by transforming $Z$ into a theory of real fields. For this we simply note that

$$Z = \prod_{\boldsymbol{x}} \left( \int_{-\infty}^{\infty} \mathrm{d}u(\boldsymbol{x})\, \delta(u(\boldsymbol{x})) \{1 + \tfrac{1}{2} [\mathrm{d}/\mathrm{d}u(\boldsymbol{x})]^2\} \right) \prod_{\boldsymbol{x},i} [1 + \beta u(\boldsymbol{x}) u(\boldsymbol{x}+\boldsymbol{i})] , \tag{8}$$

coincides with (7), since $\frac{1}{2}(\mathrm{d}/\mathrm{d}u)^2$ has the same effect upon $u^2$, in the integral $\int_{-\infty}^{\infty} \mathrm{d}u\, \delta(u)$, as $(U^*)^2$ has upon $U^2$ in the integral $\int_{-\pi}^{\pi} \mathrm{d}\theta/2\pi$. Alternatively, we can write

$$Z = \prod_{\boldsymbol{x}} \left( \int_{-\infty}^{\infty} \mathrm{d}u(\boldsymbol{x}) \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \frac{\mathrm{d}\alpha(\boldsymbol{x})}{2\pi\mathrm{i}} [1 + \tfrac{1}{2}\alpha^2(\boldsymbol{x})] \right) \exp\left(- \sum_{\boldsymbol{x}} \alpha(\boldsymbol{x}) u(\boldsymbol{x})\right) \prod_{\boldsymbol{x},i} [1 + \beta u(\boldsymbol{x}) u(\boldsymbol{x}+\boldsymbol{i})] . \tag{9}$$

The model can easily be extended to $m$ colors, by using the constraint

$$\prod_{a=1}^{m} \prod_{x} \sum_{z^a(x)=0,2} \delta_{\Sigma_i[n_i^a(x-i)+n_i^a(x)],z^a(x)} \prod_{x} \sum_{z(x)=0,2} \delta_{\Sigma_a z^a(x),z(x)} , \tag{10}$$

where the $n_i^a(x)$ can take on the values zero or one, corresponding to the link $x, x+i$ being empty or carrying color $a$. The first Kronecker $\delta$ ensures self-avoidance within each color $a$ [see (5)]. To have avoidance between different colors as well, we have to make sure that whenever a line of color $a$ passes through a site $x[z^a(x) = 2]$, no line of a different color can pass through the same site. This is guaranteed by the second Kronecker $\delta$.

In order to exhibit the underlying $O(m)$ symmetry, we also introduce the superfluous constraint

$$\prod_{x,i} \sum_{z_i=0,1} \delta_{\Sigma_a n_i^a(x) z_i(x)} . \tag{11}$$

This gives

$$Z = \prod_{x,a} \int_{-\pi}^{\pi} \frac{d\theta^a(x)}{2\pi} \prod_{x} \int_{-\pi}^{\pi} \frac{d\delta(x)}{2\pi} \prod_{x,i} \int_{-\pi}^{\pi} \frac{d\delta_i(x)}{2\pi} \prod_{x,a} \{1 + [U_a^*(x)]^2 V^2(x)\}$$

$$\times \prod_{x} \{1 + [V^*(x)]^2\} \prod_{x,i} [1 + V_i^*(x)] \prod_{x,i,a} [1 + \beta_a U_a(x) U_a(x+i) V_i(x)] , \tag{12}$$

where $V \equiv \exp(i\delta)$, $V_i \equiv \exp(i\delta_i)$. The integrals over $V$ and $V_i$ can be done and we arrive at

$$Z = \prod_{x,a} \int_{-\pi}^{\pi} \frac{d\theta^a(x)}{2\pi} \prod_{x} \left(1 + \sum_a [U_a^*(x)]^2\right) \prod_{x,i} \left(1 + \sum_a \beta_a U_a(x) U_a(x+i)\right) . \tag{13}$$

This is the direct generalization of (7) to $m$ colors. The same generalization takes place in the real field representations (8) and (9) with $u$ and $\alpha$ becoming real $O(m)$ vector fields. This symmetry determines the universality class of the critical indices. There is no problem of allowing for the possibility of break-up of chains.by inserting magnetic fields $-\Sigma_{x,a} h_a(x) U_a(x)$, such that the complete partition function of self-avoiding random chains with $m$ colors is

$$Z = \prod_{x,a} \int_{-\infty}^{\infty} du_a \int_{-i\infty}^{i\infty} \frac{d\alpha_a}{2\pi i} \prod_{x} \left(1 + \sum_a \tfrac{1}{2}\alpha_a^2\right) \exp\left(-\sum_{x,a} [\alpha_a(x) + h_a(x)]\, u_a(x)\right)$$

$$\times \prod_{x,i} \left(1 + \sum_a \beta_a u_a(x) u_a(x+i)\right) . \tag{14}$$

It is useful to compare this with the $O(m)$ spin model

$$Z_{O(m)} = \prod_{a=1}^{m} \prod_{x} \int d\Omega(x) \exp\left(\beta_m \sum_{x,i,a} S_a(x) S_a(x+i)\right) , \tag{15}$$

in which case there is a well-known similar field theory

$$Z_{O(m)} = \prod_{x,a} \int_{-\infty}^{\infty} du_a \int_{-i\infty}^{i\infty} \frac{d\alpha_a}{2\pi i} \prod_x (\tfrac{1}{2}m - 1)!(\tfrac{1}{2}|\alpha|)^{-(m/2-1)} I_{m/2-1}(|\alpha|)$$

$$\times \exp\left(-\sum_{x,a} [\alpha_a(x) + h_a(x)] u_a(x)\right) \prod_{x,i} \exp\left(\sum_a \beta_a u_a(x) u_a(x+i)\right). \tag{16}$$

Here, the expansion of the Bessel factors

$$\prod_x \left[1 + \frac{(m/2-1)!}{(m/2)!} \sum_a \tfrac{1}{4}\alpha_a^2 + \frac{(m/2-1)!}{(m/2+1)!2!} \left(\sum_a \tfrac{1}{4}\alpha_a^2\right)^2 + \ldots\right] \tag{17}$$

gives rise to all possible multiple occupancies of sites.

The case $m = 1$ reduces to the Ising model

$$Z_{O(1)} \equiv Z^{\text{Ising}} = \prod_x \int_{-\infty}^{\infty} du \int_{-i\infty}^{i\infty} \frac{d\alpha}{2\pi i} \prod_x \operatorname{ch} \alpha \exp\left(-\sum_x [\alpha(x) + h(x)]\, u(x)\right) \prod_{x,i} \exp[\beta_1 u(x) u(x+i)]\,. \tag{18}$$

Since the integration of the $\alpha$ variables restricts $u$ to the values $\pm 1$, we can write

$$\prod_{x,i} \exp[\beta_1 u(x) u(x+i)] = (\operatorname{ch} \beta_1)^{Nq/2} \prod_{x,i} [1 + \operatorname{th} \beta_1\, u(x) u(x+i)]\,. \tag{19}$$

Thus, apart from the trivial factor $(\operatorname{ch} \beta)^{Nq/2}$, the partition function of self-avoiding random chains with $m = 1$ can be obtained from that of the Ising model by identifying $\operatorname{th} \beta_1 \equiv \beta$ and performing a perturbation expansion in [‡1]

$$\Delta V = \log(1 + \tfrac{1}{2}\alpha^2) - \log \operatorname{ch} \alpha = -\tfrac{1}{24}\alpha^4 + \ldots\,. \tag{20}$$

The lowest contribution of $\Delta V$ is suppressed by a Boltzmann factor $\beta^8$, such that there are practically no corrections close to the critical point. In table 1 we compare the critical values obtained from $\operatorname{th} \beta_1$ with recent Monte Carlo data on random chains by Helfrich's group [8] and see that the agreement is indeed excellent [‡2].

For general $m$, there is a similar relation between (14) and (19). Expanding the exponential into Gegenbauer polynomials

$$\exp\left(\beta_m \sum_a S_a(x) S_a(x+i)\right) = \sum_{n=0}^{\infty} d_n(\beta_m)\, C_n^{(m/2-1)}(\Sigma_a S_a(x) S_a(x+i))\,, \tag{21}$$

with

$$d_0(\beta) \equiv \frac{\Gamma(m/2)}{(\beta/2)^{m/2-1}} I_{m/2-1}(\beta)\,, \quad d_1(\beta) = \frac{\Gamma(m/2)}{(\beta/2)^{m/2-1}} \frac{m}{m-2} I_{m/2}(\beta)\,,$$

we find the low temperature series

$$Z_{O(m)} = [d_0(\beta_m)]^{Nq/2} \prod_{x,i} \int d\Omega \left[1 + \sum_{\{n_i(x)=1,2,\ldots\}} \left(\frac{m}{m-2} \frac{I_{m/2}(\beta_m)}{I_{m/2-1}(\beta_m)}\right)^{n_i(x)} C_{n_i(x)}^{m/2-1}(\Sigma_a S_a(x) S_a(x+i))\right]. \tag{22}$$

‡1 Notice that the partition function of the Ising model would be obtained from the original Ansatz by allowing in the constraint (5), for all multiple occupancies of a site, i.e. by summing $Z$ over 0, 2, 4, ... . This replaces in (7) $1 + (U^*)^2$ by $1 + (U^*)^2 + (U^*)^4 + \ldots$ and in (9) $1 + \alpha^2/2$ by $1 + \alpha^2/2 + \alpha^4/4! + \ldots = \operatorname{ch} \alpha$.

‡2 Apart from their five-dimensional which must be wrong.

Table 1
Transition temperatures of self-avoiding random chains of $m$ colors on a s.c. lattice as estimated from those of the O($m$) spin model via the relation $\beta^c \approx I_{m/2}(\beta_m^c)/I_{m/2-1}(\beta_m^c)$ = th $\beta_1$, $I_1(\beta_2^c)/I_0(\beta_2^c)$, cth $\beta_3^c - 1/\beta_3^c$, ... for $m$ = 1, 2, 3, ... . The third row gives the Monte Carlo data of ref. [8] with dubious results put in parentheses. The last row contains the mean field estimates.

| $m$ | | $q/2$ | | | | | |
|---|---|---|---|---|---|---|---|
| | | 2 | 3 | 4 | 5 | ... | $\gg 1$ |
| 1 | $\beta_1^c$ | 0.4407 | 0.2217 | 0.1499 | 0.1140 | ... | $1/q$ |
| | th $\beta_1^c$ | 0.4142 | 0.2181 | 0.1488 | 0.1135 | ... | $1/q$ |
| | $\beta_{MC}^c$ | 0.42 | 0.22 | 0.15 | (0.14) | ... | |
| 2 | $\beta_2^c$ | 0.75 | 0.439 | 0.298 | 0.227 | ... | $2/q$ |
| | $I_1(\beta_2^c)/I_0(\beta_2^c)$ | 0.35 | 0.24 | 0.15 | 0.11 | ... | $1/q$ |
| | $\beta_{MC}^c$ | (0.45) | | | | | |
| 3 | $\beta_3^c$ | | 0.694 | 0.457 | 0.341 | ... | $3/q$ |
| | cth $\beta_3^c - 1/\beta_3^c$ | | 0.224 | 0.150 | 0.113 | ... | $1/q$ |
| | $\beta_{MC}^c$ | | | | | ... | |
| all | $\beta_{MF}^c$ | 0.25 | 0.167 | 0.125 | 0.1 | ... | $1/q$ |

For $\beta \ll \beta_c$, the diagrams are dominated by $n_i(x) = 1$ loops. In this case since $C_1(z) = (m - z)z$, the d$\Omega$ integrals produce all self-avoiding loops of $m$ colors.

$$Z_{O(m)} \sim [d_0(\beta_m)]^{Nq/2}\left(\sum_{\{L\}} m^{n[L]}\,[I_{m/2}(\beta_m)/I_{m/2-1}(\beta_m)]^{\,l}\right), \tag{23}$$

where $n[L]$ is the number of closed loops in the ensemble $\{L\}$. Corrections arise only to order $(I_{m/2}/I_{m/2-1})^8$. Thus we may use the critical temperatures of O($m$) spin models and estimate $\beta_c$ from the relation

$$\beta_c = I_{m/2}(\beta_m^c)/I_{m/2-1}(\beta_m^c)\,.$$

This gives the numbers shown in table 1. Our model can easily be studied by mean field methods. This gives a critical point at $\beta_c^{MF} = 1/q$ as compared with the O($m$) value $m/q$. For large $\beta$, the total loop length approaches $N$, which is in contrast to the O(1) model where it is $Nq/2$ since then, multiple occupancies of each site allow to fill each link.

Fluctuation corrections to the mean field solution will be given elsewhere.

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