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LETTER TO THE EDITOR

Statistics of nested spiral self-avoiding loops: exact results on the square and triangular lattices

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Abstract. The statistics of nested spiral self-avoiding loops, which is closely related to the partition of integers into decreasing parts, has been studied on the square and triangular lattices. The number of configurations with N steps is $c_N \simeq (\sqrt{2}/24) N^{-3/2} \exp(\pi\sqrt{\frac{2}{3}}\, N^{1/2})$ and their average size $X_N \simeq (1/2\pi)\sqrt{\frac{3}{2}}\, N^{1/2} \ln N$ to leading order on the square lattice while the corresponding values for the triangular lattice are $c_N \simeq (3^{3/4}/16)\, N^{-5/4} \exp((\pi/\sqrt{3})\, N^{1/2})$ and $X_N \simeq 1/(\pi\sqrt{3})\, N^{1/2} \ln N$.

Some years ago, the number of N-step spiral self-avoiding loops have been calculated for the square and triangular lattices (Manna 1985, Lin *et al* 1986). These works followed the introduction of the spiral self-avoiding walk (Privman 1983) for which a lot of exact results were obtained by a succession of authors (Blöte and Hilhorst 1984, Whittington 1984, Guttmann and Wormald 1984, Joyce 1984, Guttmann and Hirschhorn 1984, Lin 1985, Joyce and Brak 1985, Lin and Liu 1986). While the number of spiral self-avoiding loops grows with N like a non-universal, i.e. lattice-dependent power, the number of spiral self-avoiding walks also behaves in an unusual way

$$c_N \simeq A N^{-\theta} \exp(\lambda N^{1/2}) \tag{1}$$

where both θ and λ are lattice-dependent quantities. It follows that the asymptotic entropy per step decays as $N^{-1/2}$ instead of giving a constant as in the ordinary or directed self-avoiding walks. Following the work of Privman, a close connection between this problem and the theory of partitions of integers (Andrews 1976) was noticed (Derrida and Nadal 1984, Redner and de Arcangelis 1984, Klein *et al* 1984).

In this letter we present some exact results concerning the statistics of nested spiral loops which are self- and mutually avoiding and piled up around a site chosen as the origin. We study such spirals on the square lattice where on a loop only 90° turns in the same direction are allowed so that the loops are rectangular-shaped (figure 1) and on the triangular lattice where the restriction to 120° turns leads to triangles among which one only keeps those pointing up (figure 2).

Let us introduce the generating function

$$G_L(z, \omega) = \sum_{N,X} c_N(L, X) z^N \mathrm{e}^{\omega X} \tag{2}$$

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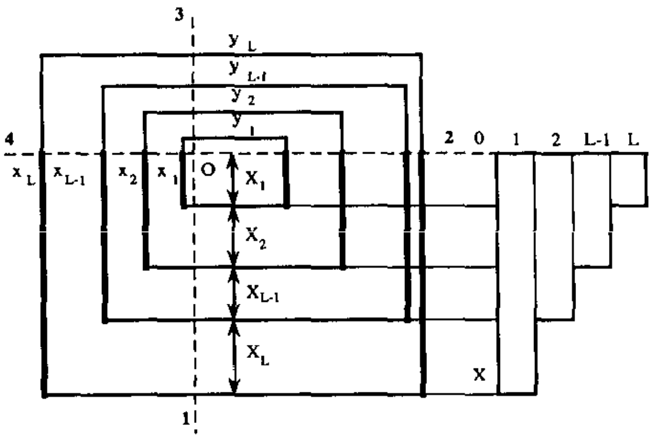

Figure 1. Nested spiral self-avoiding loops on the square lattice: with 90° turns in the same direction, rectangular-shaped loops are obtained. Each step is assigned a weight z and the size is $X=\Sigma_{k=1}^{L} X_k$. The nested-loop configuration corresponds to four independent partitions of integers into decreasing parts numbered 1 to 4 and each partition is duplicated (heavy lines).

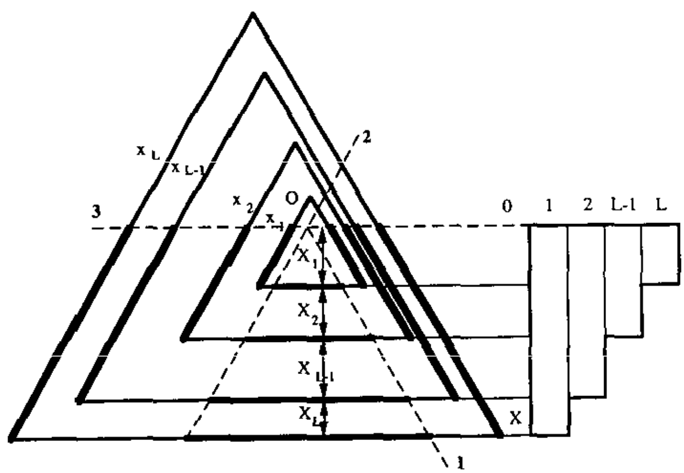

Figure 2. Nested spiral self-avoiding loops on the triangular lattice: with 120° turns in the same direction, triangular-shaped loops are obtained. Each step is assigned a weight z and the size is $X=\Sigma_{k=1}^{L} X_k$. The nested-loop configuration corresponds to three independent partitions of integers into decreasing parts numbered 1 to 3 and each partition is triplicated (heavy lines).

for the number of configurations with N steps, L loops and size $X=\Sigma_{k=1}^{L} X_k$ where X is the distance from the origin to the Lth loop. On the square lattice, with the notation of figure 1, one may write

$$G_L^{\mathrm{sq}}(z,\omega)=\sum_{x_1=2}^{\infty}\sum_{y_1=2}^{\infty}(y_1-1)\sum_{X_1=1}^{x_1-1}\sum_{x_2=x_1+2}^{\infty}\sum_{y_2=y_1+2}^{\infty}(y_2-y_1-1)\sum_{X_2=1}^{x_2-x_1-1}$$
$$\cdots\sum_{x_L=x_{L-1}+2}^{\infty}\sum_{y_L=y_{L-1}+2}^{\infty}(y_L-y_{L-1}-1)\sum_{X_L=1}^{x_L-x_{L-1}-1} z^{2\Sigma_{k=1}^{L}(x_k+y_k)}\,\mathrm{e}^{\omega\Sigma_{k=1}^{L}X_k}. \qquad (3)$$

Introducing

$$m_k = x_k - x_{k-1} \qquad x_0 = 0 \tag{4a}$$

$$n_k = y_k - y_{k-1} \qquad y_0 = 0 \tag{4b}$$

one gets

$$\sum_{k=1}^{L} (x_k + y_k) = \sum_{k=1}^{L} (L-k+1)(m_k + n_k) \tag{5}$$

and the generating function may be factorized as

$$G_L^{\mathrm{sq}}(z,\omega) = \prod_{k=1}^{L} \left[\sum_{m_k=2}^{\infty} z^{2(L-k+1)m_k} \left(\frac{\mathrm{e}^{\omega} - \mathrm{e}^{m_k\omega}}{1-\mathrm{e}^{\omega}} \right) \sum_{n_k=2}^{\infty} (n_k - 1) z^{2(L-k+1)n_k} \right] \tag{6}$$

or

$$G_L^{\mathrm{sq}}(z,\omega) = \prod_{k=1}^{L} \frac{\mathrm{e}^{\omega} z^{8k}}{(1-z^{2k})^3(1-z^{2k}\,\mathrm{e}^{\omega})}. \tag{7}$$

In the same way, on the triangular lattice with the notation of figure 2, one has:

$$\begin{aligned} G_L^{\mathrm{tr}}(z,\omega) = {} & \sum_{x_1=3}^{\infty} \sum_{X_1=1}^{x_1-2} (x_1 - X_1 - 1) \sum_{x_2=x_1+3}^{\infty} \sum_{X_2=1}^{x_2-x_1-2} (x_2 - x_1 - X_2 - 1) \\ & \ldots \sum_{x_L=x_{L-1}+3}^{\infty} \sum_{X_L=1}^{x_L-x_{L-1}-2} (x_L - x_{L-1} - X_L - 1) z^{3\sum_{k=1}^{L} x_k} \mathrm{e}^{\omega \sum_{k=1}^{L} X_k} \end{aligned} \tag{8}$$

so that using (4*a*):

$$G_L^{\mathrm{tr}}(z,\omega) = \prod_{k=1}^{L} \left[\sum_{m_k=3}^{\infty} \frac{(m_k-2)\,\mathrm{e}^{\omega} - (m_k-1)\,\mathrm{e}^{2\omega} + \mathrm{e}^{\omega m_k}}{(1-\mathrm{e}^{\omega})^2} z^{3(L-k+1)m_k} \right] \tag{9}$$

and finally

$$G_L^{\mathrm{tr}}(z,\omega) = \prod_{k=1}^{L} \frac{\mathrm{e}^{\omega} z^{9k}}{(1-z^{3k})^2(1-\mathrm{e}^{\omega} z^{3k})}. \tag{10}$$

These results may be obtained more directly by noticing the connection with the number of partitions of integers into L decreasing parts which is illustrated in figure 1, for the square lattice and figure 2 for the triangular lattice. Nested loops configurations are in one-to-one correspondence with four independent partitions in the first case and three independent partitions in the second case. The generating functions for the nested-loop problem are directly obtained as powers of the generating function for the partition of integers into L decreasing parts (Andrews 1976):

$$\begin{aligned} g_L(t) &= (t + t^2 + t^3 + \ldots)(t^2 + t^4 + t^6 + \ldots) \ldots (t^L + t^{2L} + t^{3L} + \ldots) \\ &= \prod_{k=1}^{L} \frac{t^k}{1-t^k} \end{aligned} \tag{11}$$

multiplied by a modified generating function for which a partition of size X is, as in (3) and (8), weighted by $\mathrm{e}^{\omega X}$ so that

$$\begin{aligned} g_L(t,\omega) &= (t\,\mathrm{e}^{\omega} + t^2\,\mathrm{e}^{2\omega} + \ldots)(t^2\,\mathrm{e}^{\omega} + t^4\,\mathrm{e}^{2\omega} + \ldots) \ldots (t^L\,\mathrm{e}^{\omega} + t^{2L}\,\mathrm{e}^{2\omega} + \ldots) \\ &= \prod_{k=1}^{L} \frac{\mathrm{e}^{\omega} t^k}{1-\mathrm{e}^{\omega} t^k}. \end{aligned} \tag{12}$$

One may verify that the mapping requires $t=z^2$ for loops on the square lattice (figure 1) and $t=z^3$ on the triangular lattice (figure 2); it follows that

$$G_L(t,\omega)=[g_L(t)]^{p-1}g_L(t,\omega)|_{t=z^q} \tag{13}$$

with $p=4$, $q=2$, on the square lattice and $p=3$, $q=3$, on the triangular lattice in agreement with (7) and (10).

Let us first consider the generating function $G(t)$ for the number of configurations $c_N=\Sigma_{L,X}\, c_N(L,X)$ with N steps and any number of loops which is given by

$$G(t)=\sum_{L=1}^{\infty} G_L(t,\omega)|_{\omega=0}=\sum_{L=1}^{\infty}[g_L(t)]^p|_{t=z^q}. \tag{14}$$

The behaviour of c_N for large N values is governed by the behaviour of $g_L(t)$ in the vicinity of its singularity at $t=1$. With $t=1-\eta$ and $\eta\to 0^+$, the main contribution to the sum in (14) comes from values of L near $L_0=\ln 2/\eta$ for which $g_L(\eta)$ is maximum in L (Blöte and Hilhorst 1984, des Cloizeaux and Jannink 1987) and an expansion of $\ln g_L(\eta)$ near L_0 (see the appendix) leads to

$$\ln g_L(\eta)\simeq\frac{\pi^2}{12\eta}-\tfrac{1}{2}\ln\left(\frac{2\pi}{\eta}\right)-\frac{1}{\eta}(L\eta-\ln 2)^2 \tag{15}$$

so that the sum over L in $G(t)$ may be transformed into a Gaussian integral and one gets

$$G(t)=\sum_{L=1}^{\infty}\exp[p\ln g_L(t)]\simeq(2p)^{-p/2}\left(\frac{p\eta}{\pi}\right)^{(p-1)/2}\exp\left(\frac{p\pi^2}{12\eta}\right) \tag{16}$$

for the leading contribution. With $n=N/q$, the generating function may be written as

$$G(t)=\sum_{n=0}^{\infty} c_{N=qn}t^n \tag{17}$$

so that the number of configurations is given by the Cauchy formula

$$c_{N=qn}=\frac{1}{2\pi \mathrm{i}}\oint_{(C)}\mathrm{d}t\,\frac{G(t)}{t^{n+1}} \tag{18}$$

where (C) is a circle of radius $r<1$ centred at the origin. The integral may be evaluated using the saddle-point method by deforming the contour. Through a Gaussian integration near the saddle-point at $t=1-\pi(p/12\eta)^{1/2}$ one gets

$$c_N\simeq\frac{(pq)^{p/4}(q/p)^{1/2}}{2^{p+1}3^{p/4}}N^{-(p+2)/4}\exp\left(\pi\sqrt{\frac{p}{3q}}N^{1/2}\right) \tag{19}$$

to leading order. With the appropriate p and q values one gets

$$c_N^{\mathrm{sq}}\simeq\frac{\sqrt{2}}{24}N^{-3/2}\exp(\pi\sqrt{\tfrac{2}{3}}\,N^{1/2}) \tag{20a}$$

$$c_N^{\mathrm{tr}}\simeq\frac{3^{3/4}}{16}N^{-5/4}\exp\left(\frac{\pi}{\sqrt{3}}N^{1/2}\right). \tag{20b}$$

For both lattices, the exponential term is the same as for the outward spiral self-avoiding walk (Blöte and Hilhorst 1984, Joyce 1984, Guttmann and Wormald 1984, Joyce and Brak 1985, Lin and Liu 1986) whereas the power of N in the prefactor is different.

According to (2), the mean size for L-loop configurations is given by

$$X_L(t) = \left.\frac{\partial \ln G_L(t,\omega)}{\partial \omega}\right|_{\omega=0} = \sum_{k=1}^{L} \frac{1}{1-t^k} \tag{21}$$

and may be rewritten as

$$X_L(t) = \sum_{k=0}^{\infty} \frac{t^k(1-t^{Lk})}{1-t^k} \tag{22}$$

where the first term in the sum should be understood as the limit of the ratio when $k \to 0$. When L is unrestricted, the mean size becomes

$$X(t) = \frac{\sum_{L=1}^{\infty} G_L(t) X_L(t)}{G(t)} = \sum_{k=0}^{\infty} \frac{t^k}{1-t^k} \frac{\sum_{L=1}^{\infty} G_L(t)(1-t^{Lk})}{G(t)}. \tag{23}$$

Changing the sum over L into an integral, the value $L_0 = \ln 2/\eta$ corresponding to the maximum in L of $G_L(t)$ is selected and

$$X(t) \simeq \sum_{k=0}^{\infty} \frac{t^k(1-2^{-k})}{1-t^k}. \tag{24}$$

Putting apart the first term and rearranging the sum, one gets

$$X(\eta) \simeq \frac{\ln 2}{\eta} + \sum_{k=1}^{\infty} \left(\frac{1}{1-t^k} - \frac{1}{1-t^k/2}\right). \tag{25}$$

The sum may be evaluated using the Euler–Maclaurin formula and

$$X(\eta) \simeq \frac{1}{\eta} \ln\left(\frac{1}{\eta}\right) \tag{26}$$

to leading order. On the other hand the number of steps reads

$$N(\eta) = \left.\frac{\partial \ln G(z^q)}{\partial \ln z}\right|_{z^q=1-\eta} \simeq \frac{pq\pi^2}{12\eta^2} \tag{27}$$

so that

$$X_N \simeq \frac{1}{2\pi} \sqrt{\frac{12}{pq}}\, N^{1/2} \ln N \tag{28}$$

and

$$X_N^{\mathrm{sq}} \simeq \frac{1}{2\pi} \sqrt{\tfrac{3}{2}}\, N^{1/2} \ln N \tag{29a}$$

$$X_N^{\mathrm{tr}} \simeq \frac{1}{\pi\sqrt{3}} N^{1/2} \ln N. \tag{29b}$$

One recovers the characteristic behaviour of the spiral self-avoiding walk (Blöte and Hilhorst 1984, Liu and Lin 1985) with an exponent $\nu = \frac{1}{2}$ and a logarithmic correction.

Appendix

Using (11) with $t = 1-\eta$ in the limit $\eta \to 0^+$ one has

$$\ln g_L(t) = -\sum_{k=1}^{L} \ln(t^{-k}-1) \simeq -\sum_{k=1}^{L} [\ln(e^{k\eta}-1) - \ln k\eta] - \sum_{k=1}^{L} \ln k\eta. \tag{A1}$$

The first sum may be replaced by an integral using

$$\sum_{k=1}^{L} f(k) \simeq \frac{1}{\eta} \int_{\eta/2}^{(L+1/2)\eta} f(u)\, \mathrm{d}u + \frac{\eta}{24}\left[f'\left(\frac{\eta}{2}\right) - f'((L+\tfrac{1}{2})\eta)\right] \tag{A2}$$

so that

$$\ln g_L(\eta) = -\frac{1}{\eta} \int_0^{(L+1/2)\eta} [\ln(\mathrm{e}^u - 1) - \ln u]\, \mathrm{d}u - L \ln \eta - \ln(L!) + \mathrm{O}(\eta). \tag{A3}$$

Integrating the second term and using Stirling's formula, one gets to leading order

$$\ln g_L(\eta) \simeq -\frac{1}{\eta} \int_0^{(L+1/2)\eta} \ln(\mathrm{e}^u - 1)\, \mathrm{d}u - \tfrac{1}{2} \ln\left(\frac{2\pi}{\eta}\right). \tag{A4}$$

Expanding the remaining integral, considered as a function of its upper limit, near $u_0 = L_0\eta = \ln 2$ with

$$\int_0^{\ln 2} \ln(\mathrm{e}^u - 1)\, \mathrm{d}u = -\frac{\pi^2}{12} \tag{A5}$$

one finally gets

$$\ln g_L(\eta) \simeq \frac{\pi^2}{12\eta} - \tfrac{1}{2} \ln\left(\frac{2\pi}{\eta}\right) - \frac{1}{\eta}(L\eta - \ln 2)^2. \tag{A6}$$

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