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The projected area of the three-dimensional self-avoiding polygons in a plane

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Abstract. We have calculated the exponent θ_S governing the growth of the projected area of the three-dimensional self-avoiding polygons in a plane. Our series result suggests that $\theta_S < 2\nu_{SAP}$, where ν_{SAP} is the correlation length exponent of the three-dimensional self-avoiding polygons.

The self-avoiding walk (SAW) has been the subject of extensive studies. Much work has been focused on the size of the SAW and the size of the self-avoiding polygons (SAP). The size of the SAW is characterized by the exponent ν_{SAW} which relates the mean square end-to-end distance $\rho(n)$ of the n-step SAW as follows:

$$\rho(n) \sim n^{2\nu_{SAW}}. \tag{1}$$

The size of SAP can be defined through the mean square radius of gyration of the n-step SAP in similar fashion to (1). It is generally believed that the size exponent, ν, for SAP is the same as that for SAW. Previous series analyses [1, 2] on an FCC lattice and Monte Carlo methods [3, 4] in three dimensions yield a larger exponent for SAP than for SAW. Recently, Privman and Rudnick [5] and Enting and Guttman [6, 7] studied SAP in two dimensions using the series analysis. Their results are in good agreement with the theoretical expectation $\nu_{SAP} = \nu_{SAW}$. Most recently, there have been interests [8–10] in the area of the SAP in two dimensions. The theoretical analysis of Duplantier [10] shows that $\theta_S = 2\nu_{SAW}$ in two dimensions. In this paper, we study the projected area of three-dimensional SAP in a plane which is defined as follows:

$$S_n = \iint \hat{z} \cdot \mathrm{d}\boldsymbol{S} = \oint \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{l} \tag{2}$$

where $\nabla \times \boldsymbol{A} = \hat{z}$. Setting $\boldsymbol{A} = (\boldsymbol{R} \cdot \hat{x})\hat{y}$ (where $\boldsymbol{R}$ is the position vector), we obtain

$$S_n = \sum_{l=1}^{n} (y_{l+1} - y_l)x_l. \tag{3}$$

From the dimension of the area of the SAP, we expect the exponent for the area to be equal to that of the SAP multiplied by two. We have calculated the series up to 18 bonds for the projected area of the SAP on a cubic lattice in the x–y plane. We found that $\theta_S < 2\nu_{SAP}$. However, it should be noted that the area and the mean square radius of gyration are essentially different quantities. This will be clear when we consider clusters with no free ends. Then the summation in (3) should range from $l = 1$ to $l = m$, where $l = 1, 2, \ldots, m$ denote the exterior boundary sites of the clusters with no free

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ends. Therefore, S_n is more like a surface quantity. We also note that S_n is a global quantity in the sense that one has to specify the exterior site before calculating S_n.

Assuming that

$$S(n)=\left(\sum_{\gamma_n} S_{\gamma_n}\right)(C(n)\sim n^{\theta_S})^{-1} \tag{4}$$

where $C(n)$ is the number of the n-step SAP, γ_n denotes all of the n-step SAP, and θ_S is the exponent of interest.

The series coefficients are listed in table 1. We have also listed $\rho_3(n)$, the series of the radius of gyration for SAP on the cubic lattice. The calculations took about 30 hours of CPU time on a Masscomp 5700. We analysed the series using the Padé approximant and the differential Padé approximant [11]. Specifically, we have analysed χ_1 and χ_2 defined as

$$\chi_1=\sum_n S_3(n)K^n\sim|K-1|^{-\theta_S-1} \tag{5}$$

$$\chi_2=\sum_n \rho_3(n)K^n\sim|K-1|^{-2\nu_{\mathrm{SAP}}-1}. \tag{6}$$

Since the pole is exactly one, the exponent (residue) can be read off from the pole-residue plot. For χ_1 and χ_2 we obtained $\theta_S=1.026\pm0.007$ and $2\nu_{\mathrm{SAP}}=1.206\pm0.019$, respectively. The value ν_{SAP} is consistent with $\nu_{\mathrm{SAW}}=0.592\pm0.002$ [12, 13] within the error bar. The value of θ_S is smaller than $2\nu_{\mathrm{SAP}}$. This may be due to the shortness of the series.

Table 1. The coefficients of the series, where $C_3(n)$ is the number of n-step SAP in three dimensions, $S_3(n)$ is the corresponding area projected in the x–y plane, and $\rho_3(n)$ is the mean square radius of gyration.

n	$C_3(n)$	$C_3(n)S_3(n)$	$C_3(n)\rho_3(n)$
4	3	1	1.500
6	22	16	16.833
8	206	230	225.375
10	2 367	3 526	3 377.465
12	30 390	56 593	53 847.619
14	418 842	937 389	891 873.995
16	6 088 162	15 943 435	15 199 347.398
18	92 263 998	277 324 490	265 012 864.303

For the SAP, this exponent, θ_S, is also related to the exponent corresponding to the diamagnetic susceptibility of the superconducting rings. The Hamiltonian of this system is defined as

$$H=-\sum_{\langle i,j\rangle} J_{ij}\cos(\phi_i-\phi_j-A_{ij}) \tag{7}$$

where

$$A_{ij}=\frac{2\pi}{\Phi_0}\int_i^j \boldsymbol{A}\cdot\mathrm{d}\boldsymbol{l} \tag{8}$$

where A is the vector potential and $\Phi_0 = hc/2e$ is an elementary flux quantum. It is readily shown that the total diamagnetic susceptibility, χ, of a polygon is [14, 15] $\chi \sim S^2/P$, where P is the perimeter of the polygon. Assuming that $\chi(n)$ for the n-step SAP obeys the following scaling form:

$$\sum_{\gamma_n} \chi(\gamma_n)/C(n) \sim n^{\phi}. \tag{9}$$

Now we construct a series where each superconducting polygon is weighted by the number of its bonds. Comparing (4) and (9) and using the fact that $\chi = S^2/P$, we then obtained $\phi = 2\theta_S - 1$. Hence, $\phi(d=2) = 2$ since $\theta_S = 3/2$ in two dimensions and our numerical estimate yields $\phi(d=3) = 1.052 \pm 0.014$.

In summary, we have calculated the projected area of the three-dimensional SAP in a plane. Our result suggests that $\theta_S < 2\nu_{\mathrm{SAP}}$ in three dimensions. We have also estimated the exponent for the diamagnetic susceptibility of the superconducting rings.

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