

Mean Area of Self-Avoiding Loops

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The mean area of two-dimensional unpressurized vesicles, or self-avoiding loops of fixed length N , behaves for large N as $A_0 N^{3/2}$, while their mean square radius of gyration behaves as $R_0^2 N^{3/2}$. The amplitude ratio A_0/R_0^2 is computed exactly and found to equal $4\pi/5$. The physics of the pressurized case, in both the inflated and collapsed phases, may be usefully related to that of a complex $O(n)$ field theory coupled to a $U(1)$ gauge field, in the limit $n \rightarrow 0$.

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Self-avoiding loops, or lattice polygons, have been studied extensively as models for planar vesicles. In a pioneering paper, Leibler, Singh, and Fisher (LSF) [1] considered the statistics of the area and shape of such loops, subject to an osmotic pressure difference \bar{p} and controlled by a rigidity parameter κ . While much of the interesting physics arises as a result of the variation of this latter quantity, these authors also observed interesting scaling behavior as a function of \bar{p} when $\kappa=0$. Specifically, they found, on the basis of Monte Carlo studies and exact enumerations, that for an ensemble in which the total length, or mass, N of the loop is fixed, the mean area and squared radius of gyration behave as

$$\langle A \rangle_N \sim A_0 N^{2\nu_A} Y(x), \quad \langle R_G^2 \rangle_N \sim R_0^2 N^{2\nu} X(x), \quad (1)$$

where $x = \bar{p} N^{\nu}$ and $\nu = \frac{3}{4}$ is the usual self-avoiding walk exponent in two dimensions [2]. The scaling functions are normalized so that $X(0) = Y(0) = 1$. LSF argued that $\nu = 2$, and conjectured $\nu_A = \nu$, a result which was derived indirectly by Duplantier [3] on the basis of Coulomb gas arguments. These results were confirmed and extended to measures of the shape dependence by Camacho and Fisher [4], and the lattice enumeration studies were carried to higher orders in papers by Conway, Enting, Fisher, Guttmann, and Whittington [5-8]. One result of these studies [4,6,9] was the apparent universality of the ratio A_0/R_0^2 .

This Letter describes an analytic approach to this problem. Generalizing the well-known correspondence of the de Gennes [10], the problem of self-avoiding loops at fixed \bar{p} and fixed monomer fugacity u (conjugate to N) is shown to be equivalent to a complex $O(n)$ spin model coupled to a $U(1)$ gauge field. This field-theoretic formulation of the problem immediately establishes the scaling forms in Eq. (1). Moreover, using the methods of two-dimensional conformal field theory and the Coulomb gas mappings of Nienhuis [11], the ratio A_0/R_0^2 may be computed exactly to be $4\pi/5$.

For the sake of definiteness, consider oriented self-avoiding polygons on a honeycomb lattice. The correspondence to a (complex) $O(n)$ spin model [10,11] is as follows. Suppose that $s_a(r)$ label the components ($a = 1, \dots, n$) of a complex-valued spin at the site r . These

spins are normalized so that $\text{Tr} s_a^*(r) s_b(r') = \delta_{ab} \delta_{rr'}$ and $\text{Tr} s_a(r) s_b(r') = \text{Tr} s_a^*(r) s_b^*(r') = 0$. Then the partition function $Z \equiv \text{Tr} \prod_{r,r'} [1 + u \sum_a s_a^*(r') s_a(r) + \text{c.c.}]$ gives, in the limit $n \rightarrow 0$, the generating function for the number p_N of (unoriented) self-avoiding loops per site, $Z = 1 + 2n \mathcal{N} \sum_N p_N N^N + O(n^2)$, where \mathcal{N} is the total number of sites. Up to this point, the complex $O(n)$ model is completely equivalent to the usual real $O(2n)$ model. Consider now a unit current J_μ flowing along each link of a polygon in the direction of its orientation [9,12,13]. An explicit expression for this current, when inserted into correlation functions of the lattice $O(n)$ model, is $J_\mu(r, r') = u(r' - r)_\mu \sum_a [s_a^*(r') s_a(r) - \text{c.c.}]$, where the lattice spacing has been taken equal to unity. In the continuum spin version of the $O(n)$ model, in which the spins are replaced by a field $\Phi_a(r)$, J_μ is just the $U(1)$ current, $(1/2i) \sum_a (\Phi_a^* \partial_\mu \Phi_a - \Phi_a \partial_\mu \Phi_a^*)$, whose space integral generates the global $U(1)$ symmetry $\Phi_a(r) \rightarrow e^{i\alpha} \Phi_a(r)$. The area of a given loop is now given by

$$A = -\frac{1}{2} \int |r_1 - r'_1| \delta(r_0 - r'_0) J_0(r) J_0(r') d^2 r d^2 r' \quad (2)$$

introducing Cartesian coordinates $r = (r_0, r_1)$. This expression is valid for any non-self-intersecting loop (but not, in general, for loops which do self-intersect, since it weights different regions by the modulus of the winding number of the loop around them). It differs from that for the *signed* area, which is proportional to $\epsilon_{\mu\nu} \int r_\mu J_\nu(r) d^2 r$. This latter quantity was used in Ref. [14] to study ordinary intersecting loops as a model of vesicles. However, in the absence of any pressure difference its mean, after averaging over orientations of the loop, vanishes identically, and it is therefore not a suitable measure of the area.

In fact, Eq. (2) is readily recognized as the expectation value of the polygon regarded as a Wilson loop in a $U(1)$ gauge theory,

$$A = \int \langle A_\mu(r) A_\nu(r') \rangle J_\mu(r) J_\nu(r') d^2 r d^2 r', \quad (3)$$

in the gauge $A_1 = 0$, where $\langle A_\mu(r) A_\nu(r') \rangle = -\frac{1}{2} \delta_{\mu 0} \delta_{\nu 0} \times |r_1 - r'_1| \delta(r_0 - r'_0)$. It is straightforward to check that a similar result holds also in a covariant gauge, where $\langle A_\mu(r) A_\nu(r') \rangle = (1/2\pi) (\delta_{\mu\nu} \ln|r - r'| - r_\mu r_\nu / r^2)$. This is

important, since in this gauge the rotational invariance of the final result in the continuum limit is manifest.

In the continuum limit near its critical point, the $O(n)$ lattice model corresponds to a field theory with $O(n)$ symmetry, which has been studied extensively in two dimensions [13,15,16]. This continuum theory will possess a conserved $U(1)$ current J_μ . It then follows from the above discussion that the continuum version of the generating function for self-avoiding loops weighted by $e^{\bar{p}A}$ is given by the $n \rightarrow 0$ limit of an $O(n)$ theory, described by an action S_0 , coupled to an Abelian gauge field,

$$Z = \text{Tr} \int \mathcal{D}A_\mu \exp \left[-S_0 + ie \int J_\mu A_\mu d^2r - \frac{1}{4} \int F_{\mu\nu}^2 d^2r \right], \tag{4}$$

where, as usual, $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. Integrating out the gauge field yields the identification $\bar{p} = -e^2/2$. Several remarks may be made at this point. First, since A_μ is dimensionless and J_μ , being a conserved Noether current, retains its canonical dimension of inverse length, it follows that \bar{p} has renormalization group eigenvalue $\nu_{\bar{p}} = 2$. From this and sample renormalization group scaling arguments, follow the scaling laws in Eq. (1) with $\nu_A = \nu$ and $\varphi = 2$. Second, the ‘‘physical’’ region of the $U(1)$ gauge theory, in which the gauge coupling e is real and opposite charges attract, corresponds to a negative internal osmotic pressure difference. In that region, LSF find that for large enough N the loops collapse and behave like branched polymers. This is to be expected from the field theory, since in $1+1$ dimensions a $U(1)$ gauge field provides a confining potential so that the only asymptotic states are neutral. The world lines of these bound states correspond to the filaments of the branched polymer. The inflated phase, corresponding to $\bar{p} > 0$, does not strictly make sense in the field theory, since the vacuum would become unstable to charge separation. As is well known [17], the singularity in the free energy for $e^2 < 0$ may be described in weak coupling by an instanton calculation. For $\bar{p} > 0$ it should be possible to neglect the self-avoiding constraint, so that the action S_0 may be replaced by that of n free complex scalar fields. In the first quantized picture, the instanton configuration corresponds to a particle-antiparticle pair being created at some imaginary time r_0 and annihilating at time r'_0 , their world lines describing a circle of radius R (fixed by extremizing the total action) in Euclidean space. This corresponds exactly to the physical picture of an inflated vesicle.

Now return to the case $\bar{p} = 0$, and the expression Eq. (2) for the mean area. It is easier to work in the axial gauge, although the same results are obtained in the covariant gauge. Averaging Eq. (2) over the ensemble of all self-avoiding loops,

$$2nN \sum_N p_N \langle A \rangle_N u^N = -\frac{1}{2} \int |r_1 - r'_1| \delta(r_0 - r'_0) \times \langle J_0(r) J_0(r') \rangle d^2r d^2r', \tag{5}$$

where J is now the $U(1)$ current of the complex $O(n)$ theory, in the limit $n \rightarrow 0$. Thus

$$n \sum_N p_N \langle A \rangle_N u^N = -\frac{1}{2} a_0 \int_0^\infty r_1 \langle J_0(r_1, 0) J_0(0, 0) \rangle dr_1, \tag{6}$$

where a_0 is the area per site. In general, by current conservation and dimensional analysis, the correlation function $\langle J_\mu(r) J_\nu(0) \rangle$, evaluated in the massive $O(n)$ field theory, has the form $(\partial_\mu \partial_\nu - \delta_{\mu\nu} \partial^2) f(m|r)$, where m is the mass and f is a dimensionless scaling function, whose large r asymptotic behavior may be evaluated nonperturbatively using the form factor approach described in Ref. [13]. However, at short distances, it becomes independent of m , and therefore has the form [12] $k(n)(r_\mu r_\nu - \frac{1}{2} r^2 \delta_{\mu\nu})/r^4$, determined, up to the constant $k(n)$, by current conservation and rotational symmetry. Since the normalization of this current is fixed by the requirement that its integral generate the $U(1)$ symmetry, the number $k(n)$ is universal. Moreover, being a short-distance limit, it should be calculable within the conformal field theory corresponding to the massless complex $O(n)$ field theory. The field theorist will recognize k as the chiral anomaly, since current conservation implies the existence of a contact term proportional to $\delta^2(r)$ in the operator product $J_L(r) J_R(0)$ of the left- and right-moving currents $J_{L,R} = J_0 \pm J_1$. [For integral values of $n > 1$ the $U(1)$ symmetry would be embedded in a Kac-Moody algebra and $k(n)$ would be proportional to the level number, but for $n < 1$ such a concept does not appear to make sense.]

Since the correlation function on the right-hand side of Eq. (6) behaves like $-k(n)/2(r^2)$, the integral appears to diverge logarithmically at short distances. In fact such a divergence must occur, since otherwise the integral would be dimensionless and therefore independent of the mass m , implying that the left-hand side has no singularity as a function of u . In fact, if b is used as a short-distance cutoff, this divergence must be of the form $\ln(mb)$. Using the fact that the mass vanishes at the critical point $u = u_c$ according to $m \sim (u_c - u)^\nu$, it follows that the right-hand side of Eq. (6) has the singular behavior $-\frac{1}{4} a_0 k(n) \nu \ln(u_c - u)$ and hence that, as $N \rightarrow \infty$,

$$p_N \langle A \rangle_N \sim \frac{1}{4} \sigma a_0 k'(0) \nu N^{-1} u_c^{-N}, \tag{7}$$

where the lattice-dependent integer σ appears [9,18] because, on non-close-packed lattices, the series is in fact in u^σ and therefore has σ equivalent singularities on $|u| = u_c$. Defining the amplitude B by $p_N \sim BN^{-2\nu-1} \times u_c^{-N}$, it follows that $BA_0 = \frac{1}{4} \sigma a_0 k'(0) \nu$, which gives $\frac{3}{8} k'(0)$ for the square lattice ($\sigma = 2, a_0 = 1$).

The next step is to evaluate $k(n)$ using Coulomb gas methods. These are explained in detail in Ref. [11] and the reader who is unfamiliar with them is referred to this article. The mapping to the Coulomb gas proceeds in two stages. On the honeycomb lattice, the expansion of the

partition function of the complex $O(n)$ model yields a sum over configurations of nonintersecting oriented loops, weighted by a factor of u for each link and n for each loop. This latter factor may be written in a local fashion by incorporating a factor $e^{\pm i\chi}$ at each occupied vertex, depending on whether the oriented loop makes a turn through $\pm\pi/3$ at that point. Thus (anti)clockwise loops accumulate factors of $e^{-6i\chi}$ or $e^{6i\chi}$, respectively. After the summation over orientations, the appropriate factor of $2n$ per loop may be recovered by choosing $n = \cos 6\chi$. This model may then be mapped onto a solid-on-solid (SOS) model by assigning heights $\phi(r)$ (which are conventionally chosen to be integer multiples of π) to the sites of the dual lattice. Neighboring heights on either side of an oriented bond differ by $\pm\pi$; otherwise they are equal. By convention, the higher side is on the right, looking along the oriented bond. This model is then supposed [11] to renormalize in the long wavelength limit onto a Gaussian model with action $S_G = (g/4\pi) \times \int (\partial\phi)^2 d^2r$, where $g = 1 - 6\chi/\pi$. However, there is a caveat: In the SOS model the factors $e^{\pm i\chi}$ lead to the result $\langle e^{-12i\chi\phi(r)/\pi} \rangle = 1$, as may be seen by direct calculation in the fugacity expansion. In the Coulomb gas language, where ϕ is interpreted as an electrostatic potential, this phenomenon corresponds to a total electric charge $12\chi/\pi$ on the boundary, which preserves overall neutrality. Thus all nonzero correlation functions must correspond to a total charge $-12\chi/\pi$ in the interior.

How should the $U(1)$ current of the complex $O(n)$ model be represented in the SOS model? The naive candidate is simply $J_\mu^{\text{SOS}} \equiv (1/\pi)\epsilon_{\mu\nu}\Delta_\nu\phi$, where Δ_ν denotes a lattice difference between sites of the dual lattice. This current is conserved and has the property of taking the values ± 1 as required. But it is nevertheless incorrect, since clockwise and anticlockwise loops are counted with different phase factors, resulting in a net clockwise current of $e^{6i\chi} - e^{-6i\chi} = 2i \sin 6\chi$ around each loop. In addition, it may be seen that the correlation function $\langle J_\mu^{\text{SOS}}(r)J_\nu^{\text{SOS}}(r') \rangle$ receives contributions when the links r and r' are on different loops, a feature which is absent in the $O(n)$ model. This correlation function also suffers from having net charge zero, so the charge on the boundary is not cancelled.

However, as shown by other examples discussed in Ref. [11], the nature of the mapping between the operators of the $O(n)$ model and those of the SOS model is not one to one. The only requirement is that the correlation functions of the $O(n)$ model correspond to correlation functions in the SOS model. In order to reproduce the correlation function $\langle J_\mu(r)J_\nu(r') \rangle$ of the $O(n)$ model, it is simply necessary to find operators A and B of the SOS model such that $\langle A(r)B(r') \rangle$ gives the required result in the sum over graphs. The above argument shows that taking $A=B=J^{\text{SOS}}$ does not work. However, there is another conserved current $\tilde{J}_\mu^{\text{SOS}} \equiv \lambda\epsilon_{\mu\nu}\Delta_\nu(e^{-12i\chi\phi/\pi})$, where the constant λ is to be fixed. This has the property that its expectation value around a given loop vanishes, as re-

quired, on summing over both orientations, since this is proportional to $(e^{-12i\chi} - 1)e^{6i\chi} + (e^{12i\chi} - 1)e^{-6i\chi} = 0$. Now consider the current-current correlation function, which is the expectation value of $J_\mu(r)J_\nu(r')$ in the $O(n)$ model. For a given configuration in the loop gas, after summing over both orientations, this quantity takes the values $2n\hat{r}_\mu\hat{r}'_\nu$ if r and r' lie on the same loop (where \hat{r} is a unit vector along the link r), and is zero if they lie on different loops. A suitable candidate for this in the SOS model is therefore

$$\langle \tilde{J}_\mu^{\text{SOS}}(r)J_\nu^{\text{SOS}}(r') \rangle = (\lambda/\pi) \langle \epsilon_{\mu\gamma}\Delta_\gamma e^{-12i\chi\phi(r)/\pi} \epsilon_{\nu\delta}\Delta_\delta \phi(r') \rangle, \quad (8)$$

since the quantity in $\langle \dots \rangle$ is zero when r and r' are on different loops, for the same reason as above, and when they are on the same loop, it takes the value

$$\pi\hat{r}_\mu\hat{r}'_\nu(e^{-12i\chi} - 1)e^{6i\chi} - \pi(e^{12i\chi} - 1)e^{-6i\chi} \\ = -4\pi i\hat{r}_\mu\hat{r}'_\nu \sin 6\chi.$$

Thus one should choose $\lambda = in/(2\sin 6\chi)$. It is somewhat curious that it is necessary to use different currents J and \tilde{J} in this expression, but such a result is consistent with the requirement that the total charge be $-12\chi/\pi$ for the correlation function to be nonzero.

It is now straightforward to evaluate Eq. (8) in the Gaussian model with action S_G , replacing the lattice differences by derivatives, and using the operator product expansion

$$\partial'_\mu\phi(r')e^{-12i\chi\phi(r)/\pi} \sim (-12i\chi/g\pi)(r-r')_\mu(r-r')^{-2} \\ \times e^{-12i\chi\phi(r)/\pi}.$$

The result is of the form expected, with

$$k(n) = \frac{12n\chi}{\pi^2 g \sin 6\chi} = \frac{2n \arccos n}{\pi\sqrt{1-n^2}(\pi + \arccos n)}, \quad (9)$$

where $0 \leq \arccos n \leq \pi$. For $n=1$, the model describes a single species of charged boson with repulsive interactions, whose infrared behavior is that of free fermions. In that case, one finds $k=2/\pi^2$, as may be checked independently. For $n \rightarrow 0$, Eq. (9) gives $k'(0) = 2/3\pi$, so that $BA_0 = \sigma a_0/8\pi$.

In order to eliminate the lattice-dependent factors from this otherwise universal result, it may be combined with the relation $BR_0^2 = 5\sigma a_0/32\pi^2$, which follows from a sum rule [19] which is a consequence of Zamolodchikov's c -number theorem [20]. This amplitude relation was first derived for the square lattice in Ref. [21], and generalized in Ref. [9]. The main result given in the introduction then follows. Table I shows the comparison of these predictions with results of lattice enumerations and a Monte Carlo simulation of a continuum model. The agreement is very satisfactory.

It is interesting to note that random loops with self-intersection, for which $\langle R^2 \rangle_N \sim N$, correspond to a free $O(n)$ theory, for which the current-current correlation

TABLE I. Most accurate existing estimates of the amplitudes B , A_0 , and $R\delta$ and their universal ratios compared with the predictions of this work.

	Square	Triangular	Continuum	Prediction
σa_0	2	$\sqrt{3}/2$...	
B	0.5623 ⁸	0.2640 ⁶	...	
A_0	0.1416 ⁵	0.131 ⁶	0.314 ± 3^4	
$R\delta$	0.05631 ¹⁸	
$BA_0/\sigma a_0$	0.03981	0.0399	...	$1/8\pi=0.0397887$
$A_0/R\delta$	2.515	...	2.55 ± 5^4	$4\pi/5=2.51327$

function behaves as $r^{-2}\ln r$ at short distances [12]. As a result, the mean area of such walks (weighted as discussed earlier) behaves as $N \ln N$ for large N . This is not surprising, since, as mentioned above, such loops are weighted by their winding number, whose average grows logarithmically [22]. In higher dimensions, Eq. (6) may be generalized to relate the generating function for the mean area of a loop *projected* onto a fixed plane to a similar integral over the current-current correlation function. Unfortunately, for $d > 2$ the singular behavior of this integral does not come entirely from the short-distance behavior, and therefore the whole scaling function $f(mr)$ is required, rather than just the coefficient of its short-distance behavior, which was calculated in an ϵ expansion by Miller [12]. However, this argument does imply that the mean projected area grows as $N^{2\nu}$, in contradiction to the numerical findings (with rather short series) of Ref. [23].

In this Letter I have shown how the theory of pressurized two-dimensional vesicles without rigidity may be given a field-theoretic basis. For zero pressure, this leads to an exact prediction for the universal amplitude ratio $A_0/R\delta$. In the inflated phase $\bar{p} > 0$, instanton techniques are applicable and should yield an asymptotic expansion for the crossover functions in Eq. (1) for large argument x . This work is currently in progress. The collapsed phase $\bar{p} < 0$ corresponds to confinement, and may provide an alternative field-theoretic way of describing the so far only partially solved problem of two-dimensional branched polymers. Branched polymer behavior has also been found recently in a slightly different model of self-avoiding loops [24], in which the loops are allowed to move in a background of random impurities under the constraint that the loop should contain no impurities. These may be incorporated into the above model by allowing them to act as the sources for the U(1) gauge field. Preliminary work suggests that this will lead to results similar to those obtained from a coupling to the area.

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Note added.—After this work was completed, Ref. [25] was brought to my attention. The authors of this paper study the deflated regime, using a gauge field in order to generate the area term, but they use a lattice formulation with a Z_2 rather than a U(1) gauge field. They also conclude that the pressure p has renormalization group eigenvalue $y_p = 2$. In general, the use of a U(1) field seems more suited to an analytic, continuum approach.

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