Area and Perimeter Distribution of a Surface in Two Dimensions

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We consider the number of configurations of a surface in two dimensions that has a prescribed length and encloses a prescribed perimeter with respect to a baseline. An approximate analytical treatment in a semi-continuum compares favourably with results from an exact algorithm for the discrete lattice. This work is relevant for finding the entropy associated with macroscopic configurations of such systems as domain growth problems, evaporation-deposition problems, membrane physics, or polymer physics.

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I. INTRODUCTION

In statistical mechanics, one very often performs averages over ensembles of microscopic configurations. Since this is usually very difficult, it is common to replace the ensemble of microscopic quantities by an ensemble of macroscopic quantities. For instance, a spin Hamiltonian may be replaced by one that depends only on magnetization. This paper, we address the problem of a surface in two dimensions with fixed endpoints where the macroscopic quantities are the perimeter of the surface and the area enclosed by it. Such a problem would arise, for example, if one is given a Hamiltonian for a system that consists of a area term and a surface term, i.e.

$$\mathcal{H} = J f_s(S) - P f_a(A)$$  \hspace{1cm} (1)

where $S$ is the perimeter of the surface and $A$ is the area between it and some substrate, $J$ is the surface tension, $P$ the pressure, and $f_s$, $f_a$ general functions of $S$ and $A$ respectively. These types of Hamiltonians could arise in domain roughening problems \cite{5,6}, wetting problems, evaporation–deposition problems, the physics of membranes, or polymer physics \cite{7,8}. We were motivated by an investigation of the random field Ising model \cite{9,10}.

To find the free energy of such a system and thus any relevant macroscopic quantities at a finite temperature, one would like to know the associated entropy $S = k_B \ln \Omega_L(S, A)$. Here, $\Omega_L(S, A)$ is the number of surface configurations with the given perimeter $S$ and enclosed area $A$ and which begin and end at the ends of a line of length $L$; this is the quantity that shall be of interest to us.

A slightly different version of this problem\footnote{They studied “bar graph polygons” wherein the domain wall heights are not allowed to go below the baseline. In our model, the heights of the surface can be both positive and negative.} has been solved exactly by Owczark and Prellberg \cite{11} by finding the generating function of $\Omega$. However, the solution was in terms of the $q$–series deformation of a hypergeometric function. While informative, this result is very complex and difficult to use in our analysis. Our aim is to find a simple form for $\Omega$ that can be easily manipulated.

We use an approximation to translate the problem into one of simple Riemannian geometry that can be solved using the familiar tools of vector analysis. The result is the pleasingly elementary form

$$\Omega(S, A) = f \left( g^2 S^2 - \frac{A^2}{L^2} \right)^{\frac{L+3}{2}}$$  \hspace{1cm} (2)

where $f$, $L$ and $g$ are functions of $L$ only. This result compares favourably with exact numerical results.

II. DEFINITION OF THE PROBLEM

We consider a surface with fixed endpoints such that it has an end to end distance of $L$. The surface may take any path between these endpoints as long as there are no overlaps or overhangs (i.e. it is a directed random walk). This should be a reasonable approximation in the limit of weak disorder. We label the straight line between the endpoints with the integer $i \in [0, L]$ and the height of the surface at each point by $h_i$, a single valued real number. Figure \ref{fig:example} illustrates these definitions. The quantities $A$ and $S$ may be written as functions of these variables.

$$A = \sum_{i=0}^{L} h_i$$  \hspace{1cm} (3a)

$$S = \sum_{i=0}^{L} |h_i - h_{i-1}|$$  \hspace{1cm} (3b)

where $S$ is the actual length of the surface less $L$ (since any surface that covers the baseline distance must be at least $L$ long).

The problem is simplified somewhat by the introduction of the variables $R_i = h_i - h_{i-1}$. Like $h_i$, $R_i$ is a real number with $i \in [1, L]$ an integer. Under this change of variables, equation (3b) becomes

$$A = \sum_{i=1}^{L} (L - i) R_i$$  \hspace{1cm} (4a)

$$S = \sum_{i=1}^{L} |R_i|.$$  \hspace{1cm} (4b)

There is also an additional constraint that the surface finish at height $h_L = 0$. This introduces the auxiliary equation

$$\sum_{i=1}^{L} R_i = 0.$$  \hspace{1cm} (5)

Consider an ensemble of surfaces all with various $(A, S)$ and subject only to the constraint (4). In terms of the definitions above, we wish to know how many different values of $R_i$ satisfy equations (4a), (4b), and (5) for fixed $A$ and $S$. We solve this problem in the next section.

III. SOLUTION

The solution is further complicated by the presence of the absolute value function in (4b) and so we will make a further approximation to simplify matters. It is hoped that this will not change the essential character of the solution. Thus, we replace equation (4b) by

$$g(L)^2 S^2 = \sum_{i=1}^{L} LR_i^2.$$  \hspace{1cm} (6)
This completes the approximations in the solution. That the form factor \( g \) should only be a function of \( L \) follows from a simple scaling argument.

Clearly, equation (3) implies that the vectors \( R_i \) lie on a \( L - 1 \) dimensional hypersphere embedded in \( L \) dimensions. The other two equations (4a) and (5) introduce hyperplanes that pass through the hypersphere. Thus, vectors that satisfy all three equations lie on the intersection of the hypersphere with these two hyperplanes. This intersection is itself a hypersphere, but of dimension \( L - 3 \). Thus, the problem is reduced to finding the measure of the vectors which lie on the surface of this hypersphere. Of course, we cannot satisfy this criterion for all vectors, so we demand that it be satisfied on this hypersphere. Obviously, we cannot satisfy this criterion for all vectors, so we demand that it be satisfied on this hypersphere. Thus, the problem is reduced to finding the measure of the vectors which lie on the surface of this hypersphere.

The details of this calculation are included in appendix A and the result is

\[
\Omega_L(S, A) = f \left( \max \left( g^2 S^2 - \frac{A^2}{L^2}, 0 \right) \right) \frac{L-2}{\sqrt{2L}}.
\]

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\[
f = \pi \frac{L-2}{\sqrt{2L}} \left( \frac{L-2}{2} \right) ! (L-2).
\]

It is worth noting that the problem posed by equations (1), (4a), and (5) with \( g(L) = 1 \) is in itself worthy of consideration, and may relate to other models in statistical physics. However, since we were motivated by the random field Ising model wherein (4b) arises, we set \( g(L) \) so that (4b) maps as closely as possible back to (4). We describe how to do this in the following section.

IV. THE FORM FACTOR \( g(L) \)

One can employ simple scaling arguments on (4b) to deduce that \( g(L) \sim cL^{-1/2} \) for large values of \( L \), where we would expect \( c \) to be of order unity. But, a better estimate of \( g \) can be made. Consider the set of vectors that satisfy (4b), that is, the vectors on an \( L \) dimensional hypersphere of radius \( r = g(L)A \). To satisfy (4b) we must set \( A \) such that \( \sum_{i=1}^{L} R_i = A \) for all vectors on this hypersphere. Obviously, we cannot satisfy this criterion for all vectors, so we demand that it be satisfied on average. This presumes, of course, that all the vectors on the hypersphere have equal importance in \( \Omega_L \), which is a reasonable first approximation. Thus, we set

\[
\langle \sum_{i=1}^{L} |x_i| \rangle = A
\]

where \( \langle Q \rangle \) denotes the average value of a quantity \( Q \) over the hyperball of radius \( r \). It is a straightforward piece of mathematics to perform this calculation, the details of which are included in appendix B. The result is

\[
g(L) = \sqrt{\frac{\pi}{L}} \left( \frac{(L-1)!)^2}{(L/2)! (1 + 1/L)} \right).
\]  

Using Stirling’s approximation, we find that for large \( L \) this tends asymptotically to

\[
g(L) \rightarrow \frac{\sqrt{\pi}}{2L}.
\]  

which agrees with our earlier expectations.

V. THE NUMERICAL TREATMENT

In order to test (and possibly improve upon) the analytic results obtained above, an algorithm was devised to scan over all the random walks with perimeter \( S \) less than some preset maximum \( A^* \). To understand this algorithm, it is helpful to think of \( S \) as the length of a piece of string that we have to play with. This piece of string must start and finish on the baseline but may do anything in between (subject to the restriction that there are no overhangs or overlaps). But, the amount of string we have used up in our previous steps determines how much we have left to play with in the following steps. For instance, at the first step, the string may have any height \( R_i \in [-A^* /2, A^* /2] \). In general, if we are at position \( i \) and at height \( h_i = \sum_{j=1}^{i-1} R_j \), and have already used up a length of string \( A_i = \sum_{j=1}^{i-1} |R_j| \), then this limits the range of values \( R_i \) may have. Namely,

\[
R_i \in \left[ \frac{-A^* + A_i - h}{2}, \frac{A^* - A_i - h}{2} \right].
\]

Figure 2 illustrates this.

Furthermore, we only need to scan over various values of \( R_i \) for \( i \leq L-1 \) since \( R_L \) is determined by the condition \( \sum_{i=1}^{L} LR_i = 0 \). A general outline of the algorithm is given below:

1. Set \( R_1 \) to \(-A^*/2\)
2. Set all \( R_i \) for \( i = 2, \ldots, L-1 \) to their minimum possible value and determine \( R_L \)
3. Measure \( S \) and \( A \). Increase \( \Omega(S, A) \) by one.
4. Increase \( R_{L-1} \) by one. If \( R_{L-1} \) exceeds its maximum value then increase \( R_{L-2} \) by one and set \( R_{L-1} \) to its minimum value. If this causes \( R_{L-2} \) to exceed its maximum value, then increase \( R_{L-3} \) by one and set \( R_{L-2} \) to its minimum value. Et cetera.
5. Repeat steps 3 and 4 until \( R_1 = A^*/2 \)

A recursive program was written in C to implement this algorithm, and the program was run on Sun workstations. Data was obtained for \( A^* \) as large as 60 and for \( L \) as large as 10. It becomes increasingly difficult to get data for larger \( L \) since the number of random walks seems to grow geometrically with \( L \). Indeed, we predict that

\[
\int \Omega(S, A) dV \sim (L-2)^{L} A^{L} \alpha^{L}
\]

where \( \alpha \) is a constant of order unity.
VI. COMPARISON OF NUMERICAL AND ANALYTIC RESULTS

When viewed side by side, the two results seem to look very similar (see Figure 3). However, the scales do not agree. This is attributed to the fact that the numerical routine investigates only discrete values of \( R_i \) whereas in the analytic treatment \( R_i \) was allowed to be continuous. In both treatments \( L \) is divided into discrete intervals, so this is not a cause for worry (as long as we have \( L > 3 \)). From the point of view of our hypersphere argument, the analytic treatment has given the measure of all vectors on the surface, whereas if the components of the vectors are constrained to be integers, there are fewer vectors close to the surface of the hypersphere. Nowhere is the effect of the discretization more noticeable than in the fact that \( \Omega(S, A) = 0 \) on a discrete lattice for odd \( S \). This simply says that we need as many steps up as down if we are to return to the origin. We do not have this same constraint in the semi–continuous model. Nevertheless, the results still compare very favourably on various levels (up to this scaling factor). Three quantities were chosen for the purposes of comparison, which we list below together with their predicted values:

- The maximum value of \( \Omega \) for a given \( S \) and \( L \),
  \[
  M_m = \Omega_L(A, 0) = f(L)(g(L)A)^{L-3}. \tag{13}
  \]

- The zeroth moment of the distribution with respect to \( A \),
  \[
  M_0 = \int \Omega(S, A)dV = \mathcal{L}f(L)(g(L)A)^{L-2} \Upsilon(L). \tag{14}
  \]
  where
  \[
  \Upsilon(L) = \frac{2^{2L-5}(L-3)!(L-3)!}{(2L-5)(2L-6)!}. \tag{15}
  \]

- The second moment of the distribution with respect to \( A \),
  \[
  M_2 = \int \Omega(S, A)A^2dV = \mathcal{L}^3f(L)(g(L)A)^{L-4} \Upsilon(L) \frac{2L^3}{2L-3}. \tag{16}
  \]

Given that we expect these forms to arise, we generate these quantities from our data and fit them to a power law behaviour in \( S \) for various values of \( L \). The exponent and coefficient of this fit are then compared to the analytic predictions listed above. The results are shown in Figure 4, where one can see that the exponents, but not the coefficients, agree well (as expected from the above discussion). However, the coefficients do seem to have the correct scaling behaviour in \( L \).

VII. CONCLUSIONS

We have investigated the question of the entropy of a two dimensional surface with fixed volume and area from both the numerical and analytic viewpoints. From the analytic side, we found an elegant expression for the semi–continuum by using a single approximation. From the numerical side, we generated exact results that compared favourably with the analytic expression. However, there were certain differences noted between the two and these were attributed to differences between the discrete and semi–continuous formulations of the problem.

Nevertheless, the solution captures the important characteristics of the numerical work. It is hoped that this work will be of value to finite temperature formulations of problems in many areas of statistical mechanics where the question may be posed in terms of such macroscopic quantities as the length of a curve and the area enclosed by it.

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APPENDIX A: CALCULATION OF \( \Omega(A, V) \)

We wish to find the measure of all vectors that satisfy equations (14a), (14b), and (14c). To simplify matters, let us introduce the dimensionless variables \( r_i' = R_i/(gA) \). Working with these vectors instead of \( R_i \) introduces a change of measure and since the object we are looking at is clearly a \( L - 3 \) dimensional hypersphere, this change of measure is \( J = (gA)^{L-3} \). Written in these new coordinates the equations (14a), (14b), and (14c) become

\[
\sum_{i=1}^{L} r_i'^2 = 1, \tag{A1a}
\]
\[
\sum_{i=1}^{L} r_i' = 0, \tag{A1b}
\]
\[
\sum_{i=1}^{L} (L - i + 1)r_i' = v, \tag{A1c}
\]

where \( v = V/g(L)A \).

This change of measure associated with the change of variables is associated with the scaling behaviour of the equations. We can make this more explicit by writing

\[
\Omega_L(A, V) = J\Omega_L(1/g(L), V/g(L)A). \tag{A2}
\]
Similarly, we could have written
\[ \Omega_L(A, V) = V L^{L-3} \Omega_L(A/V, 1). \] (A3)

It is important that our final solution obey these two relations.

The path to the solution is made clearer if we rewrite the equations in \((A1)\) so that they more closely resemble the vector formalism. To achieve this, let us introduce the vectors
\[ r' = \{r'_1, r'_2, \ldots, r'_L\} \] (A4a)
\[ \mathbb{1}' = \{1, 1, \ldots, 1\} \] (A4b)
\[ L' = \{L-1, L-2, \ldots, 0\} \] (A4c)
so that \((A1)\) becomes
\[ \|r'\| = 1 \] (A5a)
\[ r' \cdot \mathbb{1}' = 0 \] (A5b)
\[ r' \cdot L' = \|L'\| \cos \theta = v \] (A5c)
where \(\|L'\|^2 = L(L-1)(2L-1)/6\).

Figure \(\text{V}\) gives a pictorial representation of these equations. Equation \((A5a)\) specifies that the vectors \(r'\) lie on a unit hypersphere, \(S^L\), of dimension \(L-1\). Equation \((A5b)\) is an orthogonality condition and is used to lower the dimension of the problem by one. Finally, equation \((A5c)\) specifies that the vectors are at an angle \(\theta\) to the vector \(L'\).

We will now employ a coordinate rotation and project our problem onto the \(L-1\) dimensional space orthogonal to \(\mathbb{1}\). The rotation is chosen to simplify the projection, e.g. we let the \(z\) axis lie parallel to the vector \(\mathbb{1}\) so that \(r' \to (r'_1, 0)\) and \(L' \to (L, L_z)\).

Now \(\hat{r}\) and \(\hat{L}\) are both \(L-1\) dimensional vectors and \(L_z\) is the component of \(\hat{L}^{'}\) parallel to \(\mathbb{1}\).
\[ L_z = \frac{\hat{L}^{'} \cdot \mathbb{1}}{\|\mathbb{1}\|} = \frac{L(L-1)}{2\sqrt{L}}. \] (A6)

Equation \((A5c)\) retains its familiar form in this new, unprimed, coordinate system
\[ \hat{r} \cdot \hat{L} = \|\hat{L}\| \cos \theta = v. \] (A7)

We want a measure of the set of all unit vectors \(\hat{r}\) that satisfy this dot product. These vectors form a hypercone with angle of opening \(2\theta\) and sides of unit length. An appropriate measure is the area of the \(L-2\) dimensional hypersphere that the tips of these vectors trace out. In general, the area of a \(d\) dimensional hypersphere of radius \(r\) is
\[ A_d(r) = \frac{\pi^{d/2} r^d}{(d/2)!}. \] (A8)

Letting \(d \to L-2\) and \(r \to \sin \theta\) we arrive at
\[ \Omega(1, v) = \pi \frac{L-2}{2} \left( \frac{L-2}{2} \right)! \left( 1 - \cos^2 \theta \right)^{\frac{L-2}{2}}. \] (A9)

We substitute for the value of \(\cos \theta\) using equation \((A7)\) and simplify the notation by letting \(L = \|\hat{L}\|\), i.e.
\[ L^2 = \|\hat{L}^{'}\|^2 - L^2 = \frac{L(L-1)(2L-1)}{6} - \frac{L(L-1)^2}{4}. \] (A10)
\[ \cos \theta = \frac{v}{L}. \] (A11)

Using the scaling relation \((A2)\) we arrive at our final form
\[ \Omega_L(A, V) = f \left( g^2(L) A^2 - \frac{V^2}{\ell^2} \right)^{\frac{L-2}{2}} \] (A12)
\[ f = \pi \frac{L-2}{2} \left( \frac{L-2}{2} \right)! \left( L - 2 \right). \]

It is simple to check that this form satisfies the scaling relations \((A2)\) and \((A3)\). Obviously, for physical reasons, we set \(\Omega(A, V) = 0\) if \(V > g(L) A \ell\).

**APPENDIX B: CALCULATION OF \(g(L)\)**

Following the philosophy outlined in section \(\text{V}\) we wish to find the sum of the absolute values of the components of a vector that lies on an \(L\) dimensional hypersphere of radius \(r\). Written in terms of spherical polar coordinates, these components are
\[ x_1 = r \cos \theta_1 \]
\[ x_2 = r \sin \theta_1 \cos \theta_2 \]
\[ \vdots \]
\[ x_i = r \prod_{j=1}^{i-1} \sin \theta_j \cos \theta_i \]
\[ \vdots \]
\[ x_L = r \prod_{j=1}^{L-1} \sin \theta_j. \] (B1)

We wish to consider \(\langle \sum_{i=1}^{L} |x_i| \rangle\) but we can take advantage of the spherical symmetry to write this as \(L \langle x_L \rangle\). All that remains is to tackle the integral
\[ I = \int G d\theta_1 d\theta_2 \ldots d\theta_{L-1} \left| \prod_{i=1}^{L-1} \sin \theta_i \right| \] (B2)
where \(G = r^{2(L-1)} \prod_{i=1}^{L-2} \sin^2(L-i-1) \theta_i\) is the metric of the surface of this hypersphere. Expanding out the integrals,
\( I = 2 \prod_{i=1}^{L-2} \int_0^\pi \sin \theta_i \sin^{L-i-1} \theta_i d\theta_i \int_0^\pi \sin \theta_{L-1} d\theta_{L-1}. \)  

(B3)

The remaining integral may be done by comparison to the area integral of the \( d \) dimensional unit sphere:

\( A_o(d) = 2\pi \prod_{i=1}^{d-2} \int_0^\pi \sin^{d-i-1} \theta_i d\theta_i = \frac{\pi^{d/2} d}{(d/2)!}. \)  

(B4)

since

\( I = 2 \prod_{i=1}^{L-1} \int_0^{L-i} \theta_i d\theta_i = \frac{A_o(L+1)}{\pi}. \)  

(B5)

Thus, the normalized average is \( \langle \sum_{i=1}^L |x_i| \rangle = LI/A_o(L) \equiv A. \) Putting \( r = Ag(L) \) we get the final form

\( g(L) = \frac{\sqrt{\pi}}{L} \left( \frac{\frac{L+1}{2}!}{(L/2)! (1+1/L)} \right). \)  

(B6)

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FIG. 1. Directed surface with area \( S \) and perimeter \( S' \).

FIG. 2. The drawing on the left shows the maximum value \( R_o \) can have, thus using up all the string. The drawing on the left show the maximum value \( R_i \) can have, so that we use up all the available string at this step.

FIG. 3. Sample data set from the numerical routine, compared with the results of the analytic calculation.

FIG. 4. Plots of the exponent and coefficient of \( M_m, M_0 \) and \( M_2 \). The data points are those values found from numerical work while the solid lines represent the theoretical prediction. The error bars represent the statistical error from the power law fit.

FIG. 5. The vector space that \( \vec{1} \) and \( \vec{L}' \) live in, showing the hyperspheres \( S \) and \( S' \).
Figure 1
Figure 2

\( R_0 = \frac{A^*}{2} \)
Figure 3

$\Omega$ for $L=8$ and $A'=60$
Figure 4
Figure 5