Exact Calculations of Membrane Areas with Simple Models.

by

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Abstract

The distinction between the true total area and the projected area is elucidated with soluble models which represent the membrane as a self-avoiding string on a plane. Constraining the total area to a predetermined value changes the averages very significantly. The latter are calculated exactly from the generating functions of self-avoiding walks and are shown as functions of activities q and r related to temperature $T = \pm 1/\log(q)$ and lateral force $f = -\log(r)$. The constraint makes the partition functions and averages valid for all $q, r > 0$ and reduces the ratio of A_{tot} to the projected area L. High temperature divergences are supressed. Possible applications to simulated bilayers/membranes are discussed.

I. Introduction

Interfaces and membranes as well all undergo shape fluctuations due to thermal motion. A twodimensional sheet such as a bilayer or a planar interface changes its shape by excursions into the third dimension; thus arises the distinction between the "true" total area A_{tru} and the "projected" area. The latter term has been coined to emphasize that the "true" (proper,intrinsic) area of a planar interface when projected onto the edge of the volume, produces A, the projected, or nominal, area. The definition of the interfacial tension, *via* the constant-volume increment δF of the free energy F

$$\delta F = \gamma \delta A \tag{1.1}$$

refers to the projected area A . Another expression that both planar interfaces and membranes share, is the limiting form of the structure factor, dominated by capillary waves.

However, there are important distinctions, essentially originating from the fact that an interface is an open system, also open with respect to particle exchange. A liquid surface fluctuates and varies its surface area by diffusion of molecules in and out of either bulk phase. A surface of a perfect crystal is an extreme example, as it varies exclusively by particle exchange with vapor phase.

In membranes or bilayers such particle migration does not occur or is very rare. Commonly membranes and bilayers are formed by self-assembling surfactant (amphiphilic) molecules, embedded in a liquid solvent. These are practically insoluble in the solvent forming a variety of micelles if not in a bilayer. Consequently the shape fluctuations of a membrane or bilayer take place *under the constraint* of a constant particle number N_s forming the surfactant sheet.

This constraint translates to a constraint of constant membrane area A_{tru}.

The common formulation of the theory of capillary waves starts with an flat interface (with its true area A_{tru} originally equal to the projected area) which increases its true area by thermal fluctuations. Thus the projected area is a given quantity whereas A_{tru} varies in time about its thermal average $\langle ... \rangle$ value.

With a membrane one must take the opposite view: the true (intrinsic, proper) area of a membrane A_{tru} is a given quantity whereas the projected area is a fluctuating quantity with a thermal average $\langle ... \rangle$.

The effects of the constraint of constant particle number in the membrane are

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discussed below. Introducing these constraints into the theory has proved difficult; practically the classical reference[1,2] is entirely up to date[3] even today. A mention of some difficulties is present in a theorerical paper[4]. A most useful source of information have been computer simulations. The areas of bilayers have also been extracted from simulation data [5−7]. Overall, the simulations of bilayers have been very numerous[5−26], but not all determined the *bilayer isotherms* i.e. lateral tension *vs.* area dependences[5,6,10,12,13,16,21−24].

Although the definition (1.1) of γ may be the same, in fact the behaviour of γ of bilayers has been so different from γ of interfaces/surfaces - that a specific terminology of "lateral tension" was introduced. The "exotic" properties of the lateral tension have been recently enumerated[26].

In this paper we find useful insights from exact solutions of simple models. The membrane is modelled as a onedimensional string embedded in a square lattice. Fig.1 shows such a string and the two areas associated with it. As calculations show, besides the the membrane/bilayer case, of chief interest, the interfacial situation can also be modelled with appropriate choice of parameters while removing the constraint.

In Section II we apply the known generating functions[27] to derive some new variants of these and then to calculate the averages: the average projected area for given full area (the membrane) and the average total area for given projected area (an interface); we illustrate the spectacular differences with Figures. Finally we consider the case of a boxed membrane/bilayer, such as is modelled in molecular dynamics simulations, for which both areas, total and projected, are given and fixed. Section III is the summary and a discussion, illuminating *i.a.* the issue of the bending (rigidity) coefficient.

II. The Random Walk and its Generating Functions.

We model the membrane as a twodimensional string in an infinite square lattice. The string is generated by a partially directed self-avoiding random walk (PDSAW). With lattice constant $a_0 = 1$, the allowed steps are: up, down, or to the right, *i.e.* $(0, +1)$, $(0, -1)$, or $(+1, 0)$, respectively. The total number of steps, N, is made of L horizontal x−steps, and of A_v vertical steps. $A_v = n_+ + n_-$ is made of positive and negative steps $n_+ \geq 0$ and $n_- \geq 0$. Thus always $N = A_v + L = n_+ + n_- + L$. Such a string is shown in Fig.1.

A string of length of N steps extends from (0,0) i.e. from $x = 0, y = h_1 = 0$, to (L, h_{last}) i.e.to $x = L, y = h_L = h_{last}$. If the string is to represent a onedimensional membrane, the length N becomes the membrane area, and L the *projected area*. The usual definition of an area of a smooth surface translates into $s^2 = \Delta x^2 + \Delta y^2$ as the surface element produced by one step; we approximate the hypothenuse s by the sum $s = \Delta x + |\Delta y|$. Thus the area is always somewhat overestimated, but the difference with the usual definition was found to be quite small. Then the total area ("true") is N, $A_{tru} \equiv N$, and $N = A_v + L$. In the membrane picture N once given is constant; it does not fluctuate. In the interface model, L is given and constant and N can take any value $N \geq L$.

The generating function is constructed as

$$G = \sum_{all\ walks} q_-^{n_-} \cdot q_+^{n_+} \cdot r^L \tag{2.1}$$

where r, q_+, q_- are weights assigned to these steps and counting parameters. Generally up (plus) steps are assigned the same weight as the down (minus) steps, i.e. $q = q_- = q_+$ and q^{A_v} is substituted for $q_-^{n_-} \cdot q_+^{n_+}$.

The parameter $r > 1$ will favor large L, i.e. extended, relatively flat configurations, whereas $r < 1$ will favor small L. The parameter $q < 1$ will favor less deviations from flatness, whereas $q > 1$ will favor configurations with many folds - which are suggestive of a crumpled membrane or floppy bilayer. Restriction of h_{last} to the value $h_{last} = h_1 = 0$ may also be imposed in order to have periodic boundary condition in the x-direction.

A still more general model would introduce the bending parameter w and a factor w^T where T is the number of turns. Here we take $w = 1$, i.e. we ignore the number of turns. The issue of bending coefficient in the context of this model is discussed in Section III.

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Clearly (2.1) can be interpreted as a grand partition function with r, q as activities; thus

$$q \equiv \exp[-\beta \epsilon_v] \qquad (2.2)$$

where $\beta \equiv 1/kT$ and ϵ_v is the energy cost of a vertical step. Now we note that $q < 1$ implies $\epsilon_v > 0$ i.e. the choice for *modelling an interface* which deviates from flatness at some cost. This cost is reflected in the positivity of γ defined by (1.1). Otherwise, $q > 1$ and $\epsilon_v < 0$ owing to attractive intermolecular forces between the segments of the bilayer or membrane.

The activity r may be interpreted as $r \equiv \exp[-\beta \epsilon_h]$ with some horizontal energy cost, but if we reintroduce the lattice constant a_0, then we see that r^L may be profitably interpreted as

$$r^L = \exp[-\beta f a_0 L] \qquad (2.3)$$

where now L is a nondimensional integer and f is a *force* in the $x-$direction. Then $r > 1$ favoring large L implies a pulling force (which is negative) whereas $r < 1$ implies a compressing force (which is positive); $r = 1$ is the locus of the *tensionless states*.

We adapt to our purposes the general solution[27] for G

$$G = (r + q_- + q_+ - (r + 2)q_- q_+)/(1 - r - q_+ - q_- + q_- q_+(1 + r)) \qquad (2.4)$$

(with $w = 1$ as mentioned above). Without distinction between positive and negative vertical steps, i.e. with $q_- = q_+ = q$,

$$G_o = (2q + r + qr)/(1 - q - r - qr) \qquad (2.5)$$

With the condition of at least one horizontal step, G is[27]

$$G_1 = (r + qr)/(1 - q - r - qr) \qquad (2.6)$$

All three generating functions impose no restrictions on the final position (L, h_{last}) attained after all N steps;

$$h_{last} = n_+ - n_- + h_1 = n_+ - n_- . \qquad (2.7)$$

For strings with periodic boundary condition, taken with Fourier analysis in view, the walk is from $(0, 0)$ to $(L, 0)$, $h_{last} = 0$. The appropriate generating functions with this constraint embedded, are derived below.

The generating function G_o counts all horizontal L steps and all vertical A_v steps which produce configurations of the string; the latter can be gathered together in the combinatorial factor $g(L, A_v)$

$$G_o(q, r) = \sum_L \sum_{A_v} g_o(L, A_v) q^{A_v} r^L \qquad N = A_v + L \qquad (2.8)$$

and similarly G_1.

Canonical averages for an interface.

The shape fluctuations of an interface take place at L fixed and constant. The statistical averages, e.g. $\langle N \rangle = \langle A_v \rangle + L$ are calculated under this condition. From the generating functions, the Taylor expansion of the generating function

$$G_o = \sum_L Z(L, q) r^L \qquad (2.9)$$

produces the partition function $Z(L, q)$. The averages are found from

$$\langle A_v \rangle = q(d \log Z(L, q)/dq) \qquad (2.10)$$

and $\langle N \rangle = L + \langle A_v \rangle$. The vertical part of N, A_v, can be any nonnegative integer. In this way, for $L \geq 2$, from (2.5-2.6)

$$Z(L, q) = ((1 + q)/(1 - q))^{(L+1)}. \qquad (2.11)$$

The same Z obtains from G_1. The average total area N follows from (2.10)

$$\langle N \rangle = L + \langle A_v \rangle = L + 2qL/(1 - q^2). \qquad (2.12)$$

The areas are best represented by a normalized quantity $\mathcal{L} = L/N = L/(A_v + L)$; always $\mathcal{L} \in [0, 1]$. Rewriting (2.12)

$$\mathcal{L} = L/(L + \langle A_v \rangle) = f_1(q) = (1 - q^2)/(1 + 2q - q^2). \qquad (2.13)$$

This expression results from both G_1 and G_o. Since L is constant, $\mathcal{L}$ is $L/\langle N \rangle = L/(L + \langle A_v \rangle)$.

For the canonical averages at given q, r, i.e. without fixing L (or N) at a predetermined value, G_1 gives $f_1(q, r)$, (2.13) again; However, from G_o by using

$$\langle L \rangle = r(dG_o/dr)/G_o \qquad (2.14)$$

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one obtains

$$\mathcal{L}_o = o_1(q,r) = (1+q)^2 r / (2q + r + 2qr + q^2 r). \tag{2.15}$$

This does not differ much from (2.13) and is quoted only for completeness. The independent variables were L, q or q, r; the length N and A_v resulted as averages, so that $\mathcal{L}$ was $\langle L \rangle / (\langle L \rangle + \langle A_v \rangle)$.

Keeping the distinction between q_+ and q_- and expanding (2.1) in powers of r, we find $Z(L, q_+, q_-) = \Psi^L$ where

$$\Psi = \frac{1 - q^2}{1 - q_+ - q_- + q^2}. \tag{2.16}$$

and the expansion of Z is

$$Z(L, q_+, q_-) = \sum g(n_+, n_-, L) q_+^{n_+} q_-^{n_-} \tag{2.17}$$

The walk beginning at (0,0) and ending at (L, h_{last}) will have $h_{last} = h_{last} - h_1 = n_+ - n_-$. Let us call this quantity n. Then in the sum we insert a Kronecker Delta ensuring that $n = n_+ - n_-$; by using its Fourier representation, putting $q_+ = q_- = q$, we obtain

$$Z(n; L, q) = (1/\pi) \int_0^\pi dk \cos(n * k) \left(\frac{1 - q^2}{1 - 2q \cos(k) + q^2} \right)^m \tag{2.18}$$

where the power m is $L, L+1, L-1$ depending on the starting generating function. The result of integration depends on the inequality $(1 + q^2) > |2q|$ which is fulfilled for all $q > 0$ except for one point $q = 1$. This point approached from below corresponds to the infinite temperature in the interface models with $q = \exp(-\beta \epsilon_v)$, $\epsilon_v > 0$; approached from above corresponds to the infinite temperature in membrane models for which $\epsilon_v < 0$. For $n = 0$ in (2.18) we obtain the partition function for an interface with periodic boundary condition; it reads

$$Z(0; L, q) = P_{m-1}(u) \quad u \equiv (1 + q^2) / (\sqrt{1 - 2q^2 + q^4}) \tag{2.19}$$

Here $P_m(u)$ is the Legendre polynomial, $u \geq 1$. The normalized average area $\mathcal{L}$ is in this case $L/(L + \langle A_v \rangle)$ and $\langle A_v \rangle$ is calculated after (2.10) as $q(d \log Z / dq)$; we find then that we must take $q < 1$. Finally

$$\mathcal{L} = (1 + u - P_{L-1}(u)/P_L(u))^{-1}. \tag{2.20}$$

As we shall see below, this quantity behaves quite unlike those $\mathcal{L}$'s constrained by the total length $N = L + A_v$. It agrees very closely with $f_1(q, r)$.

Canonical averages for a membrane/bilayer.

Alternatively, treating the string as a membrane, we impose a fixed length N. This constraint is introduced into G's. The new generating function contains a selection of terms from (2.5), such that $L + A_v = N = const.$,

$$G(N; q, r) = \sum_{L=1}^{N} g(A_v = N - L, L) q^{N-L} r^L \quad N = A_v + L = const. \tag{2.21}$$

There are two cases possible: either all L compatible with given N are allowed, or both L and N are given prescribed values. In the latter case the expansion (2.21) reduces to one term, with $(A_v = N - L, L)$. From the expansion (2.8) of G_o, in powers of r and then q, we find $g_o(A_v, L)$; alleviating the notation by writing $a \equiv A_v$, we write the explicit result

$$g_o(a, L) = \sum_{m=0}^{a} \binom{L}{m} \binom{a - m + L - 1}{L - 1} \tag{2.22}$$

For $a > L$ the upper limit of the sum is L. With g_o known, we can construct the partition function Z_o as a polynomial in q and r,

$$Z_o(N; q, r) = \sum_{L=1}^{N} g_o(N - L, N) \times q^{(N-L)} \times r^L \tag{2.23}$$

by explicit substitution of (2.22) into (2.23). Now $\langle L \rangle$ and $\langle a \rangle$ follow explicitely by (2.10) and (2.14). The same procedure works for G_1. For these averages at $q, r; N$ always $\mathcal{L} = \langle L \rangle / (\langle L \rangle + \langle Av \rangle)$.

A direct and neat way is to introduce a new counting parameter t for every step whatever it is and expand

$$G_o(t; q, r) = (2qt + rt + qrt^2)/(1 - qt - rt - qrt^2) \tag{2.24}$$

in powers of t,

$$G_o(t; q, r) = \sum_{t=1}^{\infty} Z_N(q, r) t^N \quad (N = A_v + L). \tag{2.25}$$

Z_N is used for calculations of average $\langle L \rangle$ (which must be equal to $N - \langle A_v \rangle$.

Finally, pinning both ends of the string in order to have a possiblility of p.b.c., is done in two alternative ways: either we expand (2.4) in powers of t, select the coefficient

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of t^N which is $Z_N(q_+, q_-, r)$; substitute there $q_- \to q/e$ and $q_+ \to qe$, expand in powers of q and e and select the coefficient of e^0 - it is the partition function $Z_N(q, r)$ for both ends pinned, useful for p.b.c.. Alternatively, the equality of n_+ and n_- is enforced via a Kronecker Delta and its Fourier representation as an integral. Either way, its generating function is found with a rather unusual appearance

$$G_e(q,r) = r * \sqrt{B}; B \equiv (1 - q^2)/((1 - q - r - qr)(1 + q - r - qr)). \qquad (2.26)$$

To calculate the averages at constant N, the same procedure is used as for G_o. Put $q \to qt, r \to rt$, extract the Taylor series coefficient of t^N and use (2.10),(2.14). The resulting $le(q, r)$ depends on N.

These exact enumerations can be pushed very far to $N \gg 100$ - but then simple asymptotic expressions take over. These are derived now.

Both G_1 and G_o are positive and finite for small q and r; their divergences are determined by zeros of the denominators. This condition, $1 - r - q - qr = 0$, determines a line in the q, r plane cutting diagonally from $(0, 1)$ to $(1, 0)$. We write the denominator as $\alpha(t - t_1)(t - t_2)$ where $t_{1,2}$ are its roots and split G_1 as

$$G_1 = B_1/(t - t_1) + B_2/(t - t_2) \qquad (2.27)$$

The root t_1 is always positive and $t_1 < 1/r$; the other root is always negative. G takes largest values when t is close to t_1; expanding in powers of t (as $(1 - t/t_1)^{(-1)} = 1 + (t/t_1) + \cdots$) we see that the root $t_1 > 0$ is the one that matters. From this new form of G_1 we select the coefficient of t^N and calculate $\langle L \rangle$, taking the asymptotic limit of large power of t, i.e. large N. Finally we obtain

$$\mathcal{L} \equiv f_2(q, r) = (1/2) + (1/2)(r - q)/\sqrt{(r^2 + 6rq + q^2)} \quad N = const. \to \infty. \qquad (2.28)$$

This expression, like (2.22-2.24), is valid in the entire quarter-plane ($q \geq 0, r \geq 0$). $\mathcal{L}$ from G_o attains the same asymptotic result in the limit $N \to \infty$.

An important point is that the partition functions for fixed N (total area, or length of the string) $Z_N(r, q)$ are positive and well-behaved for all $q > 0, r > 0$ whereas the generating functions $G(r, q)$, the partition functions for fixed L, $Z(L, q)$ and the averages and fluctuations derived therefrom, are well behaved and physically acceptable only in certain regions of the quarter-plane.

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Fig.2 shows five functions $\mathcal{L}$: (1) the canonical average at given q, r, N, denoted as $ll(q, r)$; eq.(2.25),(2.10),(2.14); (2) as (1) but under the periodic boundary condition (i.e.pinning both ends at $h_{last} = h_1$) - function $le(q, r)$, eq.(2.26)ff; (3) the asymptotic limit of (1) for $N \to \infty$, denoted as $f_2(q, r)$, eq.(2.27). (4) the canonical average at fixed L (and given q), any N, any h_{last}; function $f_1(q, r)$, eq.(2.13). (5) as (4) but under the periodic boundary condition $h_{last} = h_1$; eq.(2.20).

In order to be physically acceptable, each $\mathcal{L}$ must be $\mathcal{L} \in [0, 1]$ and also the averages $\langle L \rangle$ and $\langle A_v \rangle$ must be positive. This selection of 5 functions $\mathcal{L}$ are shown plotted against q, for a series of values or r. The regions $q < 1$ and $q > 1$ are smoothly joined by all averages calculated at constant N. The function f_1 behaves quite differently: its physical branch is limited to the region $0 \leq q \leq 1$. f_1 does represent an interface; the other three - a membrane. Similarly under the periodic boundary condition $\mathcal{L}(q, L)$, (eq.2.20), for either $L = 10$ or $L = 140$ does not differ visibly (on the scale of the plot) from f_1; it also represents an interface. All functions start from $A_v = 0$ at $q = 0$ but the interface fluctuations give unbounded $\langle A_v \rangle$ at $q \to 1^-$ whereas the membrane fluctuations are bounded. The three constant-N functions $ll(q, r; N), le(q, r; N)$ and $f_2(q, r)$ cross smoothly the point $q = 1$; all three are not too far away from each other. In particular the asymptotic f_2 would be merged with the other two on the scale of the Figures if the plots were not drawn for a choice of small N.

The interval $0 \leq q < \infty$ is split in two and in Fig.3 amd 4 the plots are against inverse temperature, against $b = -log(q)$ for $q < 1$; against $b = log(q)$ for $q > 1$, respectively. In Fig.3 the limiting values for $b \to 0$ (the limit of high temperatures) depend on the parameter r, except for the two cases of fixed projected area L where the limit is $\mathcal{L} = 0$, as $L=$const. and $\langle A_v \rangle$ is unbounded. The point $b = 0^+$ corresponds to $q \to 1^-$. $f_2(q = 1, r)$ (eq.2.27) is continuous and $f_2(1, 1) = 1/2$. All curves, fixed N or fixed L, merge towards $\mathcal{L} = 1$ as b increases, i.e. $kT \to 0$. Obviously, $\langle A_v \rangle$ vanishes there. In Fig.4 the function f_1 is shown and how it takes unphysical values either negative or larger than 1. The other $L-$fix average(eq.(2.20) is also unphysical in this region, unlike the three constant-N functions. At very low temperatures all three $\mathcal{L}$'s tend to zero because A_v dominates; $q \gg 1$ favors configurations with many folds for which $A_v \gg L$.

We have chosen to convert all averages to $\mathcal{L}$'s for convenience but in this way some dramatic differences in behaviour are hidden from view. Thus $\mathcal{L} = 0$ implies unbounded

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A_v at finite L or vanishing $\langle L \rangle$ at finite A_v; $\mathcal{L} = 1$ if $A_v = 0$. In the limit of high temperatures, the interfacial averages, i.e. those taken at constant L, diverge, whereas the membrane averages i.e. those at constant N, produce finite values (depending on r).

Next we change the role of variables and plot below in Fig.5 the same functions against r at several constant values of q; the logarithic scale implies that we choose force $f = -\log(r)$ as the independent variable (the ordinate).

A boxed membrane.

In simulations most often not only the number of molecules forming the bilayer/membrane is kept constant, but also the membrane or bilayer is confined to the simulation box of dimensions $L_x \times L_y \times L_z$. For our model this implies that not only N is given and constant but also L. Because in this particular model the sum $A_v + L$ coincides with N, at any given temperature the partition function and the free energy are

$$Z = g(A_v, L)q^{A_v} \quad (A_v = N - L, N = const., L = const.) \tag{2.29}$$

$$\beta F = -\log g(A_v, L) - A_v \log q \tag{2.30}$$

The activity $q \equiv \exp[\epsilon/kT] > 1$. For comparison, a boxed interface in an identical simulation box, does not keep $A_v + L$ constant and therefore

$$Z_{int} = \sum_a g(a, L)q^a \quad (L = const.) \tag{2.31}$$

$$\beta F_{int} = -\log Z_{int} \tag{2.32}$$

The lateral tension of the membrane results as

$$\hat{\Gamma} = (\frac{\partial F}{\partial L})_{T,N} = -(1/g)(dg/dL)_N \tag{2.33}$$

The derivative dg/dL of $g(A_v, L)$ is taken at constant N . Fig.5 shows $\mathcal{L}$ for a series of q's with constant N plotted against the negative of the force $(-f) = \log(r)$. The asymptotic $f_2(q, r)$ (for $N \to \infty$) is also included - it has very much the same shape, only shifted along the ordinate according to the value of q, just like all the finite$-N$ curves. For comparison also $\hat{\Gamma}$ from finite differences $(\Delta g/\Delta L)_N$ is shown demonstrating the equivalence of ensembles. The continuity w.r.to q is also seen. The pulling force raises $\langle L \rangle$ as expected and conversely; the effect of q is to shift the entire curve

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$L(f)$ to the right or to the left, without much of a visible change of shape. This can be understood by looking at the maximum term in the canonical sum for which the condition is $(d \log g/dL)_N = -f - \log q$. The parameter q shifts the curve $f^*(L)$ by a constant amount.

III. Summary and Discussion.

The model allows explicit calculations in terms of simple algebra. Its use made it possible to demonstrate the role of the membrane-constraint in the statistical mechanics of membranes or/and bilayers. The constraint of constant particle number in the membrane - no particle loss or gain to or from the surrounding solvent - calls for a corresponding approach in the calculation of the membrane thermal fluctuations. In this model this translates into a constant length of the string. Such a constraint is most natural for modelling of a polymer and we expect that the calculations for a twodimensional membrane embedded in three dimensions, will be in effect calculations for a two-dimensional polymer.

In the course of calculations we have found that relaxing the constraint of constant N and replacing it by a constraint of a fixed projection area L, leads to a very different behaviour of the averages and - a posteriori obviously - modelling the fluctuations of an interface. Thus in the same model we have the region $q > 1$ inaccessible to interfaces but typical for a membrane - and the region $q < 1$ typical for interfaces and also accessible for a membrane with a changed sign of the energy of interaction.

The equivalence of ensembles operates fully in the limit of infinite systems but not for finite sizes.

The force, pulling or compressing the string, has a direct analogy in three dimensions, as the lateral tension of the bilayer. Cutting a suitably chosen part of an S-shaped curve from Fig.5, one can get a picture very similar to the "bilayer isotherm" (which is a plot of lateral tension against the projected area). Curiously, a non-symmetric derivative $(dg/dL)_N$ i.e. $(g(L_0 + 1) - g(L_0))/g(L_0)$ assigned to the point L_0, produces such curves.

Because the string is confined to the square lattice, it has an implicit resistance to bending which is also seen in the play of the parameter w. The latter has been introduced in the generating functions of the PDSAW[27] in the form of w^T where T is the number of turns; see also[28−30]. Clearly $w \gg 1$ will favor the occurence of multifolded configurations with many turns - very low bending coefficient, low resistance to bending.

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Conversely, $w \to 0$ will favor "no turns" i.e. flat membranes which are obtained with large bending coefficients - large resistance to bending. Thus it follows that our choice of $w = 1$ does not mean "zero bending coefficient" - and the explanation lies in the implicit resistance to bending imposed by the lattice. The notions of "semiflexible" and "super-flexible" strings have been introduced[28−30].

In this context it becones necessary to mention the existence of a sizable amount of very successful work on exact enumeration - for models of polymers as strings confined to a lattice[28−34]. References to earlier work can be found there as well. However, the issues tackled in this paper were not touched in those References, where the emphasis was entirely on the important topics of phase transitions, singularities, and critical scalings.

Although the usual picture of a membrane assumes an attractive interaction between its segments - which leads to $q > 1$, it is possible to envisage a string held together by other (intramolecular) forces while the segments repel each other or a good solvent encourages extended configurations; this leads to $q < 1$ - still a membrane if N is held constant.

Incidentally we also confirm the view[26] of the tensionless state $f = 0, r = 1$ as just another point on the r axis or line on the q, r plane without any special features. Contrariwise, $q = 1$ is a very special point as discussed in Section II and shown in the Figures.

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Figure Captions.

Caption to Fig.1

The string produced by a random walk on the square lattice. The x coordinate measures the projected distance-area L, the y-coordinate is called "height" in the text. Here the walk starts at $h_1 = 0$ and ends at $h_{last} = h_1$. In the Figure the number of "horizontal" steps is 14, $n_+ = n_- = A_v/2 =$, and the walk is a PDSAW.

Caption to Fig.2

Normalized $\mathcal{L}$, $\langle L \rangle/N$, $\langle L \rangle/\langle N \rangle$ or $L/\langle N \rangle$, as function of q, r, plotted against $q \in [0, +\infty]$ for several values of r. Thick solid line: function f_1 eq.(2.13) - unrestricted canonical average at given (q, r) coincidentally equal to average at fixed L. Diamonds: fixed $L = 140$ and pinned at $h_1 = h_{last} = 0$ (for the p.b.c.);eq.(2.20). Membrane averages for fixed N: thin broken lines - asymptotic function $f_2(q, r)$ eq.(2.27); thick broken lines - function $le(r, q)$, eq.(2.26) and ff. text; thin lines - function $ll(q, r)$ - canonical average under the constraint of imposed value of N; here a small value of $N{=}10$ is chosen to emphasize the differences. All three $\mathcal{L}$'s are moving smoothly with change of the parameter r; the Figure shows $r = 0.1, 1., 9., 30.$ from lowest values to highest. See text.

Caption to Fig.3

Normalized $\langle L \rangle/N$ or $\langle L \rangle/\langle N \rangle$ or $L/\langle N \rangle$ plotted against inverse temperature $b = -\log q = \epsilon/kT$ for $0 < q < 1$. See Caption to Fig.2.Thick solid line: function f_1 eq.(2.13), fixed L; Diamonds: fixed $L = 140$ and p.b.c. ($h_{last} = 0$), eq.(2.20); the differences with f_1 cannot be seen on the scale of this graph. Thin broken lines - asymptotic function $f_2(q, r)$ eq.(2.27); thick broken lines - function $le(r, q)$, eq.(2.26) and ff. text; thin lines - function $ll(q, r)$ both for a small value of $N{=}10$. The high-temperature limits depend on r, q, except for fixed L averages where the limit is zero. The low temperature limit is unity for all five $\mathcal{L}$'s.

Caption to Fig.4

Normalized $\langle L \rangle/N$ or $\langle L \rangle/\langle N \rangle$ or $L/\langle N \rangle$ plotted against inverse temperature $b = +\log q = \epsilon/kT$ for $1 < q < \infty$. see Caption to Fig.2,3. Thick solid line: function f_1 eq.(2.13), fixed L ; all values unphysical. The other $\mathcal{L}$ at constant N: with thin broken lines - asymptotic function $f_2(q, r)$ eq.(2.27); thick broken lines - function $le(r, q)$ for pinned string, eq.(2.26) and ff. text; thin lines - function $ll(q, r)$ for floating string -

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both for a small value of $N=10$. The high-temperature limits vary with r, q. ?The low temperature limit is unity for all three averages under constant N. ?The low temperature limit is zero, as $q \gg 1$ favors multifolded configurations with $\langle A_v \rangle$ dominating over $\langle L \rangle$. See text.

Caption to Fig.5

Plot of $\mathcal{L}$ at selected values of q against r. The logarithmic scale for r produces the negative of force $-f = \log[r]$. $N = 40$, $q = 0.01, 0.1, 0.5, 0.9, 1, 100, 10^4$ (thin lines in the sequence from left to right). Change of q shifts without change in shape (see text). One asymptotic $f_2(q, r)$, eq.(2.27), is shown with a thick line. Diamonds and crosses: force from eq.(2.33) for boxed interface with $N = 40$ and $N = 60$; triangles for $N = 40$ with a different interpolation of $(1/g)(dg/dL)_N$. Also see text.