

MONTE CARLO STUDY OF A STACK OF SELF-AVOIDING SURFACES WITH EXTRINSIC CURVATURE STIFFNESS [☆]

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Stacks of fluctuating self-avoiding surfaces with extrinsic curvature stiffness show a fundamental pressure law analogous to the ideal gas law $pV = Nk_B T$ for point particles, namely $p = 2\alpha(k_B T)^2/\chi d^3$ (T = temperature, d = distance, χ = stiffness). We present a precise determination of the constant α and find $\alpha \approx 0.101 \pm 0.002$ thereby improving considerably upon an earlier number.

Much attention has recently been paid to surfaces with extrinsic curvature stiffness ^{#1} to be denoted shortly as SS's (for "stiff surfaces"). They seem to represent the sheets of color electric flux tubes between quarks in a much better way than surfaces equipped with tension only [2]. Their fluctuations have the desirable feature of being asymptotically free in the ultraviolet [1,2] so that they are able to generate a tension spontaneously just as in QCD. SS's are known to be predominant also in many other systems appearing, e.g., as domain walls in magnets, as oil water interfaces in microemulsions or as biological membranes. While the fluctuation properties of a single nearly flat SS have by now been studied up to the two-loop level in any dimension D [3] and exactly in the limit $D \rightarrow \infty$ [4], the behaviour of grand canonical ensembles of SS's is still understood quite poorly. The reason is the complexity of the functional integrals over arbitrary topologies and the many possibilities of local interactions between different surface elements. So, any limited information on multisurface systems is of potential use.

Some time ago, a simple model has been devised by two of us (J.K.) [5] that allows studying an extreme limit of these local interactions in the form of self-avoiding SS's, to be called SSS's. This was done for the particularly simple geometric configuration of

a stack of closely spaced surfaces in a box. For linearized curvature energies, the Janke-Kleinert partition function reads

$$Z = \prod_{n=1}^N \int \left(\frac{du_n(\mathbf{x})}{d} \right) \exp\left(-\frac{\chi}{2T} \sum_{n,x} (\bar{\nabla} \cdot \nabla u_n)^2\right), \quad (1a)$$

$$0 < u_1 < u_2 < \dots < u_N < (N+1)d, \quad (1b)$$

where $u_n(\mathbf{x})$ are the vertical positions of the n th surface ($n = 1, \dots, N$) over a flat background area \mathbf{x} which is approximated by an $L \times L$ square lattice of spacing a ($\bar{\nabla} \cdot \nabla$ is the usual lattice laplacian and the Boltzmann constant is taken as $k_B = 1$).

The gaussian parametrization of the surfaces ensures the intrinsic self-avoidance of each individual surface, and the inequalities (1b) guarantee mutual avoidance between the surfaces, so that there is complete self-avoidance of the ensemble. For $N=1$ we have the particularly simple model of a single SSS in a box.

A simple rescaling argument presented in ref. [5] shows that Z depends on its parameters in the following way:

$$Z \equiv Z_{\text{free}} \cdot Z_{\text{int}} \equiv \tau^{NL/2} \cdot Z_{\text{int}}(\tau, \tau/L^2), \quad (2)$$

where τ is the dimensionless variable $\tau \equiv TA/\kappa d^2$ with $A = a^2 L^2 = \text{base area}$.

One therefore only needs to study the model, for any given N at any fixed A, d as a function of the single variable T . The additional free energy per layer

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^{#1} They were investigated originally in membrane physics [1].

generated by the self-avoiding constraint (1b) is

$$\Delta F/T \equiv -(\ln Z - \ln Z_{\text{free}})/N.$$

In a large system, $A \rightarrow \infty$, it possesses the obvious asymptotic expansion in τ/L^2

$$\Delta F/T = \alpha\tau(1 + \frac{1}{2}a_1\tau/L^2 + \frac{1}{3}a_2\tau^2/L^4 + \dots) \quad (3)$$

(with exponentially small terms, $\sim \exp(-L^2/\tau)$ missed). The expansion is valid only for large area A so that $1 \ll \tau \ll L^2$. If τ is close to 1, there are also corrections of the type $\exp(-\tau)$ [6]. For the internal energy per layer, (3) implies

$$\begin{aligned} \Delta E/T &= \tau \partial(-\Delta F/T)/\partial\tau \\ &= -\alpha\tau(1 + a_1\tau/L^2 + a_2\tau^2/L^4 + \dots). \end{aligned} \quad (4)$$

The pressure $p = -\partial(N\Delta F)/\partial V$, with $V \equiv (N+1)dA$ being the volume of the total stack, is directly proportional to (4), namely

$$p = 2 \frac{N}{N+1} \frac{T}{Ad} \left(-\frac{\Delta E}{T} \right)$$

(the factor $N/(N+1)$ accounting for the difference between the number of layers and that of spacings).

The choice of the variables τ and L has the obvious advantage that for fixed τ (i.e. fixed T/χ which, incidentally, is in biological membranes at room temperature $\approx \frac{1}{5}$), also the geometry A/d^2 is fixed, so that the limit $L \rightarrow \infty$ is also equivalent to the continuum limit in the lattice spacing, $a \rightarrow 0$ (with the area $A = a^2L^2$ fixed).

The internal energy can easily be measured by Monte Carlo simulations. In an earlier [5] work, the authors took advantage of the fact that they possessed previous simulation data of a related $D=2$ defect melting model [7] which could trivially be extended to a multilayer system. The data could be reinterpreted to extract a first estimate of the number α , namely $\alpha \approx 0.074$, about three times smaller than Helfrich's [8] original quasi-harmonic estimate $\alpha = 3\pi^2/128 \approx 0.23$. As convenient as it was, however, the use of the melting model introduced a quantitative source of error since it was formulated with finite steps in $u_n(\mathbf{x})$. This error was assumed to be small, since the measurements were done far above the laplacian roughening transition, where the discreteness becomes irrelevant. In the present paper we eliminate this source of error and report a value of α

with an extremely high accuracy. This is achieved by means of a detailed finite step-size, finite N , and finite-size L analysis of the system and separate runs with continuous $u_n(\mathbf{x})$'s, using the Metropolis algorithm^{#2}. It turns out that removing the steps in $u_n(\mathbf{x})$ increases α by the sizeable amount of $\approx 30\%$ to

$$\alpha = 0.101 \pm 0.002 \quad (N = \infty). \quad (5a)$$

For $N=1$, the previous discrete u estimate $\alpha \approx 0.060$ is raised by about the same fraction to

$$\alpha = 0.079 \pm 0.002 \quad (N=1). \quad (5b)$$

Let us start with the $N=1$ case using, as before, discretized displacements $u(\mathbf{x}) \equiv u_1(\mathbf{x}) = h(\mathbf{x})/h_{\text{max}}$ with integer-valued $h(\mathbf{x}) \in [-h_{\text{max}}, h_{\text{max}}]$. We investigate the dependence on h_{max} of the internal energy ΔE for h_{max} between 3 and 15. Fig. 1a shows $(\Delta E/T)/\tau = -(\alpha + \alpha_1\tau + \dots)$ plotted versus $\tau/16^2$, on a 16×16 square lattice. We have divided out the lattice size, 16^2 , so that $\tau/16^2$ is of unit order of magnitude. In these runs, at least 50000 configurations were used for measurements after discarding 10000 sweeps for thermalization. For updating the discrete displacements we employed the standard heat-bath algorithm which is straightforward to implement in this case. Our error bars are estimated by dividing each run into blocks of several sweeps, calculating the block-average, and taking the variance of these partial energies. By varying the block-lengths, we checked that the block-averages are sufficiently uncorrelated to allow for reliable error estimates. Since the intercept of smooth fits through the data in fig. 1a corresponds directly to the pressure coefficient α , it is easy to see that our new, much more accurate data for $h_{\text{max}}=5$ are consistent with our former measurements.

The new data show a strong dependence on the step-size even for larger h_{max} . This is why we decided to simulate the system once more with continuous $u(\mathbf{x})$'s using the standard Metropolis algorithm. The result is fitted well by the solid curve whose intercept gives $-\alpha$ (and whose slope gives $-\alpha_1$). The corrections due to the discreteness of $u(\mathbf{x})$ die out only like $1/h_{\text{max}}$. This is demonstrated in fig. 1b where we plot

^{#2} The algorithm consists of choosing trial values for new $u_n(\mathbf{x})$'s randomly from an interval $[u_n(\mathbf{x}) - \Delta u, u_n(\mathbf{x}) + \Delta u]$ at each site. The parameter Δu was adjusted to ensure an overall acceptance around 50%.

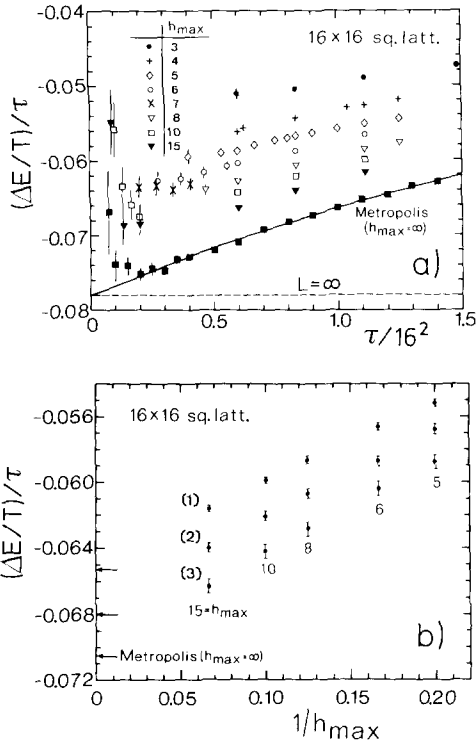


Fig. 1. (a) $(\Delta E/T)/\tau$ versus $\tau/16^2$ for discrete displacements with h_{\max} ranging from 3 to 15. Note that the intercept of the smooth interpolation gives directly the value of the pressure coefficient α . Also shown is the limiting case $h_{\max} \rightarrow \infty$ (with continuous displacements). The solid line is a fit of these data in the range $\tau/16^2 = 0.4-1.5$ to the form $-\left[\alpha + \bar{\alpha}_1 \tau/L^2 + \bar{\alpha}_2 (\tau/L^2)^2\right]$ with $\alpha = 0.078$, $\bar{\alpha}_1 = -0.0137$, $\bar{\alpha}_2 = 0.0020$. The dashed line indicates the spatial continuum limit $L \rightarrow \infty$, for fixed $\tau \equiv TA/\kappa d^2$. (b) Dependence of $(\Delta E/T)/\tau$ on the step-size of discrete displacements for $\tau/16^2 = 1.1111$ (1), 0.8333 (2), 0.6 (3). Straight line extrapolations to $1/h_{\max} = 0$ are consistent with the results for continuous displacements, indicated by the arrows at the y-axis.

$(\Delta E/T)/\tau$ versus $1/h_{\max}$ for three values of $\tau/16^2$. Obviously, simple straight line extrapolations to $1/h_{\max} = 0$ are consistent with the simulations with continuous displacements, indicated by arrows on the ordinate.

In the latter simulations we averaged, for most temperatures, the results of two runs with different start configurations (typically an ordered, random, or gaussian distribution). Each run consisted of averages over at least 500 000 configurations, after discarding 100 000-250 000 sweeps for thermalization. We further performed a finite-size scaling study

(which is simultaneously a continuum limit study) of $\Delta E/T$ on square lattices of linear size $L = 12, 16, 24, 32, 48$ (see fig. 2a, notice that we have kept the same x-axis as in fig. 1a for an easier comparison). For each lattice-size separately, we have fitted the data in fig. 2a to a polynomial $p(\tau) = -(\alpha_{-1} + \alpha\tau +$

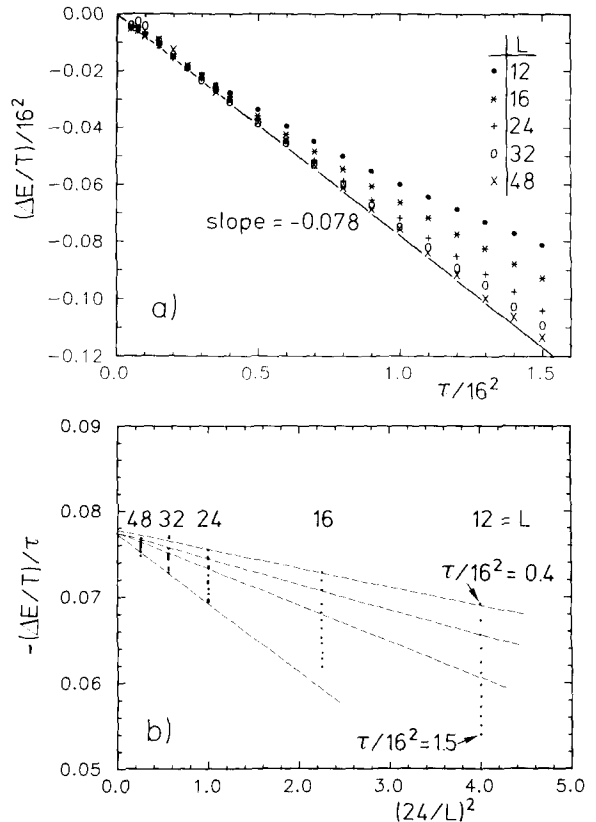


Fig. 2. (a) $\Delta E/T$ versus $\tau/16^2$ on square lattices obtained in the simulations with continuous displacements. For fixed $\tau \equiv TA/\kappa d^2$, increasing the number of lattice sites, L^2 , corresponds to approaching the continuum limit. This is shown as a straight line with slope $-\alpha = -0.078$, determined from fits to the data as explained in the text. With $T/\kappa = \frac{1}{5}$, one finds in the range $\tau/16^2 \approx 0.3-1.0$ the ratio $\sqrt{A}/d \approx 20-36$, i.e. the linear size of the basis plane is indeed much larger than the layer spacing. In this range, $L=48$ is almost sufficient to reach the continuum limit. For $\tau < 1$ (i.e. very small $\tau/16^2 < 0.004$), deviations from the simple linear law are expected due to physical finite-size effects ($A < (\kappa/T)d^2$ at fixed κ/T). (b) Scaling of the data in (a) with $1/L^2$ for fixed τ . Since we have scaled the ordinate by τ , it gives directly the slope of the straight line in (a). This plot confirms that extrapolations of the data in (a) along the vertical direction to $L = \infty$, reproduce the linear continuum law $\Delta E/T = -\alpha\tau$ with $\alpha = 0.078$.

$\alpha_1 \tau^2 + \dots$) where $\alpha_1 \sim 1/L^2$, $\alpha_2 \sim 1/L^4$, ..., parameterize the deviations from continuum behaviour. Performing ANOVA (analysis of variance) tests [9], we determined the optimal degree of our polynomial ansatz and verified that $\alpha_{-1} = 0$ is statistically significant. Since we do not observe any definite trend of α as function of L , we are able to give as final result for α , from an average over the five lattices studied, the very accurate value

$$\alpha = 0.078 \pm 0.001 \quad (N=1, \text{ square lattice}). \quad (6a)$$

The graphical $1/L^2$ extrapolations for fixed τ , shown in fig. 2b, confirm this value. We then checked the dependence of our result on the use of a square lattice by doing the same analysis once more on a triangular lattice with sizes $L=12, 24, 48$. Here we find the value, consistent with (6a),

$$\alpha = 0.080 \pm 0.001 \quad (N=1, \text{ triangular lattice}). \quad (6b)$$

Combining (6a) and (6b) we arrive at the result quoted in (5b).

Let us now turn to our simulations of stacks of surfaces (with continuous u 's). Guided by the experience with the $N=1$ case we confined ourselves to a 24×24 square lattice. Data were taken in a thermal "half"-cycle starting at large τ with 500000 sweeps for measurements and 100000 sweeps for equilibration at each temperature. With stabilizing walls at $z=0$ and $z=(N+1)d$, the number of layers was varied between $N=3, 5, 7$. Measurements of the average spacings of the layers confirmed the intuitive expectation that a neighboring SSS is slightly more repulsive than a neighboring wall. For small N , the layer-layer distance is about 25% larger than the wall-layer distance. We have therefore replaced the naive distance d by the true, measured layer-layer distance d_{\parallel} in all formulae. Furthermore, for all N we have used in our final analyses only the data for the central SSS. Since it is always in contact with two other fluctuating SSS's the addition of further outer SSS's has negligible influence apart from decreasing further the mean layer-layer distance. This picture is completely consistent with our data for the innermost SSS, plotted in fig. 3, which cluster around a common curve, after the abscissa is corrected for the increased layer-layer distance, i.e. $\tau \equiv TA/\chi d^2 \rightarrow \tau^{\text{corr}} \equiv TA/\chi d_{\parallel}^2$, as just explained. Fitting the data for each N separately

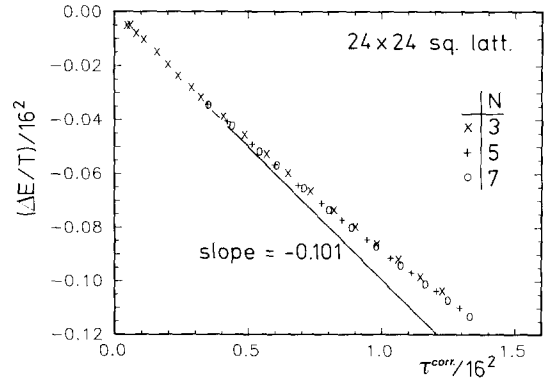


Fig. 3. $\Delta E/T$ for the central surface in stacks with $N=3, 5$ and 7 layers. Here, $\tau^{\text{corr}} \equiv TA/\chi d_{\parallel}^2$ with $d_{\parallel} (\approx d+25\%)$ the measured distance of the central surface to its neighbors. As in fig. 2a, the straight line with slope -0.101 shows the continuum limit determined from various fits (see the text).

with the polynomial ansatz $p(\tau)$, we find^{#3} $\alpha = 0.1002(6), 0.1022(6), 0.1009(7)$ for $N=3, 5, 7$, showing indeed no systematic N dependence. As a final result, we then give the average of these values and find the number quoted in eq. (5a).

Let us also mention that we have performed some comparative runs with periodic boundary conditions in the vertical direction (N SSS's distributed over a circle). In this case the average layer-layer distance is fixed to the initial d , so that all SSS's are on the same footing. This increases the available statistics by a factor of N . Unfortunately, however, the estimates for α using up to $N=10$ layers turn out to depend linearly on $1/N$ (as can easily be understood theoretically), so that it is much more economic to work with the fixed-wall case combined with the above distance corrections.

We close by remarking that although α is a fundamental constant of SSS physics, it will not be easy to measure it in real membrane systems. The non-linearities in the curvature energy with their asymptotic freedom cause a very fast crossover of the $1/d^3$ pressure law to an exponential falloff over a length scale of a few membrane thicknesses [10]. Thus there really is too little distance to see a clean $1/d^3$ dependence.

^{#3} The numbers in parentheses are the errors in the last digit.

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