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Triangular Lattice Foldings—a Transfer Matrix Study.

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Abstract. – Connection between discrete and continuum models of polymerized (tethered) surfaces has been investigated by applying a transfer matrix method to a discrete rigid-bond triangular lattice, which is allowed to fold on itself along its bonds in a two-dimensional embedding space. As its continuum counterpart, the model has an extensive entropy and the mean squared distance between two sites of a folded lattice increases logarithmically with the linear distance between the sites in the unfolded state. The model lattice with bending rigidity remains unfolded at any finite temperature, unlike real polymerized surfaces.

Properties of polymerized or tethered membranes (surfaces) have been an object of numerous recent studies [1-6]. We can view the polymerized surfaces as a generalization [1] of linear polymers [7]. This analogy has been used [3] to investigate the properties of self-avoiding tethered surfaces. However, unlike in the linear polymers, the long length-scale behavior of tethered surfaces strongly depends on the details of the Hamiltonian. In particular, very rigid surfaces exhibit a nontrivial [6] flat one. As the rigidity of a surface changes it undergoes a second-order phase transition [1, 4, 5] from a crumpled (linear-polymerlike) phase to a flat phase. Neither the flat phase nor the crumpling transition has an analogy in linear polymers.

The theoretical treatment of long length-scale properties of *linear* polymers rests on a firm foundation, since in the absence of self-avoiding (excluded volume, steric) interactions their properties can be calculated exactly. In particular, it can be shown that the end-to-end distance (both in continuum and on a discrete lattice) of a long polymer described by any local Hamiltonian obeys the Gaussian probability distribution. Thus on sufficiently long length-scales the polymer can be described by an effective Hamiltonian $H_1 = = Kk_B T \int dx(d\boldsymbol{r}/dx)^2$, where $\boldsymbol{r}$ is the position of a monomer in the d-dimensional embedding space, while x is the *internal* coordinate (label) of a monomer.

A straightforward generalization of H_1 assumes that at long length-scale two-dimensional ($2d$) polymerized membranes without self-avoiding interactions will be described by $H_2 \equiv Kk_B T \int d^2x(\nabla \boldsymbol{r})^2$, where x is the *internal* coordinate of a monomer, *i.e.* its position in the $2d$ network, while $(\nabla \boldsymbol{r})^2 \equiv (\partial \boldsymbol{r}/\partial x_1)^2 + (\partial \boldsymbol{r}/\partial x_2)^2$. This expression has indeed been confirmed by Monte Carlo simulations and by an approximate Migdal-Kadanoff renormalization group treatments for a $2d$ network embedded in a continuous three-dimensional space for several types of intermonomer potentials [1], and has been used as a starting point in the theoretical treatment of self-avoiding membranes [3]. The validity of H_2 also has been demonstrated in the limit of the infinite embedding dimension for quite a large class of models [8]. Obviously this cannot be a general result for an arbitrary microscopic Hamiltonian in an arbitrary embedding space dimension, because the mere presence of the crumpling transition and of the flat phase indicates that the longh length-scale limit does depends on the details of the microscopic Hamiltonian. One may also question the equivalence of discrete and continuum models, and wonder whether a situation resembling roughening transition in solid interfaces [9] may also be present in tethered surfaces. Actually, one can easily find a discrete example of a different behavior [4]: consider a two-dimensional square lattice embedded in two dimensions and free to fold on itself along its bonds. The folds of the lattice can be only along infinite straight lines, thus, configurations of such a lattice can essentially be represented by an external product of two one-dimensional random walks. The number of distinct folded configurations of a finite $L \times L$ lattice is 4^L, meaning that the entropy of the system increases as its *linear* size and therefore the entropy per unit area vanishes as $L \to \infty$. The mean-squared distance $\langle r^2 \rangle$ between two points of the lattice increases linearly with the internal separation w between the points, as opposed to the prediction $\langle r^2 \rangle \sim \ln w$ following from the continuum Hamiltonian H_2. If one introduces a bending rigidity by assigning energy $\varkappa$ per unit length of a fold, one can easily see that the lattice remains flat at any finite temperature T, because the energetic cost of a single fold $\varkappa L$ cannot be offset by the gain in the entropy. One may wonder, whether such a pathological behavior of a square lattice characterizes all discrete systems.

We consider all possible foldings of a $w \times L$ parallelogram excised from a triangular lattice in the limit $L \to \infty$. Figure 1*a*) depicts such a lattice before the folding, while fig. 1*b*) shows the same lattice in the folded state. Each site of the lattice is identified by a number. Each permitted folding, which maintains the correct distances between the neighboring sites, is assumed to have the same weight. Two configurations are identical if the positions of all corresponding sites coincide. (We disregard the differences caused by a uniform translation, rotation or inversion of the entire lattice.) Our definition of the identical configurations does not distinguish between the different manners of folding which lead to the same final state. The bold lines in fig. 1*a*) indicate the positions of the folds required to create the configuration in fig. 1*b*). The «+» and «−» signs indicate the «up» or «down» orientation of the triangles in the folded configuration. While the signs in fig. 1*a*) resemble Ising variables, the set of all possible configurations, obviously, cannot be obtained by

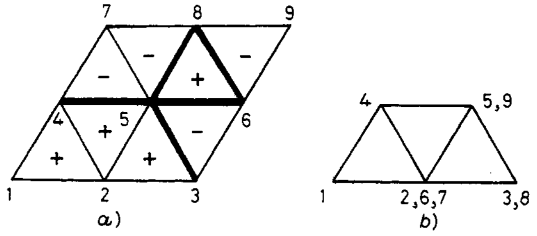

Fig. 1. – Triangular lattice in *a*) unfolded and *b*) folded states (see text).

applying a local construction rule to those variables. On the other hand, we may consider six bonds entering a particular site (*e.g.* site 5 in fig. 1*a*)): each bond can be either folded or not. However, one can easily verify, that out of 64 possible surroundings of such a site only 11 local environments are permitted. Thus one may attempt to construct the configurations using 11-state «Potts variables» assigned to the sites. Unfortunately, even such a description requires a nonlocal rule, although the nonlocality is much more subtle, than in the «Ising-like» description. (Details will be given elsewhere [10].) It seems that the nonlocality is inherent in this problem, and the only reasonable (but extremely inconvenient) description of a configuration consists of an explicit list of all folds which have been made.

We resorted to a thermodynamic transfer matrix method (see, *e.g.*, ref. [11]) to investigate the properties of lattice foldings. This method permits an *exact* solution of an *infinite* strip of a finite width w. By comparing the results obtained for various values of w we extract the results for an infinite triangular lattice. The folded configuration can be described as follows: consider a set of all parallel lines in the original lattice, such as the line joining sites 1-2-3, line 4-5-6 and line 7-8-9. The configuration can be described by giving the shape of each of these lines in the folded states, as well as their relative positions and orientations. The shape of a single line can be described by listing the «turns» it makes in the folded state. A pair of neighboring bonds can either be parallel or form a $\pm 2\pi/3$ angle. The shape of a line of length w is given by $w-1$ numbers describing the relative orientations of bond pairs. The relative position and orientation of two neighboring lines is determined by the (up or down) orientation of two triangles situated between the first bonds of the lines. *E.g.*, the relative position and orientation of lines 1-2-3 and 4-5-6 in fig. 1 is given by the orientation of the triangles 1-2-4 and 2-5-4. Each line can be in $4\cdot 3^{w-1}$ states, and the folded configuration is described by a list of all states. Transfer matrix element $T^{(w)}_{\alpha\beta}$ is 1 if the two neighboring lines are permitted to be in the states α and β, and vanishes otherwise. Whether or not $T^{(w)}_{\alpha\beta}=1$ can be determined by a direct examination of the two lines [10]. A folded configuration consisting of the lines in states $\alpha_1\alpha_2\alpha_3\ldots\alpha_L$ is permitted only if $T^{(w)}_{\alpha_1\alpha_2}T^{(w)}_{\alpha_2\alpha_3}\ldots T^{(w)}_{\alpha_{L-1}\alpha_L}=1$. The total number of permitted states $N_L^{(w)}$ is obtained by summation of this product over all values of all α_i. Thus $N_L^{(w)}$ is essentially a sum of all elements of a matrix obtained by multiplying $L-1$ matrices $T^{(w)}$. If the largest eigenvalue $\lambda(w)$ of $T^{(w)}$ is not degenerate (as indeed is the case [10]), then, for a very large L, the result will be solely governed by that eigenvalue: $N_L^{(w)}\sim\lambda^L$. Thus the total number of states in an infinite strip of width w is determined by λ. We found the largest eigenvalues of $T^{(w)}$ for strip widths $w=2, 3, \ldots, 7$. (The matrices have several symmetry properties which can be used to reduce the size of the matrix which actually needs to be diagonalized [10].) Figure 2 depicts the w-

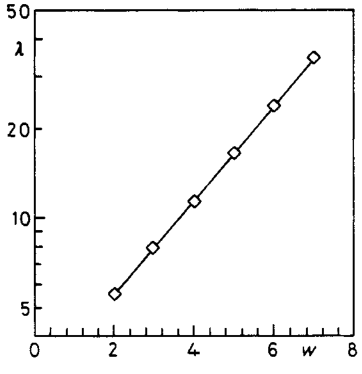

Fig. 2. – Largest eigenvalue λ of the transfer matrix *vs.* the width w of the infinite strip.

dependence of λ on a semilogarithmic scale. If the entropy of the lattice is extensive we expect $N_L^{(w)} \sim \exp[\gamma wL] \equiv q^{2wL}$, with $\exp[\gamma w] = \lambda$. From fig. 2 we find $\gamma = 0.386 \pm 0.002$, *i.e.* each triangle in a large lattice can «on the average» be in $q = 1.21$ states. Thus, the number of states increase exponentially with area as one would expect in a continuum system, and as opposed to the result of a square lattice where $\gamma = 0$.

One may apply a similar method to determine the mean square width $\langle r^2 \rangle$ of the infinite strip. If the squared end-to-end distance of a line (across the strip) in the state α is r_α^2, then, for a very large L, the ensemble average $\langle r^2 \rangle = \sum_\alpha \tilde{v}_\alpha r_\alpha^2 v_\alpha$, where v and $\tilde{v}$ are the (bi-normalized) left and right eigenvectors of $T^{(w)}$ corresponding to the largest eigenvalue λ_w. We calculated $\langle r^2 \rangle$ for $2 \leqslant w \leqslant 7$ and found a logarithmic dependence $\langle r^2 \rangle = B \ln w$, with $B \approx 0.6$. This result is, again, consistent with the prediction of the continuum Hamiltonian H_2.

So far the results of the discrete model were consistent with our expectations for the behavior of a polymerized membrane. However, an introduction of bending energy proportional to the total number of folded bonds, produces a situation, which is different from the regular case of rigid membranes: the lattice remains «flat», *i.e.* unfolded, at any finite temperature. Like in the case of a square lattice, the lowest-energy excitations (folds) require energy proportional to the linear dimensions of the system, and that cost cannot be offset by entropy. Unlike the square lattice, in already folded configurations it is possible to create excitations, whose energy is independent of the lattice size. However, the temperature T, at which such excitations become important increases with the system size [10]. Thus, we expect the infinite lattice to remain unfolded at any finite T. This result does not necessarily contradict the predictions regarding the finite-T crumpling transition [1] in polymerized membranes because: *a*) the bending rigidity of membranes in continuous spaces was «Heisenberg-like», *i.e.* it was proportional to the continuously varying scalar product between the neighboring normals to the surface [2], while the model considered in this work has an «Ising-like» bending energy; *b*) the transition temperature of a continuous membrane is expected to increase [4, 6] with increasing in-plane elastic constants, whereas our model might be thought of (at least, approximately [10]) as having an infinite in-plane stiffness, leading to an infinite transition temperature.

In this work we considered the statistical mechanics of a simple discrete model of a polymerized membrane, when our goal was both to understand the physics underlying the continuum surfaces and to inquire whether one can define a model which can be used in numerical investigations of such surfaces. We conclude that triangular lattice possesses only part of the properties expected of continuum systems. It is conceivable that the finite crumpling transition temperature is «restored» in the rigid-bond model in the *continuous* three-dimensional space with «Heisenberg-like» bending rigidity. However, the results of numerical methods in a discretized space will have only a limited applicability to real systems.

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