

## Excess surface free energy in a two-dimensional model of a biomembrane

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LETTER TO THE EDITOR

Excess surface free energy in a two-dimensional model of a biomembrane

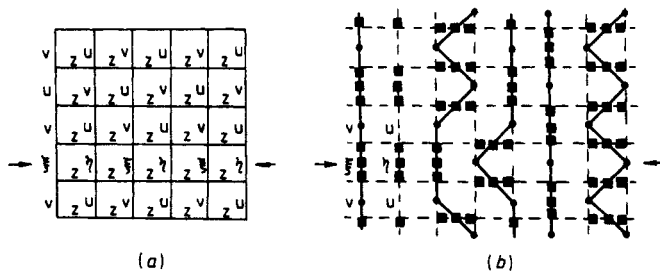
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**Abstract.** The staggered quadratic dimer model of a biomembrane is considered in the case of a lattice with modified activities of the vertical bounds in a selected row. An exact expression for the excess surface free energy is obtained and its dependence on the bulk parameters which control the density, flexibility and ordering of the polymer chains is investigated.

Two-dimensional lattice models occupy an important place among the statistical models of biomembranes [1, 2] due to the possibility of obtaining an exact solution. Most of them belong to the class of ‘free-fermion’ models [3], the well known representative of which is the two-dimensional Ising model. Free-fermion models of polymers are usually formulated in terms of dimer problems on different lattices with various distributions of weights over the lattice bonds. The choice of the lattice and the weight distribution determines the configurational properties of the polymers, reflecting in three main features: density, flexibility and degree of ordering. Nagle [1] has suggested a sufficiently simple model on the square lattice which incorporates all of the three desirable features and represents a generalisation of the previously introduced dimer model studied by Kasteleyn on the honeycomb lattice (*K*-model). In the review article [4], which summarises the achievements in the study of dimer models on anisotropic lattices, this model is called the staggered quadratic Kasteleyn model; here we will refer to it as the sq model. The sq model is defined on a quadratic lattice with a chessboard alternation of the activities *u* and *v* of vertical bonds and activity *z* of all the horizontal bonds; see figure 1(a). The correspondence between the dimer and



**Figure 1.** The staggered quadratic model with a linear defect—the row of modified vertical bounds is indicated by arrows. (a) The distribution of bond activities. (b) The correspondence between the dimer and polymer representations of the model.

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polymer representations of this model [1, 4] is shown in figure 1(b). The number of polymers on the lattice is determined by the difference between the dimer occupation numbers of  $u$ - and  $v$ -bonds in a row. The number of gauche bonds of the polymer chains (strictly speaking, the number of slanted chain links) is determined by the number of horizontal dimers, each of weight  $z$ . A completely ordered state corresponds to all vertical  $u$ -bonds being occupied.

Most of the solutions obtained so far for biomembrane models, including the sq model, pertain to the translationally invariant case when the two-dimensional lattice is wrapped on a torus. However, the study of the surface tension  $\sigma$  of the membrane, as well as the interaction of membrane polymers with macroscopic impurities, requires the solution for a lattice with boundaries. In [5] the  $K$ -model with a boundary parallel to the main polymer orientation has been solved and it has been found that  $\sigma \sim \rho^2$ ,  $\rho$  being the polymer density, whereas in the three-dimensional case  $\sigma \sim \rho^{3/2}$ . Of considerably greater interest is the investigation of the natural membrane surface, i.e. a boundary perpendicular to the polymer orientation. The main purpose of this work is to study the effect of the bulk polymer statistics on the surface tension due to the presence of such a boundary.

The unit cell of the translationally invariant sq model contains four lattice sites. The introduction of a boundary would require the change of the vertical bonds in a selected row from their bulk values  $u$  and  $v$  to some new values  $\xi$  and  $\eta$ . Clearly, this would lead to the problem of diagonalising a rather unwieldy matrix. A radical simplification of the problem may be achieved if we note that between the partition function of the sq model with a linear defect,  $\Lambda_{\text{sq}}(z, u, v; \xi, \eta)$ , and the partition function of the homogeneous dimer model (hq-model) with  $u = v = y$  having the same defect  $\Lambda_{\text{hq}}(z, y; \xi, \eta)$ , there exists a simple one-to-one correspondence. This correspondence arises due to the conservation law formulated in [4]: for each lattice row the difference between the number of dimers on  $u$ -bonds and the number of dimers on  $v$ -bonds is the same. Naturally, this conservation law reflects the continuity of the polymer chains.

Consider the dimer problem on a square lattice of size  $M \times N$  wrapped on a torus. Let the activities of the lattice bonds be distributed according to figure 1(a). Under multiplication of all the activities by a constant  $\lambda$ , the partition function of the model changes by a trivial factor  $\lambda^{2MN}$ . If one chooses  $\lambda = (uv)^{-1/2}$  and takes into account that  $n_u - n_v = (N-1)\Delta$ , where  $n_u$  ( $n_v$ ) is the total number of dimers on the  $u$ -bonds ( $v$ -bonds), and  $n_\xi - n_\eta = \Delta$ , then one obtains

$$\Lambda_{\text{sq}}(z, u, v; \xi, \eta) = \sum_{\{c\}} z^{n_z} u^{n_u} v^{n_v} \xi^{n_\xi} \eta^{n_\eta} = (uv)^{-MN} \sum_{\{c\}} \tilde{z}^{n_z} [\tilde{\xi} u^{(N-1)}]^{n_\xi} [\tilde{\eta} v^{(N-1)}]^{n_\eta}. \quad (1)$$

Here the summation is carried over all dimer configurations and the symbol 'tilde' means that the corresponding activity has been multiplied by  $\lambda$ . Consider now the homogeneous model (hq model) with activity of the horizontal bonds  $x$ , of the vertical bonds  $u = v = y$  and with the same linear defect. Its partition function is

$$\Lambda_{\text{hq}}(x, y; \xi, \eta) = \sum_{\{c\}} x^{n_x} y^{n_y} \xi^{n_\xi} \eta^{n_\eta}. \quad (2)$$

By comparison of the right-hand sides of equations (1) and (2) we establish the relationship

$$\Lambda_{\text{sq}}(z, u, v; \xi, \eta) = (uv)^{-MN} \Lambda_{\text{hq}}(x, 1; \xi_0 e^{\alpha N}, \eta_0 e^{-\alpha N}) \quad (3)$$

where

$$x = z(uv)^{-1/2} \quad \xi_0 = \xi/u \quad \eta_0 = \eta/v \quad \alpha = \frac{1}{2} \ln(u/v). \quad (4)$$

This relationship allows one to study the simpler model, the HQ model with a linear defect. The latter problem has been already considered in our paper [6] with relation to the dimer model of crystallisation suggested there. In the limit of an infinitely long cylinder ( $\infty \times N$ ), exact expressions have been obtained for the densities  $\rho_\xi^{(N)}$ ,  $\rho_\eta^{(N)}$  of dimers on the  $\xi$ ,  $\eta$  lattice bonds, valid for any even  $N$ :

$$\rho_\xi^{(N)}(x, y; \xi, \eta) = \frac{\xi}{2(\xi+x)} \left( 1 - \frac{1}{\pi} \int_0^\pi d\varphi \frac{y(y-\eta) + y(y+\eta)R(\varphi)[1+2\delta_N(\varphi)]}{y^2 + \xi\eta + (y^2 - \xi\eta)R(\varphi)[1+2\delta_N(\varphi)] + 2(\xi+y)(\eta+y)\delta_N(\varphi)[1+\delta_N(\varphi)]} \right) \tag{5}$$

Here

$$R(\varphi) = x|\sin \varphi| (y^2 + x^2 \sin^2 \varphi)^{-1/2} \tag{6}$$

$$\delta_N(\varphi) = y^N \{ [x|\sin \varphi| + |y^2 + x^2 \sin^2 \varphi|^{1/2}]^N - y^N \}^{-1}.$$

The expression for  $\rho_\eta^{(N)}$  may be obtained from (5) by interchanging  $\xi$  and  $\eta$ .

Starting from the definition of the excess surface free energy in the SQ model and taking into account equation (3), we obtain

$$\begin{aligned} \sigma_{SQ}^{(N)}(z, u, v; \xi, \eta) &= \ln[\Lambda_{SQ}^{(N)}(z, u, v; u, v) / \Lambda_{SQ}^{(N)}(z, u, v; \xi, \eta)] \\ &= - \int_1^{\xi_0} \rho_\xi^{(N)}(x, 1; \xi'_0 e^{\alpha N}, e^{-\alpha N}) \frac{d\xi'_0}{\xi'_0} - \int_1^{\eta_0} \rho_\eta^{(N)}(x, 1; \xi_0 e^{\alpha N}, \eta'_0 e^{-\alpha N}) \frac{d\eta'_0}{\eta'_0} \end{aligned} \tag{7}$$

where the parameters  $x$ ,  $\xi_0$ ,  $\eta_0$  and  $\alpha$  have been defined in (4). In the thermodynamic limit  $N \rightarrow \infty$  equation (7) leads to the expression

$$\begin{aligned} \sigma_{SQ}(z, u, v; \xi, \eta) &= -|\Delta| \left\{ \begin{aligned} &\ln(\xi/u) \\ &\ln(\eta/v) \end{aligned} \right\} \\ &\quad - \frac{1}{2\pi} \int_{\pi|\Delta}^{\pi(1-|\Delta|)} d\varphi \ln \left[ \frac{1}{2} \left( 1 + \frac{\xi\eta}{uv} \right) + \frac{1}{2} \left( 1 - \frac{\xi\eta}{uv} \right) \frac{z \sin \varphi}{(uv + z^2 \sin^2 \varphi)^{1/2}} \right] \end{aligned} \tag{8}$$

where the parameter  $\Delta$  is a linear function of the polymer density  $\rho$ ,  $\rho = \frac{1}{2} + \Delta$  and depends only on the bulk lattice activities:

$$\Delta = \begin{cases} \frac{1}{\pi} \sin^{-1} \left( \frac{u-v}{2z} \right) & |u-v| \leq 2z \\ \frac{1}{2} \operatorname{sgn}(bu-v) & |u-v| \geq 2z. \end{cases} \tag{9}$$

In the right-hand side of (8)  $\ln(\xi/u)$  should be taken when  $u \geq v$  and  $\ln(\eta/v)$  when  $u \leq v$ . We emphasise that here the density  $\rho$  has been defined as the number of polymer chains per unit length of the cross section perpendicular to their main orientation and, therefore, it differs from the chain density used by Nagle [1].

The behaviour of the excess surface free energy at a small polymer density,  $\rho \rightarrow 0$  when  $v - u \rightarrow 2z$ , is given by the expansion:

$$\sigma_{\text{SQ}}(z, u, v; \xi, \eta) = -\frac{1}{2} \ln\left(\frac{\eta}{v}\right) + \ln\left[\frac{\eta(u+v)}{v^2 + \xi\eta}\right] \rho + \mathcal{O}(\rho^2). \quad (10)$$

It is seen that  $\sigma_{\text{SQ}}$  depends linearly on  $\rho$  unlike the  $\sigma \sim \rho^2$  dependence in the case of a boundary parallel to the chain orientation [5]. The sign of the proportionality coefficient depends on the relative magnitude of the bulk parameters  $u, v$  and the boundary parameters  $\xi, \eta$ , i.e. on the properties of the boundary. The conservation law excludes the possibility of speaking about 'attracting' or 'repelling' boundary conditions, since the number of polymer chains is conserved in each cross section of the membrane. It is convenient instead to introduce the notion of 'complementary' boundary conditions. To clarify the physical meaning of this notion, let us consider small deviations from the translationally invariant case by setting  $\xi = u + du, \eta = v + dv$ . Then, the coefficient of  $\rho$  in the expression (10) equals  $-(du - dv)/(u + v)$ . Using (9), this can be written as

$$-\frac{1}{u+v}(du - dv) = -\frac{2\pi z \cos[\pi(\rho - \frac{1}{2})]}{u+v} d\rho \approx -\frac{2\pi^2 z}{u+v} \rho d\rho. \quad (11)$$

Therefore, if  $du$  and  $dv$  are sufficiently small and  $du > dv$ , which corresponds to an increase of the polymer density  $\rho$ , the coefficient of  $\rho$  in (10) is negative. So in this case the replacement of the bulk activities  $u, v$  by the corresponding surface values  $\xi, \eta$  results in a decrease in the excess free energy. Such boundaries we call complementary to the bulk with respect to the polymer density. In the opposite case,  $du < dv$ , the coefficient of  $\rho$  is positive and the excess free energy increases.

Similarly, in the limit of close polymer packing,  $\rho \rightarrow 1$  when  $u - v \rightarrow 2z$ , we obtain

$$\sigma_{\text{SQ}}(z, u, v; \xi, \eta) = -\frac{1}{2} \ln\left(\frac{\xi}{u}\right) - \ln\left(\frac{u^2 + \xi\eta}{\xi(u+v)}\right) (1 - \rho) + \mathcal{O}[(1 - \rho)^2]. \quad (12)$$

It can be readily checked that the same correspondence between complementarity of the boundary conditions and the sign of the coefficient of  $\rho$  also holds in this case.

Consider now the excess surface free energy in the limit of small polymer flexibility. As a measure of flexibility we choose the density of the horizontal dimers in the SQ model, for which Nagle [1] has obtained the expression (in our notation)

$$\rho_z(z, u, v) = \frac{1}{2} \left[ 1 - \frac{1}{\pi} \cos^{-1} \left( 1 - \frac{(u+v)^2}{2(uv+z^2)} \right) \right]. \quad (13)$$

In the limit  $\rho_z \rightarrow 0$ , when  $z(uv)^{-1/2} \rightarrow 0$  at a fixed polymer density  $\rho$ , we obtain

$$\sigma_{\text{SQ}}(z, u, v; \xi, \eta) = \sigma_{\text{SQ}}^{(0)} + \frac{\xi\eta - uv}{\xi\eta + uv} \rho_z + \mathcal{O}(\rho_z^2). \quad (14)$$

For interpretation of the sign of the linear term in (14) we turn again to the notion of complementarity. Note that due to (9) the flexibility  $\rho_z$  at constant  $\rho$  is a monotonically increasing function of the parameter  $x = z(uv)^{-1/2}$ . Let us replace  $u, v$  by the corresponding surface values  $\xi, \eta$  and consider the new value of this parameter  $x' = z(\xi\eta)^{-1/2}$ . If  $x' > x$ , that replacement would lead to an increase in the density of horizontal dimers, i.e. to an increase in the number of slanted polymer links. We call such a boundary complementary to the bulk with respect to flexibility. Then the

coefficient of  $\rho_2$  in expansion (14) is negative for complementary boundary conditions and positive for non-complementary.

Naturally, the results obtained here for the surface tension of a two-dimensional membrane have a purely model character. A derivation of similar relationships for the three-dimensional model of a biomembrane suggested by Izuyama and Akutsu in [7] would bring the theory closer to real experiments.

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