Phase Transitions in Multicomponent String Model

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Abstract

We propose a one-dimensional model of a string decorated with adhesion molecules (stickers) to mimic multicomponent membranes in restricted geometries. The string is bounded by two parallel walls and it interacts with one of them by short range attractive forces while the stickers are attracted by the other wall. The exact solution of the model in the case of infinite wall separation predicts both continuous and discontinuous transitions between phases characterised by low and high concentration of stickers on the string. Our model exhibits also coexistence of these two phases, similarly to models of multicomponent membranes.

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The functional renormalization group calculations showed that the continuous unbinding transitions of fluid membranes are characterised by the same fixed points as those of one-dimensional strings governed by a finite tension \cite{1}. However, one-dimensional strings attracted to a flat substrate by finite-range forces exhibit only continuous unbinding transitions while two-dimensional fluid membranes can undergo also discontinuous unbinding transitions in this case \cite{2}. Moreover, recent computer simulations indicated that models for multicomponent membranes show complex phase diagrams which contain both continuous and discontinuous unbinding transitions \cite{3}. The aim of this letter is to present a model for two-component, one-dimensional string fluctuating between two parallel walls with which it interacts. This model is solved exactly in the case of infinite wall separation and exhibits phase transitions similar to multicomponent membranes.

Any membrane present in biological cells is composed of a lipid bilayer which provides its basic structure, and which contains different proteins \cite{4}. The proteins anchored in the lipid bilayer are large molecules which can usually freely diffuse within the fluid membrane. These macromolecules protrude from the
Figure 1: One-dimensional lattice model for a string with stickers. Position of the string at site number $i$ is denoted by $l_i$, and $n_j = 1$ (or 0) indicates presence (or absence) of a sticker at the $j$-th site.

bilayer and may interact with another membrane, or a substrate, by a short-range forces and, thus, act as local stickers or repellers. To investigate the influence of this interaction on membrane adhesion phenomenon various models for membranes with stickers in contact with a planar substrate were used recently [3, 5, 6]. In these models a membrane with zero spontaneous curvature is usually considered and adhesion molecules of only one sort are taken into account. The state of the membrane is specified then by two fields: the local separation between the membrane and the substrate and the local concentration of the stickers. As already mentioned, both continuous and discontinuous membrane unbinding transitions were found for such models, and separation into the unbound phase with low average concentration of stickers and the bound phase with higher average sticker concentration was observed.

In this letter we consider a model of a string containing specific adhesion molecules (stickers). The string with attached stickers fluctuates in a two-dimensional space between two parallel, one-dimensional walls (slit geometry). The walls are separated by distance $L$. In the present lattice model (see Fig. 1) the string separation from the bottom wall is described by the set of discrete variables $l_i$, where the lattice site number $i = 1, \ldots, N$ measures the distance along the one-dimensional walls. Each of the $N$ variables $l_i$ can take $L + 1$ values: $l_i = 0, \ldots, L$. The stickers’ degrees of freedom are specified by the set of occupation numbers $n_i$ and each of these variables can be either 0 or 1. The value $n_i = 1$ indicates the presence of a sticker on the string above the $i$-th lattice site while the value $n_i = 0$ indicates that there is no sticker at that position.
In the present model we assume that the string itself interacts with the upper wall via a pinning potential while the stickers attached to the string interact only with the bottom wall by another pinning potential. The corresponding Hamiltonian takes the following form

$$H = \sum_{i=1}^{N} \left[ J|l_{i+1} - l_i| - n_i W_1 \delta_{i,0} - W_2 \delta_{i,L} \right].$$

The first term describes the bending energy of the string, and $J$ is the stiffness parameter. The second and the third terms correspond to the interaction of the stickers with the bottom wall and the interaction of the string with the upper wall, respectively; we assume that $W_1 > W_2 > 0$.

The grand partition function

$$Z(T, \mu, N) = \sum_{\{n_i\}} \sum_{\{l_i\}} \exp \left[ -\beta \left( H - \mu \sum_{i=1}^{N} n_i \right) \right],$$

where $\beta = \frac{1}{k_B T}$ and $\mu$ denotes the chemical potential of the stickers, will be evaluated for periodic boundary conditions along the walls. To this aim we first sum out the stickers degrees of freedom $\{n_i\}$, and then - using transfer matrix method - trace out all possible string configurations $\{l_i\}$. We additionally assume that the string does not fluctuate too violently, and so its positions at the neighbouring sites differ at most by one, i.e., $|l_{i+1} - l_i| = 0, 1$. In this way we arrive at the modification of the restricted solid-on-solid model \cite{7}. This leads to the following exact result

$$Z(T, \mu, N) = (1 + e^{\beta \mu})^N \sum_{i=0}^{L} (\lambda_i)^N,$$

where the quantities $\lambda_0 \geq \lambda_1 \geq \ldots \geq \lambda_L$ are the eigenvalues of the corresponding transfer matrix. It is given explicitly by the following expression

$$T_{m,n} = (\delta_{m,n} + j \delta_{|m-n|,1}) \sqrt{w_1^{\delta_{m,n+\delta_{n,0}}} w_2^{\delta_{m,L+\delta_{n,L}}}},$$

where

$$j = e^{-\beta J}, \quad w_1 = \frac{1 + e^{\beta (W_1 + \mu)}}{1 + e^{\beta \mu}}, \quad w_2 = e^{\beta W_2},$$

and $\delta_{i,j}$ is Kronecker delta. A transfer matrix of similar structure was discussed in \cite{8} in the context of the wetting phenomena in the slit geometry.

In the thermodynamic limit $N \to \infty$ the free-energy density

$$f = -k_B T \log[\lambda_0(1 + e^{\beta \mu})],$$

and the parallel correlation length of the string

$$\xi_{||} = \left[ \log \left( \frac{\lambda_0}{\lambda_1} \right) \right]^{-1},$$
are determined by the two largest eigenvalues of the transfer matrix. The average sticker concentration \( n \) can be obtained as the derivative of the free-energy density \( f \) with respect to the chemical potential \( \mu \),

\[
n = - \frac{\partial f}{\partial \mu} .
\]  

(8)

The unbinding transition, by definition, occurs when the average separation of a membrane from a substrate becomes infinite. The discussion of this phenomenon within the present model is only possible if the distance between the walls is made infinite, \( L = \infty \). In this limiting case the spectrum of the transfer matrix \( T \) consists of infinite number of eigenvalues homogeneously distributed in the segment \( [1 - 2j, 1 + 2j] \), and - in addition - of at most two eigenvalues which can be larger than \( 1 + 2j \). We arrive at this result using the same methods as discussed in detail in [8]. The two largest eigenvalues of the transfer matrix are expressed in terms of two auxiliary parameters \( \sigma_1 \) and \( \sigma_2 \)

\[
\lambda_0 = \max [\sigma_1, \sigma_2] , \quad \lambda_1 = \min [\sigma_1, \sigma_2]
\]  

(9)

where

\[
s_k = \left\{ \begin{array}{ll}
\frac{w_k}{2} \left[ 1 + \sqrt{1 + \frac{4j}{w_k - 1}} \right] & \text{for } w_k \geq \frac{1 + 2j}{1 + j} \\
1 + 2j & \text{for } w_k < \frac{1 + 2j}{1 + j}
\end{array} \right.,
\]  

(10)

for \( k = 1, 2 \). The parameters \( \sigma_k \) have continuous first derivatives with respect to \( w_k \), and for \( w_k \geq \frac{1 + 2j}{1 + j} \) one has \( \sigma_k \geq 1 + 2j \), and \( \frac{d\sigma_k}{dw_k} \geq 0 \).

The unbinding phase transition is indicated by divergence of the parallel correlation length, when the two largest eigenvalues of the transfer matrix become equal, \( \lambda_0 = \lambda_1 \). Upon changing the model parameters the two largest eigenvalues \( \lambda_0 \) and \( \lambda_1 \) may both become equal either (i) to the value \( 1 + 2j \), which leads to the continuous unbinding transitions, or (ii) to the value located inside the segment \( [1 + 2j, +\infty] \), and then the string unbinds discontinuously from one of the walls and becomes pinned to the other one; these scenarios were discussed in [8]. Thus the discontinuous unbinding transitions caused by energetic competition between the infinitely separated walls occur when \( w_1 = w_2 > \frac{1 + 2j}{1 + j} \), while the continuous de-pinning transitions driven by the string thermal fluctuations take place when \( w_1 = \frac{1 + 2j}{1 + j} > w_2 \) or \( w_2 = \frac{1 + 2j}{1 + j} > w_1 \), see Eq. (10). A straightforward analysis of the above inequalities – based on definitions (5) – leads to the conclusion that unbinding of the string from the bottom wall is either the discontinuous transition, which occurs when \( \mu = \mu_I(T) \) and \( \mu_J(T) > \mu_{II}(T) \), or the continuous transition, which takes place when \( \mu = \mu_{II}(T) \) and \( \mu_I(T) < \mu_{II}(T) \), where

\[
\mu_I(T) = - \frac{1}{\beta} \log \frac{e^{\beta W_1} - e^{\beta W_2}}{e^{\beta W_2} - 1} ,
\]  

(11)

and

\[
\mu_{II}(T) = - \frac{1}{\beta} \log \left[ (e^{\beta J} + 1) (e^{\beta W_1} - 1) - 1 \right] .
\]  

(12)
Figure 2: Phase diagram in coordinates $T - \mu$ plotted for fixed values of model parameters: $W_1 = 2J$, $W_2 = \frac{4}{3}J$. The chemical potential $\mu$ is given in energy units of the stiffness parameter $J$ and the temperature $T$ is given in units of $J/k_B$. Unbinding of the string form the bottom wall is discontinuous for low temperatures ($T < T_2$) and continuous for high temperatures ($T_2 < T < T_1$).

The tricritical point is determined by equation $\mu_I(T) = \mu_{II}(T)$ and the corresponding temperature will be denoted as $T_2$.

The corresponding phase diagram plotted in the variables $T$ and $\mu$ (for fixed values of model parameters $J$, $W_1$, and $W_2$) which contains the relevant parts of curves $\mu = \mu_I(T)$ and $\mu = \mu_{II}(T)$ is displayed in Fig. 2. The area above the curve corresponds to the states for which the string is bound to the bottom wall. The area under the curve corresponds to the states for which the average distance between the string and the bottom wall is infinite. For temperatures $T < T_2$ the curve represents the locus of discontinuous phase transition while for $T > T_2$ it represents the continuous transitions. The continuous transition line has the vertical asymptote $T = T_1$, which is determined by condition $\mu_{II} = \infty$.

To construct the phase diagram in coordinates $T - n$ we have to make use of Eq. (8) which together with Eqs (6) and (4) leads to the following relation

$$n = \frac{1}{1 + e^{-\beta\mu}} + \frac{e^{-\beta\mu}(e^{\beta W_1} - 1)}{(1 + e^{-\beta\mu})^2} \frac{1}{\lambda_0} \frac{\partial \lambda_0}{\partial w_1}.$$  (13)

The derivative $\frac{\partial \lambda_0}{\partial w_1}$ is not equal to zero only if $\lambda_0 = \sigma_1 > 1 + 2j$, i.e., when the string is bound to the bottom wall. In all other cases $\frac{\partial \lambda_0}{\partial w_1} = 0$ and then the average sticker concentration is equal $(1 + e^{-\beta\mu})^{-1}$. It means that the configurations when the string is bound on the bottom wall correspond to the phase with high concentration of stickers, while configurations where the average distance of the string from the bottom wall is infinite correspond to the phase with low sticker concentration.

The continuous unbinding transitions line $\mu_{II}(T)$ is determined by equations $w_1 = \frac{1 + 2j}{1 + j}$ and $\lambda_0 = \sigma_1$. When this conditions are fulfilled then it follows from Eq. (10) that $\frac{\partial \lambda_0}{\partial w_1} = 0$. Thus, upon crossing the continuous transitions line
\( \mu_{II}(T) \) the average sticker concentration changes continuously.

On the other hand, the discontinuous unbinding transitions take place when \( w_1 > \frac{1+2j}{2j} \). In this case \( \frac{\partial \lambda_0}{\partial \mu} > 0 \) for \( \lambda_0 = \sigma_1 \), and \( \frac{\partial \lambda_0}{\partial \mu} = 0 \) for \( \lambda_0 = \sigma_2 \), which means that upon crossing the discontinuous unbinding transitions line, \( \mu_1(T) \), the average stickers concentration changes discontinuously.

The above predictions can be made more explicit by evaluating the derivative \( \frac{\partial \lambda_0}{\partial w_1} \) along both transitions lines. In this way one finds the stickers concentration on both sides of curves \( \mu_{II}(T) \) and \( \mu_{I}(T) \). A straightforward calculation leads to the conclusion, that along the continuous transitions line, on both sides of the curve \( \mu_{II}(T) \), the average stickers concentration is given by the following expression

\[
n_{II}(T) = \frac{1}{(e^{\beta J} + 1)(e^{\beta W_1} - 1)} .
\] (14)

On the other hand, the average stickers concentration along the discontinuous transitions line, \( \mu_{I}(T) \), on the side of the phase poor in stickers, is equal

\[
n_{-I}(T) = \frac{e^{\beta W_2} - 1}{e^{\beta W_1} - 1} ,
\] (15)

and on the side of the phase rich in stickers it is equal

\[
n_{+I}(T) = n_{-I}(T) + \Delta n(T) ,
\] (16)

where the jump of stickers concentration, \( \Delta n \), is given by formula

\[
\Delta n(T) = \frac{e^{\beta W_2} - e^{\beta W_1}}{2(e^{\beta W_1} - 1)} \left[ 1 - 2e^{-\beta W_2} + \left(1 + \frac{4e^{-2\beta J}}{e^{\beta W_2} - 1}\right)^{-\frac{1}{2}} \right] \geq 0 .
\] (17)

One can check that \( \Delta n(T_2) = 0 \), and show that the derivative \( \left( \frac{\partial}{\partial T} \Delta n \right)_{T=T_2} \) is always negative. It means that while approaching the tricritical point the jump of the sticker concentration vanishes linearly with temperature, \( \Delta n \sim T_2 - T \).

An example of phase diagram, which contains the relevant parts of curves \( n_{-I}(T) \), \( n_{+I}(T) \), and \( n_{II}(T) \), is shown in figure[2]. The curve \( n_{II}(T) \) separates the regimes which correspond to phases rich and poor in stickers. The area limited by curves \( n_{-I}(T) \), \( n_{+I}(T) \) and the \( n \) axis is the coexistence region of these two phases.

In summary, by analogy with some models for multicomponent membranes, we consider a one-dimensional model of a string with stickers attached to it. The string is confined between two parallel walls of different properties: the bottom wall interacts only with the stickers, and the upper wall only with the string itself. In the case when the distance between the walls is infinite, the string unbinding transitions take place for certain values of temperature and the sticker chemical potential. At low temperatures (\( T < T_2 \)) the transitions are discontinuous while for higher temperatures (\( T_2 > T > T_1 \)) they are continuous. We show that the configurations for which the string is bound to the bottom wall correspond to the phase with high concentration of stickers while
Figure 3: The phase diagram in coordinates $T - n$ for fixed values of model parameters: $W_1 = 2J$ and $W_2 = \frac{1}{3}J$. The temperature $T$ is given in units of $J/k_B$. The lines $n_{II}(T)$, $n_I^-(T)$, and $n_I^+(T)$ separate the sticker-rich phase, the sticker-poor phase, and the coexistence region of these two phases.

configurations where the average separation between this wall and the string is infinite correspond to the phase with low sticker concentration. We find both discontinuous and continuous transitions between phases rich and poor in stickers. The phase diagram on Fig. 3 indicates regimes corresponding to these two phases as well as the two-phase coexistence region and the continuous transitions line. In this respect it resembles phase diagrams for some models of multicomponent membranes [3].

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