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Morphological transitions of the fixed-point potential of the renormalization group

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Abstract. Interactions between fluid membranes are studied by renormalization group techniques. To make the zero-flow condition at the origin compatible with the renormalization, there should be a non-renormalizable region near the origin. The renormalization procedure involving such a region picks up an inhomogeneous contribution which will also be recast during the renormalization. This paper gives an example to show how the morphology of the fixed-point potential undergoes a series of transitions due to this inhomogeneous contribution.

The shape of fluid membranes and the interactions between membranes are of fundamental significance in biological processes such as assembles of cells, communication among cells etc [1]. Membranes in solution exhibit direct interactions such as Van de Waals, hydration and electrostatic forces [2]. In addition, membranes suffer shape fluctuations due to thermally-excited modes, which represent an effective repulsive interaction and renormalize the direct interactions [2, 3]. From a physical point of view, synthesizing these interactions is a challenging problem, because it involves many scales from the size of the molecules (1 nm) to the size of the membrane (typically 1–10 μm). As adding these forces together cannot directly give the right answer, one is naturally led to study the behaviour of the interactions under scaling transformations. Provided the shape fluctuations are scaling invariant, the renormalization group technique has been applied to this problem and had a number of successes. For example, a general nonlinear renormalization group method was developed in [4] and a whole line of fixed-point potentials was obtained in which several subregimes could be discriminated [5]. In the strong fluctuation subregime, the membranes undergo a second-order transition from a bound state to an unbound state. Multicritical phenomena were also found when the dimension approaches three [6]. Earlier three very different scaling behaviours were predicted by the linear renormalization group for wetting transitions in $d = 2 + 1$ [7]. An exact result for $d = 1 + 1$ wetting transitions was also obtained by the transfer-matrix method [8, 9]. Recently, a new renormalization group theory was developed to study wetting transitions in $d = 2 + 1$ [10]. To proceed, I follow [4, 5] to let $x = (x^1, x^2, \ldots)$ be the longitudinal coordinates and $l(x)$ the local separation between two membranes. Two lengths are of interest: $L_\parallel$ the longitudinal correlation length; and $L_\perp$ the transverse correlation length. The roughness exponent ζ describes the fluctuations of a free membrane or interface, for lateral distance $L_\parallel$, the typical value of $L_\perp$ scales as

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$L_\perp \sim L_\parallel^\zeta$. For fluid membranes in $d = 2+1$, $\zeta = 1$. For $(d-1)$ dimensional interfaces, $\zeta = \frac{1}{2}(3-d)$.

For two parallel segments of a membrane or interface, the effective Hamiltonian reads as

$$H = \frac{1}{k_B T}\int D^{d-1}x\left[\frac{K}{2}[\nabla^n l(x)]^2 + v[l(x)]\right]. \tag{1}$$

For membranes, $n = 2$, and K is the effective bending rigidity; for interfaces, $n = 1$ and K is the interface stiffness. $v[l(x)]$ is a direct potential.

Provided shape fluctuations are scaling invariant, the uniquely correct scaling transformations are:

$$x \to x' = \frac{x}{b} \qquad l \to l' = \frac{l}{b} \tag{2}$$

where $b > 1$ is a scale constant.

In the infinitesimal limit, a very simple fixed-point equation for the potential was obtained in [4]. The next step is to integrate the fixed-point equation with the appropriate boundary condition. In [5], a boundary condition was added as a wall $v(l) = \infty$ for $l < 0$ and the integration was from an asymptotic solution near the wall. In [11], for a symmetrical potential, the boundary condition was supplemented as $v(0) =$ constant $\partial v(0)/\partial l = 0$.

Now let us point out the problems in this procedure.

First, the procedures change the zero-flow condition at $l(x) = 0$. The zero-flow condition is that the directional derivative of the energy–momentum tensor across the plane $l(x) = 0$ is zero. Certainly, there is no energy–momentum flow crossing the plane $l(x) = 0$ during the renormalization while the membranes remain at their former positions. Membranes cannot be penetrated through each other. Unfortunately, previous procedures break this requirement, moving the wall or changing the potential at $l(x) < 0$. In two-dimensional conformal field theory, the zero-flow condition will lead to non-trivial results [12].

Second, the procedures change the direct potential near $l(x) = 0$ drastically. From a physical point of view, the potential near $l(x) = 0$ is determined by the membranes themselves and it is impossible to obtain them from the fixed-point potential equation of the renormalization group based on scaling invariance. Note that the membranes arrive at this region at a very small probability and when membranes arrive at this region, most shape fluctuations are suppressed, so, by causal law, shape fluctuations will induce a very small effective repulsive interaction. In addition, this problem is basically a classical one, a finite potential is sufficient to prevent the membranes from penetrating each other.

So, it seems to me that both the renormalization and the supplemented boundary condition near $l(x) = 0$ are possibly problematic; in particular it will be difficult to involve the zero-flow condition in the renormalization procedure. In this paper, I tentatively proposed a new renormalization procedure in which the zero-flow condition is automatically preserved but at the expense of an inhomogeneous item involved in the renormalization.

I suggest a new renormalization procedure as follows.

(i) There exists a small region which cannot be renormalized by shape fluctuations, and in which the Hamiltonian is generally unknown. The potential in this region should be great enough to prevent penetration. Hence, the zero-flow condition will automatically be satisfied during renormalization.

(ii) Such a rigid region 'twists' renormalization and contributes a non-zero item to the potential during renormalization.

(iii) To protect the group property, the twisting contribution will also be recast during renormalization.

In what follows, I will use linear renormalization group theory as an example to show how to realize this new procedure.

In linear renormalization theory, the potential recursion equation is [4, 7, 11]

$$v^{(N+1)}(z) = b^{d-1} \exp\left[\frac{1}{2}\bar{a}^2 \frac{\mathrm{d}^2}{\mathrm{d}z^2}\right] v^{(N)}(z) \tag{3}$$

where $z = b^{\zeta} l$ and $b > 1$ a scale factor

$$\begin{aligned}\bar{a}^2 &= \frac{k_{\mathrm{B}}T}{K} \int_{\Lambda/b}^{\Lambda} \mathrm{d}^{d-1} p/(2\pi)^{d-1} p^{2n} \\ &= \frac{k_{\mathrm{B}}T}{\pi K} a(b-1) \qquad n = 1, d = 2 \\ &= \frac{k_{\mathrm{B}}T}{\pi K} a^{2\zeta}(b^2 - 1) \qquad n = 2, d = 3\end{aligned} \tag{4}$$

where $\Lambda \approx 1/a$ is the large momentum cut-off and a the short-distance cut-off.

In the non-renormalizable region, after recovery of scale, the Hamiltonian is the same (suffering no renormalization), so the zero-flow condition is automatically satisfied. However, renormalization will change the boundary of the rigid region and the matching condition between the direct potential and the rigid region; to compensate for this, the rigid region will 'twist' any renormalization irreversibly. So, I insert an item $R(b) f^{(N)}(z)$ which represents this twisting effect on the renormalization into the recursion equation (4) and transform it into

$$v^{(N+1)}(z) = b^{d-1} \exp\left[\frac{1}{2}\bar{a}^2 \frac{\mathrm{d}^2}{\mathrm{d}z^2}\right] \left[v^{(N)}(z) + R(b) f^{(N)}(z)\right] \tag{5}$$

where $R(b)$ is a scaling factor.

The twisting effect depends on both the direct potential and the specific renormalization procedure. To keep the procedure simple at this stage, in this paper I assume that at every step the rigid region twists renormalization locally, i.e. the $f(z)$ are short-range functions. Hence, to linear order, I assume that the $f(z)$ are independent of the direct potential and *are only subject to the constraints of the renormalization group. Then to protect the group* property, $f^{(N)}(z)$ is 'renormalized' as

$$f^{(N+1)}(z) = b^{d-1} \exp\left[\frac{1}{2}\bar{a}^2 \frac{\mathrm{d}^2}{\mathrm{d}z^2}\right] f^{(N)}(z). \tag{6}$$

At the end of this paper, I will discuss the validity of this linear approximation. Using the relation from (4),

$$\bar{a}^2(b_1) b_2^{2\zeta} + \bar{a}^2(b_2) = \bar{a}^2(b_1 b_2)$$

and selecting

$$R(b_1) + R(b_2) = R(b_1 b_2)$$

one can easily prove the semigroup property of the recursion.

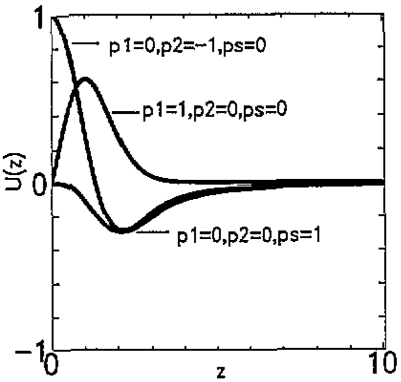

Figure 1. Three parts of the FPP.

In the infinitesimal limit $b = e^{\delta t}(\delta t \to 0)$ and setting $\lim_{\delta t\to 0} R(b)/\delta t = 1$, we obtain two very simple flow equations:

$$\frac{\partial v(l)}{\partial t} = (d-1)v(l) + \zeta l \frac{\partial v(l)}{\partial l} + \tfrac{1}{2}A^2 \frac{\partial^2}{\partial l^2} v(l) + f(l) \tag{7}$$

$$\frac{\partial f(l)}{\partial t} = (d-1)f(l) + \zeta l \frac{\partial f(l)}{\partial l} + \tfrac{1}{2}A^2 \frac{\partial^2}{\partial l^2} f(l) \tag{8}$$

where

$$A^2 = \frac{k_B T}{2\pi K} a^{2\zeta}.$$

Expressed in dimensionless variables $z = \sqrt{2\zeta l}/A$, the fixed-point potential (FPP) equations read as

$$2U(z) + z\frac{\partial U(z)}{\partial z} + \frac{\partial^2}{\partial z^2}U(z) + F(z) = 0 \tag{9}$$

$$2F(z) + z\frac{\partial F(z)}{\partial z} + \frac{\partial^2}{\partial z^2}F(z) = 0. \tag{10}$$

It is interesting to see the non-trivial results from this procedure. Equation (10) has two linearly independent solutions:

$$\varphi_1 = z\exp(-\tfrac{1}{2}z^2) \qquad \varphi_2 = z\exp(-\tfrac{1}{2}z^2)\int \frac{\exp(\frac{1}{2}z^2)}{z^2}\,dz. \tag{11}$$

Let us confine ourselves to the short-range solution φ_1, then we have

$$F(z) = p_s z\exp(-\tfrac{1}{2}z^2) \tag{12}$$

$$U(z) = p_1\varphi_1(z) + p_2\varphi_2(z) - p_s\varphi_1(z)\int \frac{\exp(\frac{1}{2}z^2)}{z^2}\left[\int z^2\exp(-\tfrac{1}{2}z^2)\,dz\right]dz. \tag{13}$$

It is more convenient to integrate (9), incorporating $F(z)$ and the boundary condition as $U(0) = -p_2$, $\partial U(0)/\partial z = p_1$.

The three parts of $U(z)$ are schematically represented in figure 1.

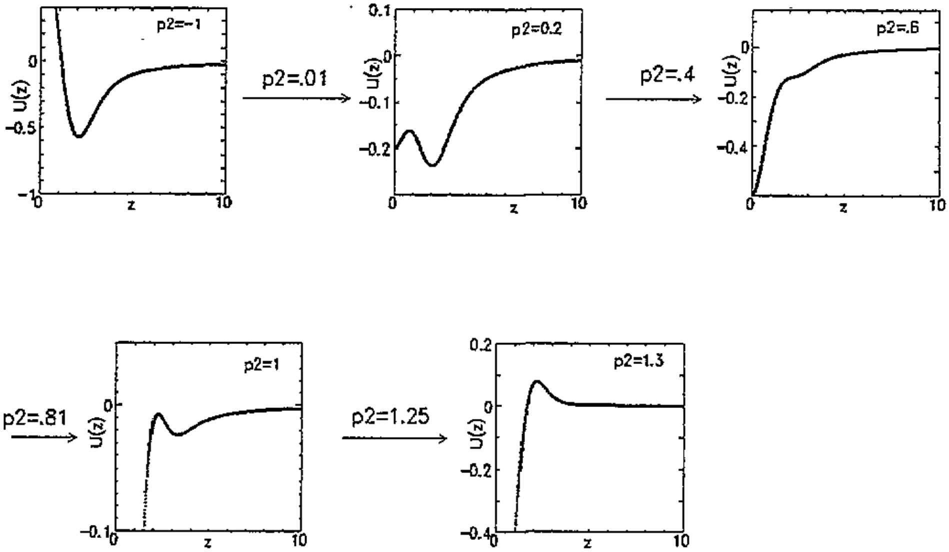

Figure 2. Morphological transitions of FPP ($p_1 = 0$, $p_s = 1$).

The first part in (13) is short-ranged, the second and third parts are both long-ranged and decay as $1/z^2$ at large z.

When the three constants change, the morphology of the FPPs can undergo transitions and several series can be identified.

(i) Series 1. $p_2 = 0$ or $p_s = 0$. This series falls into competition between a short-ranged and a long-ranged part. There is always a maximum or a minimum if $p_2 \neq 0$ or $p_s \neq 0$.

(ii) Series 2. $p_1 = 0$. There is no short-range part. We can set $p_2 = 1$ or $p_s = 1$, and change p_s or p_2, we have a series of morphological transitions (see figure 2). The parameter values above the arrows are the critical values at which the transitions occur.

(iii) Series 3. $p_1 = 1$ $p_2 > 0$. We can set p_2, and vary p_s to see the morphological transitions of the FPPs. It is interesting to see a bifurcation. When $p_2 < p_2^{\Delta} = 11.18$, the morphological transitions only involve the creation or annihilation of a minimum far away from the origin as in figure 3.

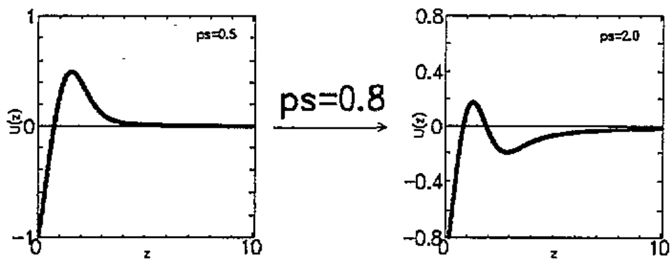

Figure 3. Morphological transition of FPP ($p_1 = 1$, $p_2 = 1$).

When $p_2 > p_2^{\Delta} = 11.18$, the transitions also involve the creation and annihilation of a maximum–minimum pair. One should notice that the transition below $p_2^{\Delta} = 11.18$ is preserved when $p_2 > p_2^{\Delta} = 11.18$ (see figure 4: the first small figure shows the values of p_s at which the transitions take place).

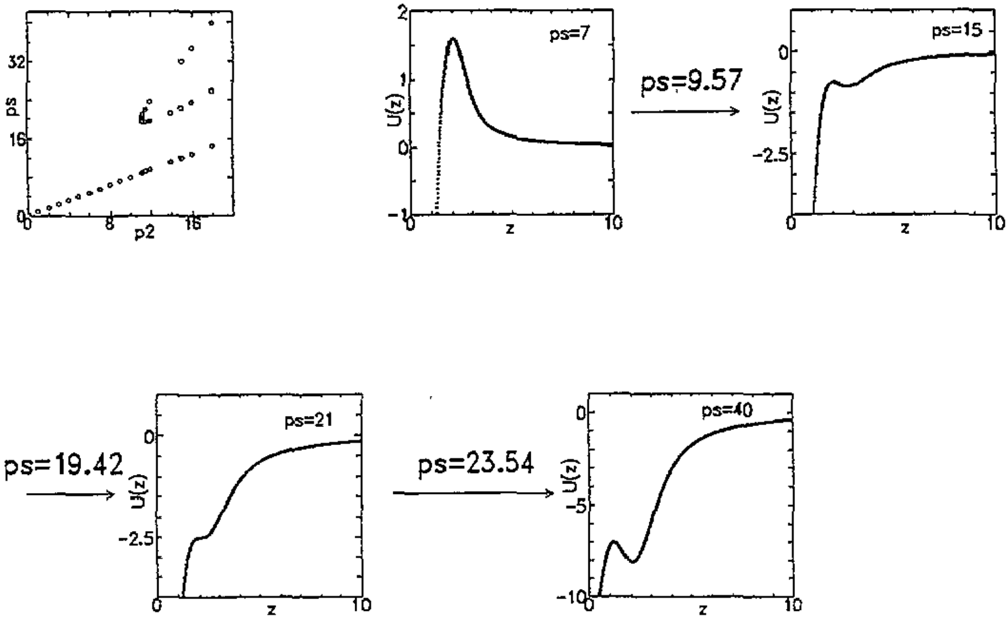

Figure 4. Morphological transitions of FPP ($p_1 = 1$, $p_2 = 12$).

(iv) Series 4: $p_1 = 1$, $p_2 < 0$. When $p_2 > \bar{p}_2 = -1.4$, the transition involves the creation or annihilation of a minimum as in figure 5. When $p_2 < p_2 = -1.4$, the transitions transform into another form in which a minimum is preserved and involve the creation or annihilation of a maximum–minimum pair. The first small figure in figure 6 shows the values of p_s at which the transitions take place.

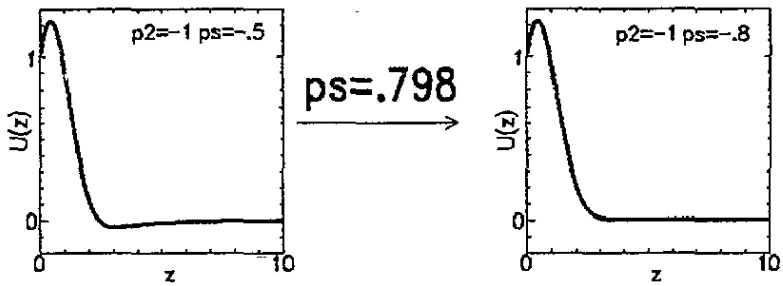

Figure 5. Morphological transitions of FPP ($p_1 = 1$, $p_2 < 0$).

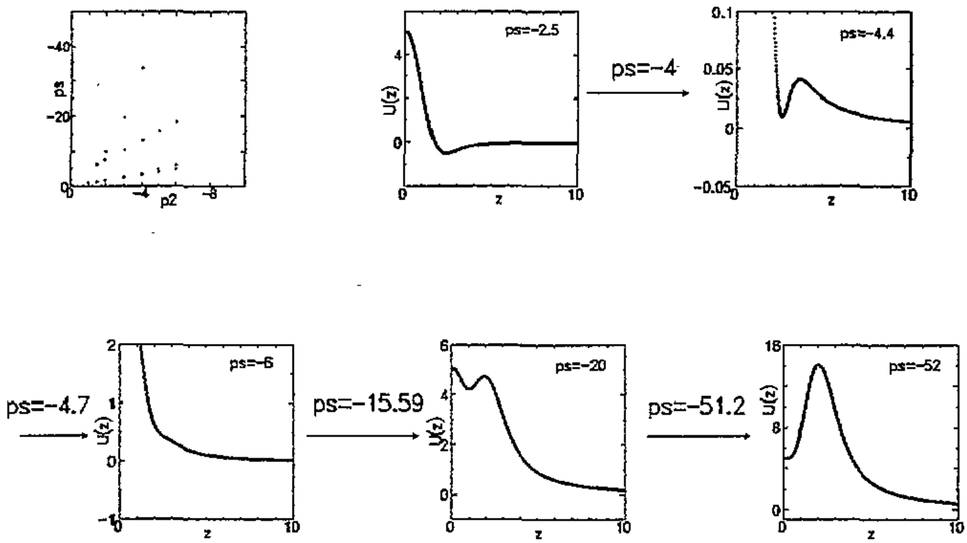

Figure 6. Morphological transitions of FPP ($p_1 = 1$, $p_2 = -5$).

Now, it is time to explain some points. Because of the linear superimposition principle, setting $p_1 = 1$ does not mean that generality is lost. Changing all the signs of p_1, p_2 and p_s is also meaningful. The real meaning of the morphological transitions of the fixed-point potentials is the creation or/and annihilation of extremes. The way in which a maximum, minimum or a maximum–minimum pair disappears or is created determines the characteristic of the transitions. Using the charts of morphological transitions of fixed-point potentials, one can easily see the transitions the membranes may undergo. When a minimum disappears at the point farthest away from the origin, one can say the membranes undergo transition from a bound state to an unbound state. Note that in our calculation, there is no indication that a minimum disappears at infinity or is created from infinity. A minimum is created or disappears at finite z, the farthest one is $z = 6.923$ when $p_s = 0.7979$ and $\partial^2 U/\partial z^2 = 1.363 \times 10^{-8}$ in series 2. When a minimum and a maximum approach one another and then annihilate $\partial^2 U/\partial z^2$ disappears, the system goes to another bound state or to infinity, but the average separation z never becomes continuously divergent. The result of nonlinear renormalization group theory is $l \sim (T - T_c)^{-\psi}$ $\psi \approx 1$ [2, 13]. The disappearance of a minimum or a maximum or a minimum–maximum pair can also cause a jump from a bound state to another bound state. In all series, a single extreme disappears or is created only far from or near to the origin, while a pair of extremes can disappear or be created in the whole range. The bifurcations in the parameter space are unexpected.

In real systems, two natural cut-offs—a, the short cut-off, and L, the long-range cut-off—are involved. Renormalization may be cut off somewhere, so the fixed-point potentials may not tell the whole story.

Conclusion and discussion

Broken symmetry and a finite non-renormalizable region can irreversibly influence the renormalization. To incorporate this a new procedure has been suggested and an example realizing it has been given in the framework of linear renormalization group theory. The morphological transitions of the fixed-point potentials and the bifurcations in the parameter space are indeed impressive. The zero-flow condition is really special, one must treat this condition and renormalization carefully. In experiments, both first- and second-order transitions from a bound state to an unbound have been observed [14–16]. A Monte Carlo experiment also showed that short-range excitations are important [17].

The fact that local twisting by a finite rigid region will lead to a long-range part in the fixed-point potentials is not trivial. For long-range direct potentials, the potentials will not be renormalized at large separation. So it is highly possible that this non-trivial effect of local twisting will be preserved in nonlinear theory in which local twisting depends on both the direct potential and the specific renormalization procedure used. Hence I believe that linear theory incorporates some important points. The induced long-range part may play an important role in many similar systems. We can say that under renormalization, a finite rigid region can influence the property of a vacuum at infinity.

Recently, A J Jin and M E Fisher [10] have developed a new renormalization group theory for wetting transitions in $d = 2 + 1$. They introduced a spatially variant interfacial stiffness. Under linear renormalization, they obtained two flow equations. Their equations are very similar to the corresponding equations in this paper, the only difference being that equation (8) in this paper has an additional item $(d-1)f(z)$. If one follows the procedure in this paper and operates a 'twisted matching procedure', just like they do, by choosing twisting $f(z)$, all the results from A J Jin and M E Fisher [10] can be obtained and, beyond these, one can obtain other results and some insights, though the procedure in the present paper is quite *ad hoc*.

I hope the results of this paper can be tested by experiments. Further study to elucidate the effects of the zero-flow condition on renormalization is needed. The idea should also be applicable to other similar physical systems.

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