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Depinning transition of a directed polymer by a periodic potential: A d-dimensional solution

S. Galluccio and R. Graber
Institut de Physique Théorique, Université de Fribourg, CH-1700, Fribourg, Switzerland

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We study the depinning phase transition of a directed polymer in a d-dimensional space by a periodic potential localized on a straight line. We give exact formulas in all dimensions for the critical pinning we need to localize the polymer. We show that a bound state can still arise even if, in average, the potential layer is not attractive and for diverging values of the potential on the repulsive sites. Our solution can be useful in the context of kinetic growth of interfaces. [S1063-651X(96)50106-6]

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The statistical mechanics of long linear chains (directed polymers) in ordered and disordered media has been an object of intense study in the past few years. One relevant problem in that large context is the study of the depinning transition of a directed line by a single extended defect embedded in a $(d+1)$-dimensional lattice. An attractive potential pins the interface (here a line) on itself suppressing wandering, but thermal fluctuations increase the configurational entropy and a phase transition takes place at a given critical temperature T_c [1]. The depinning transition of polymers by a single defect has been the object of intense work and exact results are now well established in some simple cases [2,3]. Moreover the simultaneous effect of both point and extended defects has led recently to some new results in the context of the renormalization group approach in continuum models [4].

In this article we will deal with the following problem: the depinning phase transition of a single polymer in a $(d+1)$-dimensional hypercubic lattice by a periodic potential localized on a line, i.e., a potential which is alternatively attractive and repulsive. We point out that such a potential layer can be used, for instance, to mimic the effect of two alternating kinds of pinning centers with different strengths. Moreover it is tightly linked with a simplified version of the Kardar-Parisi-Zhang (KPZ) equation for interface growth (see discussion below). Some well-known arguments show that with an n-dimensional (oriented) defect the polymer is localized for $d-n+1 \leqslant 2$ by an arbitrarily weak attractive force, while for $d-n+1>2$ a finite strength is necessary to do the work [5]. Analytical results are in general not available for such high-dimensional systems.

Our main results in this work are the following: (i) we solve the phase transition problem in *all* dimensions and we give an exact formula for the critical pinning strength necessary to localize the polymer at the origin. (ii) We surprisingly show that a bound state can always arise even though, in average, the potential layer is repulsive. This effect has been recently studied in the one-dimensional case [6]. We also prove that in *all* finite dimensions a finite strength on the attractive sites is enough to pin the polymer even in the limit of an infinite potential on the repulsive sites. (iii) The approach introduced is also interesting on its own: we use a dual space representation of the transfer matrix which enables us to simply find the critical state of the system and the partition (wave) function. This approach leads to exact results for the error-catastrophe problem in biological evolution [7].

The energy of a line of length L with extremes at $\mathbf{h}^{(0)}=\vec{0}$ and $\mathbf{h}^{(L)}=\mathbf{x}$, wandering in a $(d+1)$-dimensional space $\Omega=\mathbf{Z}^d\times\mathbf{N}$ and directed along a ''time'' axis, is given by [1]

$$\mathcal{H}(\{\mathbf{h}^{(i)}\}) = J\sum_{k=1}^{L} |\mathbf{h}^{(k)}-\mathbf{h}^{(k-1)}| - \sum_{k=1}^{L} U_k \delta_{\mathbf{h}^{(k)},\vec{0}}, \qquad (1)$$

where $\mathbf{h}^{(k)}$ is a vector identifying the position of the line in Ω at each ''time'' k. The potential is localized at the origin and it is alternatively attractive and repulsive, i.e., $U_k=u>0$ if k is even and $U_k=-v<0$ if k is odd. The directed line has no overhangs and the RSOS condition is imposed. A canonical partition function is introduced (the sum is over all possible allowed realizations of the interface ''height'' $\mathbf{h}^{(k)}$):

$$\mathcal{Z}_L(\mathbf{x}) = \sum_{\{\mathbf{h}\}} \exp[-\mathcal{H}(\{\mathbf{h}^{(k)}\})/T]. \qquad (2)$$

In the usual approach one defines a symmetrical transfer matrix $\mathbf{T}_{zz'}=\mathbf{T}_{z-z'}$ from $\mathcal{Z}$ as $\mathcal{H}=-T\ln\Sigma_z\mathbf{T}(z)\hat{S}_z$; (here $\hat{S}_z$ stands for a shift operator [1]). At finite temperatures $T>0$ the fluctuations of the interface increase the configurational entropy while large humps are unlikely since they give a higher internal energy. The final state of the polymer is the result of that competition and it is associated with the free energy density (per unit length) f. In the thermodynamic limit $(L\rightarrow\infty)$ f is dominated by the largest eigenvalue of $\mathbf{T}_{zz'}$.

For our system we see that in one step the partition function $\mathcal{Z}_L(\mathbf{x})$ obeys the following recursion relation:

$$\mathcal{Z}_{L+1}(\mathbf{x}) = [1+(a_{L+1}-1)\,\delta_{\mathbf{x},\vec{0}}]\left[\mathcal{Z}_L(\mathbf{x}) + t\sum_{i=1}^{L} [\mathcal{Z}_L(\mathbf{x}+\mathbf{e}^{(i)}) + \mathcal{Z}_L(\mathbf{x}-\mathbf{e}^{(i)})]\right] \qquad (3)$$

where the unitary vectors $\mathbf{e}^{(i)}=(0,0,\ldots,i,\ldots,0)$ have a ''1'' bit as the ith element (so as to satisfy RSOS condi-

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tions). In the above we have defined the parameters $t=\exp(-J/T)\in(0,1]$ $a_L=\exp(u/T)$ (for L even) and $a_L=\exp(-v/T)$ (for L odd). We now introduce a dual space representation of our equation in order to simplify the calculation. For the present problem we use a standard Fourier transform, but sometimes one needs different representations [7]. As the partition function $\mathcal{Z}(\mathbf{x})$ is expected to be symmetric in the arguments we introduce a cosine transform

$$\mathcal{Z}_L(\mathbf{x})=\int_0^1 d^dk\prod_{i=1}^{d}\cos(\pi k_i x_i)\,\mathcal{Z}_L(\mathbf{k}),\tag{4}$$

and its inverse. In the Fourier space Eq. (3) takes a simple form; a proper definition of the transfer matrix should anyway take into account the periodicity of the problem. If we introduce the normalized quantities $G_L(\mathbf{k})=\mathcal{Z}_L(\mathbf{k})/(1+2dt)^L$ and $\xi(\mathbf{k})=[1+2t\Sigma_{i=1}^{d}\cos(\pi k_i)]/(1+2dt)$, after two consecutive steps our equation reads

$$\begin{aligned}G_{2L+2}(\mathbf{k})&=\xi^2(\mathbf{k})G_{2L}(\mathbf{k})+A\int_0^1 d^dq\,\xi^2(\mathbf{q})G_{2L}(\mathbf{q})\\&\quad+B\xi(\mathbf{k})\int_0^1 d^dq\,\xi(\mathbf{q})G_{2L}(\mathbf{q})\\&\quad+\frac{AB}{1+2dt}\int_0^1 d^dq\,\xi(\mathbf{q})G_{2L}(\mathbf{q}),\end{aligned}\tag{5}$$

with $A=a_{2L}-1$ and $B=a_{2L+1}-1$.

In order to find the maximum eigenvalue ε we should consider the spectral equation obtained from (5) by identifying $G_{L+2}(\mathbf{k})=\varepsilon^2G_L(\mathbf{k})$. We recall that the only significant contribution in the thermodynamic limit $L\rightarrow\infty$ is the maximum eigenvalue associated with (5). In fact one can show that $f\approx-\ln\varepsilon$ is always different from 0 in the localized region ($\varepsilon>1$) while it vanishes in the unbound state for $\varepsilon\rightarrow1$. The depinning phase transition is defined at $\varepsilon=1$ [8].

The search for a general solution of the eigenvalue equation is a very hard task, nevertheless one can find the criticality condition as a function of the free parameters $\{d,t,u,v\}$ of the theory with no enormous effort. The idea is to introduce two auxiliary constants $K_{1,2}$ by integrating all the terms containing the unknown function $G_L(\mathbf{k})$:

$$K_n=\int_0^1 d^dk\,G_L(\mathbf{k})\xi^n(\mathbf{k})\quad(n=1,2).\tag{6}$$

Therefore we get a homogeneous system of two algebraic equations for K_n which must be satisfied by any general set of parameters $\{d,t,u,v\}$:

$$\begin{aligned}&\left(A\mathcal{I}_2(\varepsilon)+\frac{AB}{1+2dt}\mathcal{I}_1(\varepsilon)-1\right)K_1+B\mathcal{I}_1(\varepsilon)K_2=0,\\&\left(A\mathcal{I}_3(\varepsilon)+\frac{AB}{1+2dt}\mathcal{I}_2(\varepsilon)\right)K_1+(B\mathcal{I}_2(\varepsilon)-1)K_2=0,\end{aligned}\tag{7}$$

with

$$\mathcal{I}_n(\varepsilon)=\int_0^1 d^dk\frac{\xi^n(\mathbf{k})}{\varepsilon^2-\xi^2(\mathbf{k})}\quad(n=1,2,3).\tag{8}$$

The homogeneous system (7) admits nontrivial solutions if and only if the determinant of its coefficients vanishes. This is therefore the condition we must require in order to get the spectrum of the transfer matrix. Performing the limit $\varepsilon\rightarrow1$ we arrive at the condition which must be satisfied by any set $\{d,t,u,v\}$ at the critical point [8]. After some calculations we then get the criticality condition:

$$1-(A+B)\mathcal{I}_2'+AB\left[\mathcal{I}_2'^2-\mathcal{I}_1'\left(\mathcal{I}_3'+\frac{1}{1+2dt}\right)\right]=0,\tag{9}$$

with $\mathcal{I}_n'=\mathcal{I}_n(\varepsilon=1)$ $(n=1,2,3)$. In the following we will drop the ‘‘prime’’ from the formulas, anyway recalling that all quantities are calculated at $\varepsilon=1$. Borrowing from the thermodynamic language, Eq. (9) can be thought of as the *equation of state* at criticality: the ‘‘thermodynamic variables’’ are now those in the set $\{d,t,u,v\}$.

Despite the complexity of the high-dimensional integrals $\mathcal{I}_n$ involved in the above formula one can finally express them, after some analytical work, in the following form:

$$\mathcal{I}_1=\frac{\alpha}{2}(f-g),\quad\mathcal{I}_2=\frac{\alpha}{2}(f+g)-1,\quad\mathcal{I}_3=\mathcal{I}_1-\frac{1}{2t\alpha},\tag{10}$$

where we have defined a new constant $\alpha=(1+2dt)/2t$ and the two integrals:

$$f=\int_0^1 d^dk\frac{1}{d-\Sigma'(\mathbf{k})},\quad g=\int_0^1 d^dk\frac{t}{1+dt+t\Sigma'(\mathbf{k})}.\tag{11}$$

with $\Sigma'=\Sigma_{i=1}^{d}\cos(\pi k_i)$. By means of the above definitions our equation of state reads

$$A=\frac{B\mathcal{I}_2-1}{B(\mathcal{I}_2^2-\mathcal{I}_1^2)-\mathcal{I}_2}.\tag{12}$$

The integrals f and g are well known in the theory of random walks (RW’s) [9]; the former, in particular, has a well defined physical meaning: it gives the *mean time* spent on the origin for a random walker in a d-dimensional hypercubic lattice (times $1/d$). In other words $1-d/f$ is the probability of return of a random walker to his starting point. We use an integral representation to write them in a simpler form:

$$f=\int_0^\infty du\,e^{-du}I_0(u)^d,\quad g=\int_0^\infty du\,e^{-(d+1/t)u}I_0(u)^d.\tag{13}$$

Here $I_0(u)$ is the usual modified Bessel function of integer order. The mathematical properties of f and g are central to our solution and then we will summarize them in more detail. All results below hold in the ranges: $d\in[0,\infty)$ and $t\in(0,1]$ [8].

Both f and g are positive strictly convex decreasing functions of d, converging to 0^+ for $d\rightarrow\infty$. Moreover we have that $f>g$ $\forall t\in(0,1]$. It is interesting to look at their behavior in some extreme situations. If we perform an asymptotic development of g for t close to 0 we get the result $g=t-dt^2+O(t^3)$. Moreover we find that

$$f=\frac{1}{d}\left[1+\frac{1}{2d}+\frac{3}{4d^2}+\frac{3}{2d^3}+O\left(\frac{1}{d^4}\right)\right], \tag{14}$$

$$g=\frac{1}{d+1/t}+\frac{d}{2(d+1/t)^3}+\frac{3d^2}{4(d+1/t)^5}+O\left(\frac{1}{d^4}\right), \tag{15}$$

from the asymptotic developments at large d. Perhaps the most important property of the two above integrals is that f is a divergent integral for $d=1,2$ while it is finite for $d>2$ (e.g., see [9]). The second one, g, is finite, on the other hand, $\forall d$. In the RW theory the divergence of f for $d<3$ leads to the well-known result that the total probability of return of a random walker to his starting point is 1 only for dimensions less than 3. Our solution shows directly how this pure topological effect plays a central role in the context of the depinning transition for directed polymers.

For $d=1$, g can be explicitly calculated and by taking the dominant contribution of (12) at diverging f, the criticality condition becomes

$$\frac{u}{T}=\ln\left(1-\frac{B}{1+B(2-\sqrt{1+2t})}\right), \tag{16}$$

which confirms the result obtained by Nechaev and Zhang in the same context [6]. Let us now turn back to Eq. (12) for the general case. At $t=0$, or equivalently $J\rightarrow\infty$, the polymer is a rigid straight line and then it is in the pinned (or unpinned) phase depending on the sign of the difference $u-v$. This result is indeed contained in our solution: by asymptotically expanding g for small t (see above) we finally find

$$A=-\frac{B}{B+1}+\frac{4+4B-B^2(df-1)}{f(B+1)^2}t+O(t^2). \tag{17}$$

We see that, as expected, at vanishing hopping constant t there is no more dependence on the dimensionality; and solving for the pinning strength one gets the result that $A(B+1)=-B$ or $u=v$. The "phase diagram" on the plane u-v is then represented in this case by a single straight line bisecting the whole space (see Fig. 1). In the above semispace $(u>v)$ the polymer is in a bound state, while in the lower one $(u<v)$ it is completely delocalized.

What does happen if the hopping constant t is different from 0? In, by now, standard notation we define u_c as the value of the force on the attractive sites which satisfies (12) for a given set $\{d,t,v\}$. For $B=0$, or equivalently $v=0$, the potential layer is made of alternating attractive and neutral sites and the criticality condition reads $u_c=T\ln(1+1/\mathcal{I}_2)$. This is an exact formula valid in all dimensions. Since f (and then $\mathcal{I}_2$) diverges for $d<3$, an arbitrarily small $u=\delta>0$ is enough to localize the polymer, according to well-known general results, while for $d\geqslant 3$ we need a finite value

$$e^{u_c/T}=2d+\frac{-1+2t-2t^2}{t^2}+\frac{1-2t+t^3-3t^4}{2t^4}\frac{1}{d}+O\left(\frac{1}{t^6d^2}\right), \tag{18}$$

to do the job (this phenomenon has also a quantum mechanical counterpart [10]). Moreover that critical attractive force diverges logarithmically at large d. The same result we get in the more familiar case $v=-u$ representing an extended linear attractive defect. In this case one finds

$$\frac{u_c}{T}=\ln\left[1+\frac{1}{\mathcal{I}_1+\mathcal{I}_2}\right], \tag{19}$$

which gives, at $d=1$, a known result, i.e., $u_c=0$. Figure 2 shows the shape of u_c/T as a function of the dimension d in that case.

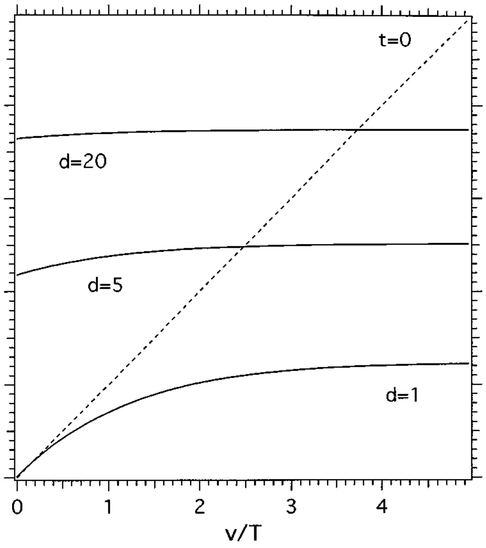

FIG. 1. Critical curves u_c/T vs v/T for different values of t and d calculated by numerically integrating f and g (see text). Above (below) them the system is in a bound (unbound) state for the partition function. At vanishing hopping constant $(t=0)$ the depinning line is the diagonal of the phase space u-v. For $t>0$ and $d>2$ we need a finite value of the potential u to pin the polymer.

An interesting aspect of our solution is that a bound state can take place at *all* finite dimensions d even if the potential

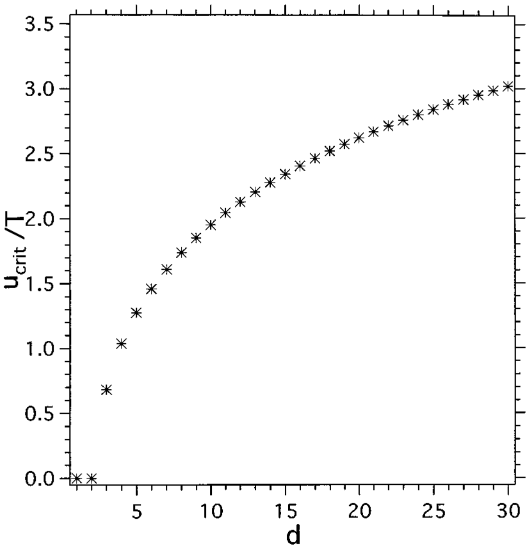

FIG. 2. The critical pinning (divided by T) necessary to localize the polymer as a function of d in the case of a uniform attractive potential (i.e., $v=-u$). The divergence of u_c/T with d is logarithmic (see text).

layer is, in average, repulsive ($v > u$). This is evident from Fig. 1 in which we have drawn the critical curves separating bound and unbound regions for different values of d as a function of the ‘‘reduced parameter’’ v/T. Above (below) the straight line $u = v$ the potential is, in average, attractive (repulsive). Then we see that for every fixed v and $\forall d$ (finite), one can find a finite value of u_c which localizes the polymer giving a bound state for the partition function. The more astonishing point is that one can simply prove from (12) that the critical curves asymptotically converge toward a finite u_c also in the extreme limit $v \to +\infty$:

$$\frac{u_c^{(\infty)}}{T} = \ln\left[1 + \frac{1+\mathcal{I}_2}{(\mathcal{I}_2^2 - \mathcal{I}_1^2) + \mathcal{I}_2}\right]. \tag{20}$$

Again, for $d = 1$, we recover the known result [6] $\exp(u_c^{(\infty)}/T) = \sqrt{1+2t}/(\sqrt{1+2t} - 1)$. The intuitive explication of this apparent paradox is that the polymer wanders in the space avoiding repulsive sites and passing through the potential layer on the attractive ones (preferentially). Some critical curves are shown in Fig. 1 for both $d < 2$ and $d > 2$ as functions of the reduced parameter v/T.

We recall that, as is obvious, instead of choosing u and v as ‘‘free parameters’’ in the above considerations, we could, in principle, directly look at the behavior of the system as a function of the temperature T [from Eq. (12)] with u and v fixed.

A potential layer breaks the translational symmetry of Ω and Goldstone modes are created, whose mass μ is finite for $T < T_c$ (i.e., in the pinned phase). The bound state can be expressed as $\mathcal{Z}(\mathbf{x}) \simeq \exp(-\mu|\mathbf{x}|)$ and the maximum eigenvalue as $\varepsilon \simeq 1 + \mu^2$. Moreover we have that near the transition $|f - f_c| \simeq \ln\varepsilon \simeq \varepsilon - 1$. At $d = 1$ one can show, by solving the partition sum [8], that the mass gap vanishes linearly with $(u - u_c)$, that is the phase transition is of second order and the transversal correlation length $\xi_\perp$ diverges as $(u - u_c)^{-1}$ at the critical point. At $d > 1$ the situation is less clear since integrations cannot be performed explicitly and one has to be careful in order to get the correct answers. Following Newman and Kallabis [11], we believe that one should find a very rich scenario in function of the dimensionality. In a recent work they study a deterministic KPZ equation [12] with a δ-shaped potential at the origin. The link between our model and this simplified version of the KPZ problem was already established some time ago [13]. In fact the binding-unbinding transition for a directed polymer can be mapped into the strong-weak coupling transition for the KPZ equation. We also believe that our exact solution could be useful to confirm the results of Ref. [11] in connection with the search for an upper critical dimension of the KPZ equation.

Conclusion: we have studied the problem of a polymer in a d-dimensional space in the presence of a linear extended defect with periodically arranged pinning sites and we have found the exact condition for the occurrence of the depinning transition. Exact formulas for the critical pinning are found in all dimensions. Perhaps the most interesting aspect of our system is that a bound state of the partition function can arise for all d even if the potential on the extended defect is more repulsive than attractive. As a final remark we point out that our method can also be used to get the complete form of the normalized partition sum in all dimensions; the complete calculation will appear in a forthcoming paper [8].

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