PHYSICAL REVIEW E **79**, 051127 (2009)

Directed polymer in random media with a defect

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(Received 19 February 2009; published 26 May 2009)

We investigate a directed polymer in random media with an attractive defect at the center of the one-dimensional substrate. Without the defect, the end to end distance Δx of the polymer follows $\Delta x \sim t^{1/z}$, with $z=3/2$ and t is the polymer length. When the defect strength ϵ is weak, its contribution to Δx is negligible. If $\epsilon \geq \epsilon_c$, then Δx approaches a finite value $\Delta x_{\text{sat}}(\epsilon)$ in large t limit, and we find $\Delta x_{\text{sat}} \sim (\epsilon - \epsilon_c)^{-\delta}$, with $\delta \approx 3.0$. Such transition is related to the queuing phenomena of the asymmetric simple exclusion process. The polymer energy fluctuation is also discussed.

DOI: 10.1103/PhysRevE.79.051127 PACS number(s): 05.40.−a, 68.35.Rh, 05.70.Ln

I. INTRODUCTION

A traffic jam commonly occurring in a bottleneck, behind slow moving trucks on single-lane highways, or near a road under construction is a typical example of queuing phenomena. Several attempts such as the asymmetric simple exclusion process (ASEP) [1–7] have been introduced to explain the relation between the queuing phenomena and a nonequilibrium driven dynamic process. In the ASEP with a slow bond, most particles jump into a vacant neighboring site in one direction with hopping probability one, and a fixed slow bond of hopping rate r, with $0<r<1$, plays a role of the bottleneck. Lots of studies have suggested that the critical hopping rate is one, $r_c=1$, i.e., the slow bond always gives rise to queuing phenomena [8–15]. However, some recent studies on the ASEP with a slow bond insist that a queuing transition of a jamming state exists at $r_c<1$. The overall flux passing through the slow bond is rarely influenced if the defect strength is not strong enough [16–20].

The ASEP can be mapped to the surface roughening problem of crystal growth such as the body-centered solid-on-solid interface model [21], where the height difference between the nearest neighbors is restricted by ±1. An increase (decrease) in surface height is equivalent to the presence (absence) of a particle in the ASEP. Both models belong to the Kardar-Parisi-Zhang (KPZ) universality class [22].

The directed polymer in random media (DPRM) [23,24] also has a close relation with the ASEP. An attractive line defect in two-dimensional DPRM corresponds to the slow bond in the ASEP. Here, we study the DPRM with an attractive defect in both a triangular structure and a square structure and measure various physical quantities to understand the queuing transition.

The Hamiltonian of DPRM with a defect at $\mathbf{x}=0$ is given as

$$\mathcal{H} = \int dt \left[\gamma \left(\frac{d\mathbf{x}}{dt} \right)^2 + \mu(\mathbf{x},t) - \epsilon \delta(\mathbf{x}) \right], \tag{1}$$

where $\mathbf{x}$ is the $d-1$ dimensional transverse vector, t is the polymer length perpendicular to the substrate, and $-\epsilon\delta(\mathbf{x})$ is a time-independent defect at $\mathbf{x}=0$, where ϵ controls the strength of the defect. There are three competing terms: a bending energy γ forcing the polymer straight against a transverse bending, the random potential $\mu(\mathbf{x},t)$ assigned to each point $(\mathbf{x},t)$ preferring the polymer to be deformed through the minimum potentials, and the attractive defect at $\mathbf{x}=0$ forcing the polymer return to the origin. This defect plays the same role as the slow bond in the ASEP. The random potential $\mu(\mathbf{x},t)$ is a white noise satisfying

$$\langle \mu(\mathbf{x},t)\mu(\mathbf{x}',t')\rangle = 2D\delta(t-t')\delta^{d-1}(\mathbf{x}-\mathbf{x}'). \tag{2}$$

The partition function $Z(\mathbf{x},t)$ for the polymer, starting from (0,0), and ending at $(\mathbf{x},t)$, can be written as the path integral [23]

$$Z(\mathbf{x},t) = \int_{(0,0)}^{(\mathbf{x},t)} \mathcal{D}\mathbf{x}'(t') \exp\left\{ -\frac{1}{T}\int_0^t dt' \left[\gamma\left(\frac{d\mathbf{x}'}{dt'}\right)^2 + \mu(\mathbf{x}',t') - \epsilon\delta(\mathbf{x}') \right] \right\}, \tag{3}$$

and it satisfies

$$\frac{\partial Z(\mathbf{x},t)}{\partial t} = \left[\frac{T}{2\gamma}\nabla^2 - \frac{1}{T}\mu(\mathbf{x},t) + \frac{\epsilon}{T}\delta(\mathbf{x}) \right] Z(\mathbf{x},t), \tag{4}$$

where T is the temperature. The related free energy is defined as

$$F(\mathbf{x},t) \equiv -T \ln Z(\mathbf{x},t). \tag{5}$$

Then, with $\epsilon=0$, the free energy satisfies the KPZ equation [22]

$$\frac{\partial F(\mathbf{x},t)}{\partial t} = \nu\nabla^2 F(\mathbf{x},t) + \lambda[\nabla F(\mathbf{x},t)]^2 + \eta(\mathbf{x},t), \tag{6}$$

where $\eta(\mathbf{x},t)$ is a random noise proportional to $\mu(\mathbf{x},t)$. Thus, the free energy $F(\mathbf{x},t)$ of the DPRM plays the same role as the height variable $h(\mathbf{x},t)$ of the growth model [24].

II. MODEL AND NUMERICAL RESULTS

At zero temperature the entropy is ignored and then the problem in Eq. (1) becomes much simplified by finding the

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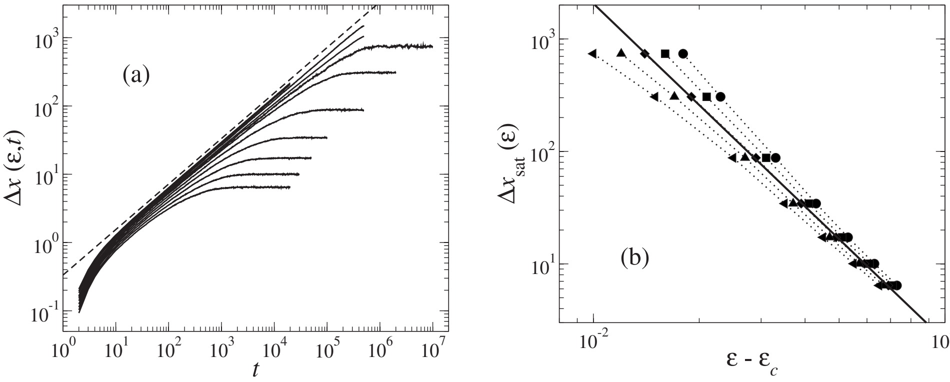

FIG. 1. (a) $\Delta x(\epsilon,t)$ as a function of t on a discrete triangular structure with ϵ=0.00, 0.01, 0.02, 0.03, 0.035, 0.04, 0.05, 0.06, 0.07, 0.08, and 0.09 from top to bottom. The data points up to $t=10^7$ are for ϵ=0.035. The dashed line has the slope of 2/3, corresponding to $1/z$ of the DPRM without defect. (b) $\Delta x_{\text{sat}}(\epsilon)$ as a function of $\epsilon-\epsilon_c$ for arbitrary critical values ϵ_c=0.011, 0.016, 0.021, 0.026, and 0.031 from right to left. The solid straight line is obtained at ϵ_c=0.021, where $\Delta x_{\text{sat}} \sim (\epsilon-\epsilon_c)^{-\delta}$ with δ=3.0.

optimal path and its energy $E(x,t)$ among all the paths arriving at (x,t). The initial energy $E(x,0)=0$ is given at $t=0$. A continuous random number between 0 and 1 with uniform distribution is assigned for the randomness $\mu(x,t)$ on a discrete structure. In addition, the attractive defect potential $-\epsilon$ is given at the center site $x=0$.

First we consider a polymer on a triangular structure. The polymer starts from $x=0$, and its path is restricted by $|x(t)-x(t+1)|=0$ or 1. There is a bending energy γ against a transverse jump $|x(t)-x(t+1)|=1$. The minimum energy $E(x,t)$ for the polymer ending at (x,t) can be obtained recursively [24] in $d=1+1$,

$$\begin{aligned} E(x,t+1) = \min\{&E(x,t) + \mu(x,t) - \epsilon\delta_{x,0}, E(x-1,t) \\ &+ \mu(x-1,t) + \gamma - \epsilon\delta_{x-1,0}, E(x+1,t) \\ &+ \mu(x+1,t) + \gamma - \epsilon\delta_{x+1,0}\}, \end{aligned} \tag{7}$$

where $\min\{A,B,C\}$ takes the minimum value among A, B, and C. We shall write $d=1+1$ to indicate that there is one transverse and one longitudinal direction. Following Eq. (7) the polymer energy at each site is updated in parallel.

We measure Δx, which is the root mean square of the end to end distance of the polymer as a function of t. In general it increases with t. Without the defect, Δx follows

$$\Delta x \sim t^{1/z}, \tag{8}$$

with $z=3/2$ [23–25]. The optimal path is affected by the strength of the defect ϵ as shown in Fig. 1(a). Its contribution to Δx seems to be negligible for small ϵ, where Δx still shows the power-law behavior with $z=3/2$. For large ϵ, Δx increases with t at initial stage and then approaches an asymptotic value Δx_{sat} in large t limit. Actually Δx_{sat} depends on ϵ. Due to the limitation of current computing power, it is hard to get Δx_{sat} for small value of $\epsilon<0.035$. We assume that Δx_{sat} diverges as ϵ approaches ϵ_c following a scaling law

$$\Delta x_{\text{sat}} \sim (\epsilon-\epsilon_c)^{-\delta}, \tag{9}$$

where ϵ_c is the critical defect strength. The log-log plot of Δx_{sat} against $(\epsilon-\epsilon_c)$ for various values of ϵ_c is given in Fig. 1(b). The most straight line is obtained for $\epsilon_c=0.021$ with $\delta=3.0$. It means that Δx_{sat} diverges at $\epsilon=\epsilon_c$. We would expect $\Delta x(t) \sim t^{2/3}$ for $\epsilon<\epsilon_c$.

Since the polymer energy $E(t)$ increases with t, we define the mean velocity of energy as $v(\epsilon,t) \equiv \partial\bar{E}(\epsilon,t)/\partial t$, which is the average energy density per unit length. It is related to the flux of the ASEP. The mean velocity depends on both the defect intensity ϵ and the polymer length t. It approaches a saturation velocity $v_s(\epsilon)$ in large t limit. We define the velocity difference due to the defect as

$$\Delta v(\epsilon) \equiv v_s(0) - v_s(\epsilon), \tag{10}$$

where $v_s(0)$ is the saturation velocity of the energy with $\epsilon=0$. If ϵ is less than ϵ_c actually, Δv approaches zero with t. Above ϵ_c, however, the defect site attracts the polymer strongly so that Δv becomes finite. We would expect

$$\Delta v \sim \begin{cases} 0 & \text{if } \epsilon<\epsilon_c \\ (\epsilon-\epsilon_c)^{\beta} & \text{otherwise}. \end{cases} \tag{11}$$

We measure Δv as a function of ϵ and plot Δv as a function of $(\epsilon-\epsilon_c)$ for various values of ϵ_c as shown in Fig. 2(a). The best power-law behavior is obtained from ϵ_c=0.021 in good agreement with the critical value obtained from Δx. The measured value of β is near 2.76.

In analogy with the surface problem, we also consider a square structure of system size L with a periodic boundary condition on the lateral direction. The mean velocity $v(L,\epsilon,t)$ depends on the system size L also. At the critical point ϵ_c=0.021, the velocity difference is expected to follow

$$\Delta v(\epsilon_c) \sim L^{-x_\Delta}. \tag{12}$$

Figure 2(b) shows $\Delta v(L,\epsilon_c)$ for various system sizes in log-log plot, where the dashed line shows a power-law behavior very well with x_Δ=0.82(2). From both Eqs. (11) and (12), one can guess a scaling form [19]

$$\Delta v(L,\epsilon) \sim L^{-x_\Delta} f[L^{y}(\epsilon-\epsilon_c)], \tag{13}$$

where $f(u)$ is u^β for $u>0$ and 0 for $u<0$ with $y=x_\Delta/\beta$. In Fig. 3 all the scaled data for various system sizes collapse very well with x_Δ=0.82, y=0.297, and ϵ_c=0.021. It seems that Δv follow the scaling behavior of Eq. (13). For $\epsilon<\epsilon_c$,

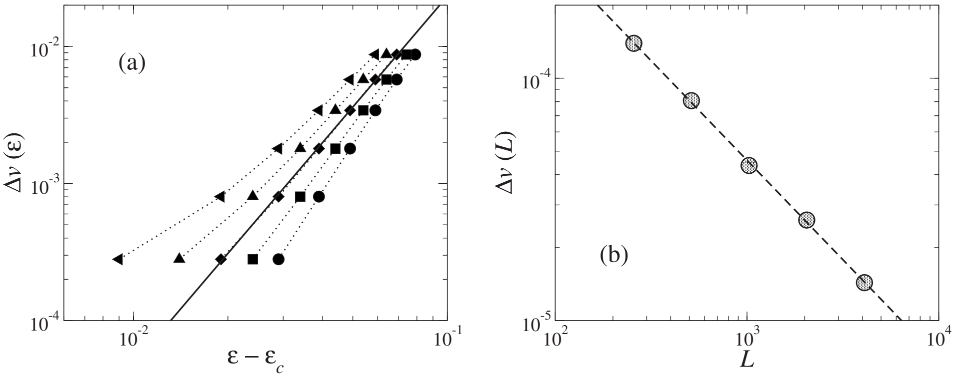

FIG. 2. (a) Δv as a function of $\epsilon-\epsilon_c$ for arbitrary values $\epsilon_c=0.011$, 0.016, 0.021, 0.026, and 0.031 from right to left. The most straight line is obtained at $\epsilon_c=0.021$, where $\Delta v\sim(\epsilon-\epsilon_c)^{\beta}$ with $\beta=2.76$. (b) The plot of Δv as a function of L at $\epsilon=0.021$, where the dashed line shows the power-law behavior $\Delta v\sim L^{-x_\Delta}$ with $x_\Delta=0.82$.

Δv remains almost zero implying that the defect does not alter the polymer energy.

Another interesting quantity in the finite system size is the fluctuation of the ground-state energies,

$$\Delta E(L,t)=\langle(E-\bar{E})^2\rangle^{1/2}, \tag{14}$$

where $\bar{E}$ denotes the mean energy averaged over the space. The angular brackets denote the configurational average, i.e., the average over many realizations of the noise. Since the energy is interpreted as the surface height of growth model, the energy fluctuation $\Delta E(L,t)$ corresponds to the surface width $W(L,t)$, the standard deviation of the height. The energy fluctuation $\Delta E(t)$ increases with t and becomes saturated in large t limit. So $\Delta E(L,t)$ is as follows [24]:

$$\Delta E(L,t)\sim\begin{cases}L^{\alpha}f(t/L^{z})\\ t^{\omega} & \text{if } t\ll L^{z}\\ L^{\alpha} & \text{if } t\gg L^{z},\end{cases} \tag{15}$$

where the scaling function $f(x)$ is x^{ω} for $x\ll1$ and constant for $x\gg1$. Without the defect ($\epsilon=0$), the exponents α, ω, and z are connected by the relation $z\omega=\alpha$ and $\alpha+z=2$ [21] which comes from the invariance of the KPZ equation for the Galilean transform. Thus, there is only one independent exponent that has to be determined. The exponents are known to be $\omega=1/3$ and $z=3/2$ in $d=1+1$.

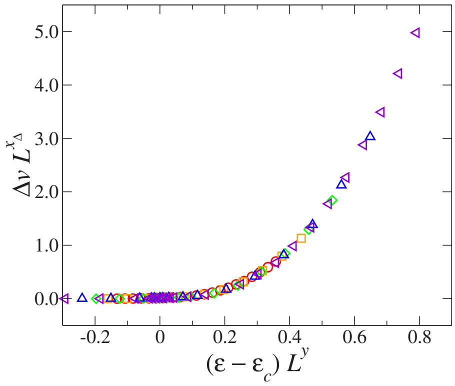

FIG. 3. (Color online) Data collapse of Δv following Eq. (13) with $x_\Delta=0.82$, $y=0.297$, and $\epsilon_c=0.021$ for $L=257$ (circles), 513 (squares), 1025 (diamonds), 2049 (up triangles), and 4097 (left triangles).

Here we also monitor $\Delta E(\epsilon,t)$ on a square lattice substrate. It increases with the strength of the line defect [20]. The inset of Fig. 4 shows that the saturation value $\Delta E_{\text{sat}}(\epsilon)$ seems to be almost independent of the defect strength ϵ for $\epsilon<\epsilon_c$ and it increases with ϵ for $\epsilon>\epsilon_c$. To check the effect of ϵ we consider a relative quantity $Q(\epsilon)$ [20],

$$Q(\epsilon)\equiv\frac{[\Delta E_{\text{sat}}(\epsilon)]^2-[\Delta E_{\text{sat}}(0)]^2}{[\Delta E_{\text{sat}}(0)]^2}, \tag{16}$$

where $\Delta E_{\text{sat}}(0)$ is the saturation energy fluctuation at $\epsilon=0$. As shown in Fig. 4, $Q(\epsilon)$ is almost zero for $\epsilon\le0.02$ and it increases with ϵ for $\epsilon>0.02$. They are consistent with the previous results that there is a phase transition near $\epsilon_c\approx0.021$.

III. SUMMARY

A directed polymer in random media with an attractive defect in the middle of one-dimensional substrate is studied. The end to end distance Δx of the polymer is measured as a function of the polymer length t and the defect strength ϵ. The contribution of the defect to Δx is negligible for $\epsilon<\epsilon_c$, so Δx still increases with t, i.e., $\Delta x\sim t^{2/3}$. For $\epsilon>\epsilon_c$, Δx increases with t at the beginning and becomes saturated for large t. There is a localization transition (the queuing transition in ASEP) at finite $\epsilon_c\approx0.021$. The polymer is not localized for small attractive defect. However, it is localized for $\epsilon>\epsilon_c$. Since there exists a mapping between the ASEP and

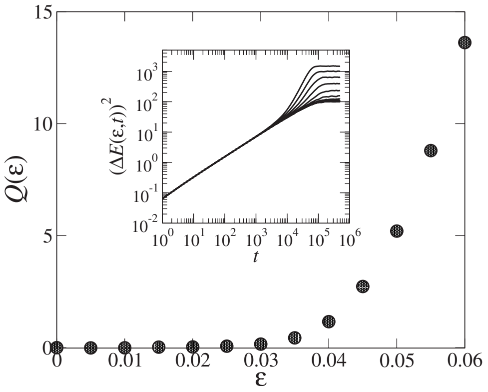

FIG. 4. The plot of $Q(\epsilon)$ as a function of ϵ from $\Delta E_{\text{sat}}(\epsilon)$. In the inset, $\Delta E(\epsilon,t)$ is monitored as a function of t for $L=4097$ with $\epsilon=0.0,0.005,0.010,\ldots,0.060$ from bottom to top.

the DPRM, we would expect the queuing transition in the ASEP. The Δx obtained in a triangular structure depends on t only. In principle, Δx_{sat} does not have any system size effect. The polymer energy per unit length in square lattice depends on both L and t. From the finite-size scaling of the mean energy velocity in square lattice, we obtain $\beta=2.76$, $x_{\Delta}=0.82$, and $y=0.297$. Our value of y exponent 0.297 is a bit higher than 0.253 in ASEP of Ref. [19]. The polymer energy fluctuation data in the square lattice also support that there exists a phase transition. Analytic works and larger simulations are required to get more accurate values of the critical exponents.

ACKNOWLEDGMENTS

We wish to thank Hwajeong Choi for numerical help and Meesoon Ha and Hyun Suk Song for useful discussion. This work was supported by Korean Government (Grant No. KRF-2008-314-C00143) and the Soongsil University Research Fund.

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