Directed polymers at finite temperatures in 1+1 and 2+1 dimensions

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We present systematic numerical simulations for directed polymers at finite temperatures in 1+1 and 2+1 dimensions. The transverse fluctuations and free energy fluctuations tend to the strong coupling limit at any temperature in both 1+1 and 2+1 dimensions for long time t. Two different definitions for energy fluctuations at finite temperatures, which are the ensemble energy fluctuations and the internal energy fluctuations, are investigated. Apart from zero temperature, the behavior of the energy fluctuations and the free energy fluctuations for directed polymers is shown to be different. At finite temperatures, the ensemble energy fluctuations in both 1+1 and 2+1 dimensions and internal energy fluctuations in 1+1 dimensions scale as $t^{1/2}$ where the free energy fluctuations in 1+1 dimensions and 2+1 dimensions scale as $t^{1/3}$ and $t^{0.2}$ respectively. As a consequence of that the specific heat in both 1+1 and 2+1 dimensions scales as t and the entropy fluctuations in 1+1 dimensions scale as $t^{1/2}$ at any finite temperature.

Introduction

Rough surfaces and interfaces are found in a wide variety of natural and industrial processes. The KPZ equation provides a good quantitative understanding of surface growth phenomena[1−5]. It is well known that the KPZ equation is equivalent to the problem of directed polymers in a random medium[6−9], which has attracted much attention in recent years. The problem of directed polymers is also relevant to many other fields ranging from paper rupture[10] and spin glasses[11] to high-T_c superconductors[12]. The KPZ equation provides the exact dynamical exponent for directed polymers in 1+1 dimesions[6−8]. A self-consistent expansion of the correlation function[13] yields results compatible with simulations for 2+1 dimensions. Above 2+1 dimensions, the behavior of directed polymers has a phase transition when temperature is raised and the system goes over from the strong coupling behavior to a perturbative behavior[13−18]. The strong coupling behavior has been studied by extensive numerical investigations for the energy fluctuation at zero temperature[6,8,19−21], which is ensemble fluctuations of the ground state energy of directed polymers. At finite temperatures, fluctuations of the free energy have been studied extensively but it seems that quantities like fluctuations of the internal energy have not received much attentions.

In this article, we present systematic numerical simulations for directed polymers in 1+1 and 2+1 dimensions. Our numerical simulations show that the transverse fluctuation and free energy fluctuation crossover to the strong coupling behavior at any finite temperature in both 1+1 and 2+1 dimensions, in agreement with the predictions of the field theory[13,22,23]. We define the energy fluctuations at finite temperatures using two different definitions: the ensemble energy fluctuations and the internal energy fluctuations. The difference between the two definitions is related to the specific heat. We find that the behavior of the energy fluctuation at finite temperatures is different from that at zero temperature. For understanding the energy fluctuations at finite temperatures, we introduce the entropy and study its fluctuation. The behavior of the energy fluctuations at finite temperatures can be understood after investigating the specific heat and the entropy fluctuations.

Model

Consider a directed polymer on a hyperpyramid lattice structure with the random energy assigned on each bond. The partition function $G(x,t)$ for directed polymers starting from $(0,0)$ and ending at (x,t) is defined by $G(x,t) = \sum_C e^{-E_C/T}$ where E_C is the sum of the energies on the path C and T is the temperature. The iteration relation for the partition function $G(x,t)$ is

$$G(x,t+1) = G(x-1,t)e^{-\epsilon_l/T} + G(x+1,t)e^{-\epsilon_r/T}, \qquad (1)$$

in which, ϵ_l and ϵ_r are the energy assigned to the left and right bonds of the point (x,t). The free energy $F(t)$ is given by $F(t) = -TlnG(t)$, where $G(t) = \sum_x G(x,t)$ is the total partition function. The transverse fluctuation Δx for the directed polymers is $(\overline{\langle x^2 \rangle})^{1/2}$ where $\langle x^2 \rangle = \sum_x x^2 G(x,t)/G(t)$ ($\overline{A}$ is the ensemble average of the quantity

A). The transverse fluctuation Δx and free energy fluctuation $\Delta F = (\overline{F^2} - \overline{F}^2)^{1/2}$ have been commonly studied. Another interesting quantity for directed polymers is the energy fluctuation. It is clear that the energy fluctuation at zero temperature is just that of the free energy. For finite temperatures, we propose two definitions for the energy fluctuations. One is the *ensemble energy fluctuation* and the other is *internal energy fluctuation*. The ensemble energy fluctuation is defined by $(\Delta E)_B \equiv (\overline{\langle E^2\rangle} - \overline{\langle E\rangle}^2)^{1/2}$, in which $\langle E\rangle$ is the internal energy:

$$\langle E\rangle = \frac{\sum\limits_x \sum\limits_C E_C e^{-E_C/T}}{\sum\limits_x \sum\limits_C e^{-E_C/T}} = T^2 \frac{\partial lnG}{\partial T} \tag{2}$$

and

$$\langle E^2\rangle = \frac{\sum\limits_x \sum\limits_C E_C^2 e^{-E_C/T}}{\sum\limits_x \sum\limits_C e^{-E_C/T}} = T^2 \frac{\partial}{\partial T}[T^2 \frac{\partial lnG}{\partial T}] + [T^2 \frac{\partial lnG}{\partial T}]^2. \tag{3}$$

The internal energy fluctuation is defined by $(\Delta E)_T \equiv (\overline{\langle E\rangle^2} - \overline{\langle E\rangle}^2)^{1/2}$. It is obvious that both the two energy fluctuations will degenerate into the fluctuation of the sum of the energy on the optimal path when temperature tends to zero. From the equations (2) and (3), we have

$$(\Delta E)_B^2 = (\Delta E)_T^2 + T^2 C(T,t) \tag{4}$$

where $C(T,t) = \frac{\partial}{\partial T}[T^2 \frac{\partial lnG}{\partial T}] = \frac{\partial \langle E\rangle}{\partial T}$ is the specific heat[24].

In order to understand the internal energy fluctuation , we use the entropy as $S = (\langle E\rangle - F)/T$ and the entropy fluctuation is $\Delta S = (\overline{S^2} - \overline{S}^2)^{1/2}$. It is easy to see that

$$(\Delta S)^2 = \frac{1}{T^2}[(\Delta E)_T^2 + (\Delta F)^2] - \frac{2}{T^2} B(T,t), \tag{5}$$

where $B(T,t) = \overline{\langle E\rangle F} - \overline{\langle E\rangle}\ \overline{F} = -\frac{1}{2} T^3 \frac{\partial}{\partial T}[(\Delta F)^2/T^2]$.

The above quantities can be calculated by the iteration relations given in Appendix. In the following, we present systematic numerical simulations based upon the equation (1) and equation (A1) and (A2) from the Appendix with the initial conditions $G(x,0) = \delta_{x,0}$, $\widehat{E}(x,0) = 0$ and $\widehat{E}_2(x,0) = 0$. The random energy assigned on the bond is assumed to be uniformly distributed in the interval (-0.5,0.5) and uncorrelated in space and time. The effective program RAN2 was used for generating the uniform distributed random number[25]. We use length up to $t = 2000$ ($d = 1+1$) and $t = 150$ ($d = 2+1$). Six thousands configurations for 1+1 dimensions and four thousands configurations for 2+1 dimensions were collected for the ensemble average. In order to avoid unstability, we normalize the partition function at every time step.

Directed polymers in 1+1 and 2+1 dimensions

At infinite temperature, directed polymers become random walks: the transverse fluctuation Δx will scales as $t^{1/2}$ and the ensemble energy fluctuation will be $(\Delta E)_B \propto t^{1/2}$ because the ensemble energy fluctuation at N time steps is only the variance of the sum of N uncorrelated random numbers at the limit. The free energy fluctuation for infinite temperature can be predicted by the Edwards-Wilkinson equation[26−28] that describes the linear surface growth phenomena. It follows that the free energy fluctuation ΔF scales as $t^{1/4}$ in 1+1 dimensions and tends to the logarithmic behavior in 2+1 dimensions.

When approaching zero temperature, the system will take the strong coupling behavior. Our simulations show that the transverse fluctuation scales as t^{ν} and both the free energy and energy fluctuations scales as t^{ω}, in which $\nu = 2/3, \omega = 1/3$ for $d = 1+1$ and $\nu \approx 0.6, \omega \approx 0.2$ for $d = 2+1$. These results are in agreement with the theoretical treatments and the previous numerical works[6−9,13,19−20].

The problem of directed polymers in 1+1 and 2+1 dimensions at finite temperatures is investigated. Our simulations show that the transverse fluctuation Δx crossovers from $t^{1/2}$ to $t^{2/3}$ and the free energy fluctuation ΔF crossovers from $t^{1/4}$ to $t^{1/3}$ in 1+1 dimensions at any finite temperature (see Fig. 1) in agreement with earlier arguments[29]. The scaling relations $\Delta x = T^2 f_1(T^{-4}t)$ and $\Delta F = T g_1(T^{-4}t)$, which describe the crossover from the Edwards-Wilkinson behavior to KPZ behavior in 1+1 dimensions given by Amar and Family using the scaling analysis[29] , are confirmed for $T > 0.25$ (see Fig. 2).

Similar to 1+1 dimensions, the transverse fluctuation Δx and free energy fluctuation ΔF crossover from $t^{1/2}$ to $t^{0.6}$ and from the logarithmic behavior to $t^{0.2}$ respectively in 2+1 dimensions (see Fig. 3). For 2+1 dimensions, we can fit the data very well using $(\Delta F)^2 = 0.0068 ln(1+20t)$ at very high temperature. Assuming the scaling relations $\Delta x = Tf_2(T^{-2}t)$ for $T > 0.1$ and $\Delta F = Tg_2(T^{-2}ln(1+20t))$ for $T > 0.2$, the data collapse very well (see Fig. 4). We note that an argument for the crossover time $lnt_\times \sim T^2$ for the free energy fluctuation has been given earlier[16,22-23]. Also note that our numerical data suggest that the crossover time for Δx and ΔF are different.

The difference between the two different definitions for the energy fluctuation is proportional to the specific heat as shown in equation (4). Our simulations shows that that specific heat $C(T,t) \to 0$ for $T \to 0$ as $O(T^\alpha)$ where $\alpha = 1.3$ for $d = 1+1$,$\alpha = 1.6$ for $d = 2+1$ and $C(T,t) \to \sigma^2/T^2$ for $T \to \infty$ where $\sigma = (\frac{1}{12})^{1/2}$ is the variance of the random numbers. We also find that the specific heat scales as t at any temperature in both 1+1 and 2+1 dimensions (see Fig. 5). Fig. 6 shows that the ensemble energy fluctuations $(\Delta E)^2_B$ scale as t as the specific heat apart from zero temperature. We find very good fit with the scaling relations $(\Delta E)^2_B = e^{1/T}h_1(e^{-1.5/T}t)$ in 1+1 dimensions and $(\Delta E)^2_B = e^{0.2/T}h_2(e^{-0.5/T}t)$ in 2+1 dimensions for $T \leq \frac{1}{3}$ (see Fig. 7). Howevever, in both 1+1 and 2+1 dimensions, the picture for the internal energy fluctuation is not clear (see Fig. 8). We note that the internal energy fluctuations is not monotonic with the temperature. But, at the two limits of zero and infinite temperatures, the internal energy and free energy fluctuations are the same in both 1+1 and 2+1 dimensions. For investigating the difference between the internal energy fluctuations and the free energy fluctuations, we study the entropy fluctuations.

Entropy is an important physical quantity for characterizing the disorderd systems. Fig. 9 shows that the entropy fluctuation has the behavior $(\Delta S)^2 \propto t$ at any temperature in 1+1 dimensions. This result is in agreement with earlier arguments of Fisher and Huse[30]. The entropy fluctuation $(\Delta S)^2$ reaches a maximum about $T = T_P = 0.2$ and tends to zero as $O(T^{-4})$ when $T \to \infty$ and as $O(T)$ when $T \to 0$ (see Fig. 10). It follows that the internal energy fluctuation and the free energy fluctuation are the same at infinite temperature and the energy fluctuation and the free energy fluctuation are the same at zero temperature. The function $B(T,t)$ in the equation (5) can also be calculated numerically. From the equation (5), it is easy to see that the function $B(T,t)$ is the same as the free energy fluctuation or the internal energy fluctuation at the two limits of zero and infinite temperature. At finite temperatures, Fig. 11a shows that the behavior of $B(T,t)$ is similar to that of the free energy fluctuation $(\Delta F)^2$ and also has a crossover from $t^{1/2}$ to $t^{2/3}$ in 1+1 dimensions. From the equation (5), we can expect that the internal energy fluctuations $(\Delta E)_T$ will scale as to $t^{1/2}$ as the behavior of the entropy fluctuations ΔS at finite temperatures in 1+1 dimensions.

Discussion

Using the iteration relations (1), (A1) and (A2), we study the problem of directed polymers in 1+1 and 2+1 dimensions. The transverse fluctuations and free energy fluctuations have a crossover from the EW behavior to KPZ behavior at finite temperatures in both 1+1 and 2+1 dimensions as predicted by the field theory. In order to understand the energy fluctuations at finite temperatures, we investigate the specific heat and the entropy fluctuations. The specific heat in both 1+1 and 2+1 dimensions and the entropy fluctuations $(\Delta S)^2$ in 1+1 dimensions scale as t at any finite temperature. As a result, the ensemble energy fluctuations in 1+1 and 2+1 dimensions and the internal energy fluctuations in 1+1 dimensions scale as $t^{1/2}$ at finite temperatures. It means that the energy fluctuations and the free energy fluctuations may have a different behavior at finite temperatures in both 1+1 and 2+1 dimensions. The behavior of the entropy fluctuations in 2+1 dimensions is more complicated than that in 1+1 dimensions. There is an indication of a phase transition in 2+1 dimensions. The phase transition occurs at the temperature where the entropy fluctuation reaches the maximum. This result will be published elsewhere[31]. Fig. 11b shows that the function $B(T,t)$ in 2+1 dimensions also has a crossover from the logarithmic behavior to $t^{0.2}$ at any finite temperature. As a result, the internal energy fluctuations in 2+1 dimensions also have a phase transition even if Fig. 8b can not show it clearly.

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Appendix: Iteration relations

As in deriving the iteration relation for the partition function $G(x,t)$ given by Eq. (1), we concentrate on the 1+1 dimensional case. The generlization to higher dimensions is obvious. In order to obtain the iteration relations for calculating the energy and entropy fluctuations, we define $\widehat{E}(x,t) \equiv \sum_{C(x,t)} E_{C(x,t)} e^{-E_{C(x,t)}/T}/G(t)$ and

$\widehat{E}_2(x,t) \equiv \sum_{C(x,t)} E^2_{C(x,t)} e^{-E_{C(x,t)}/T}/G(t)$. It is clear that $\langle E\rangle = \sum_x \widehat{E}(x,t)$ and $\langle E^2\rangle = \sum_x \widehat{E}_2(x,t)$. The derivation for the iteration relations for $\widehat{E}(x,t)$ and $\widehat{E}_2(x,t)$ are given as follows:

$$\begin{aligned}
&\widehat{E}(x,t+1) = \sum_{C(x,t+1)} E_{C(x,t+1)} e^{-E_{C(x,t+1)}/T}/G(t+1) \\
&= [\sum_{C(x-1,t)} (E_{C(x-1,t)} + \epsilon_l) e^{-(E_{C(x-1,t)}+\epsilon_l)/T} + \sum_{C(x+1,t)} (E_{C(x+1,t)} + \epsilon_r) e^{-(E_{C(x+1,t)}+\epsilon_r)/T}]/G(t+1) \\
&= [e^{-\epsilon_l/T}\widehat{E}(x-1,t)G(t) + e^{-\epsilon_r/T}\widehat{E}(x+1,t)G(t) + \epsilon_l e^{-\epsilon_l/T}G(x-1,t) + \epsilon_r e^{-\epsilon_r/T}G(x+1,t)]/G(t+1)
\end{aligned} \tag{A1}$$

and

$$\begin{aligned}
&\widehat{E}_2(x,t+1) = \sum_{C(x,t+1)} E^2_{C(x,t+1)} e^{-E_{C(x,t+1)}/T}/G(t+1) \\
&= [\sum_{C(x-1,t)} (E_{C(x-1,t)} + \epsilon_l)^2 e^{-(E_{C(x-1,t)}+\epsilon_l)/T} + \sum_{C(x+1,t)} (E_{C(x+1,t)} + \epsilon_r)^2 e^{-(E_{C(x+1,t)}+\epsilon_r)/T}]/G(t+1) \\
&= [e^{-\epsilon_l/T}\widehat{E}_2(x-1,t)G(t) + e^{-\epsilon_r/T}\widehat{E}_2(x+1,t)G(t) + 2\epsilon_l e^{-\epsilon_l/T}\widehat{E}(x-1,t)G(t) + 2\epsilon_r e^{-\epsilon_r/T}\widehat{E}(x+1,t)G(t) \\
&\quad + \epsilon_l^2 e^{-\epsilon_l/T}G(x-1,t) + \epsilon_r^2 e^{-\epsilon_r/T}G(x+1,t)]/G(t+1).
\end{aligned} \tag{A2}$$

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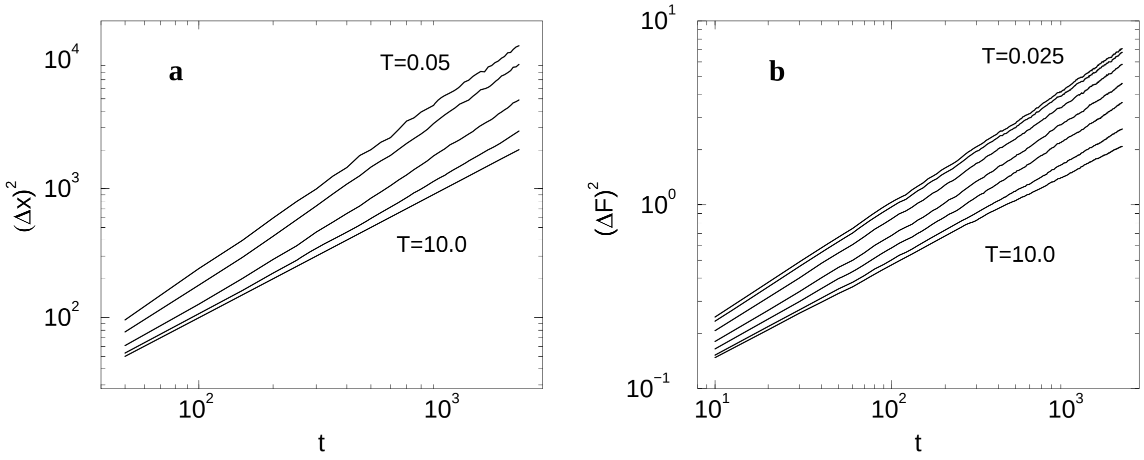

FIG. 1. (a) Plot of the transverse fluctuations $(\Delta x)^2$ as a function of time t at different temperatures $T = 10, 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{20}$ (from bottom to top) in $d = 1 + 1$ dimensions. (b) Plot of the free energy fluctuations $(\Delta F)^2$ as a function of time t at different temperatures $T = 10, 1, \frac{1}{2}, \frac{1}{3}, \frac{1}{5}, \frac{1}{10} \frac{1}{40}$ (from bottom to top) in $d = 1 + 1$ dimensions.

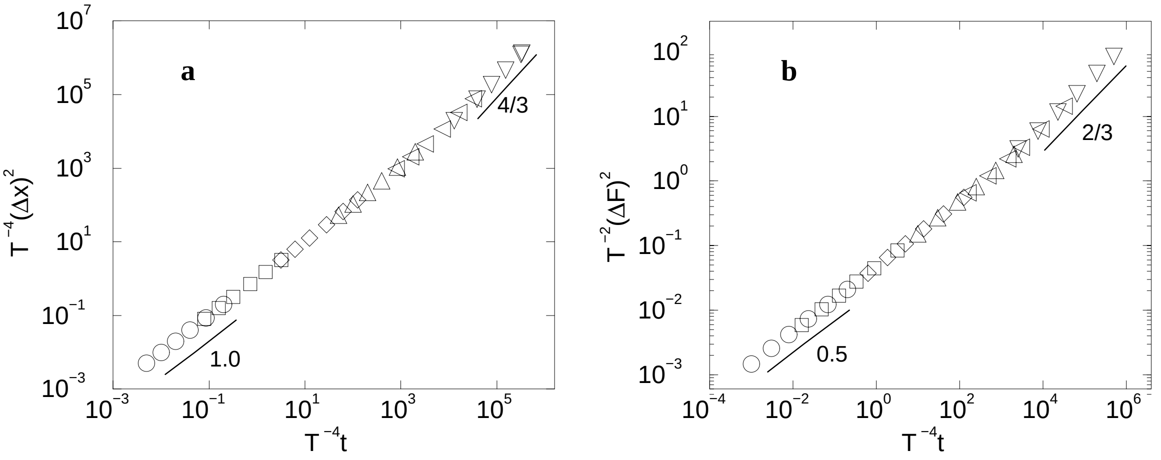

FIG. 2. Scaling plot for the transverse fluctuations $(\Delta x)^2$ shown in Fig. 1a and the free energy fluctuations $(\Delta F)^2$ shown in Fig. 1b for $d = 1 + 1$ dimensions where circle, square, diamond, triangle up, triangle left, triangle down correspond to different temperatures $T = 10, 5, 2, 1.0, 0.5, 0.25$ respectively.

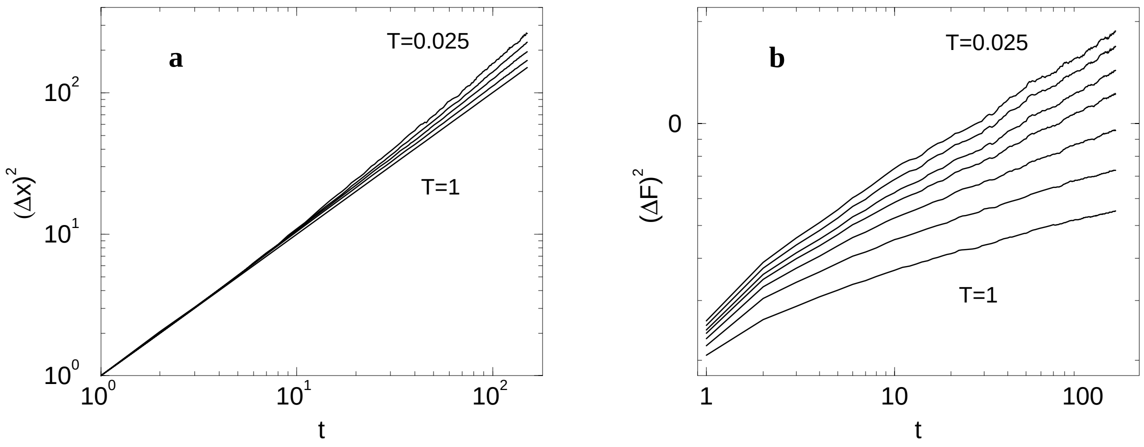

FIG. 3. (a) Plot of the transverse fluctuations $(\Delta x)^2$ as a function of time t at different temperatures $T = 1, \frac{1}{5}, \frac{1}{7}, \frac{1}{10}, \frac{1}{40}$ (from bottom to top) in $d = 2+1$ dimensions. (b) Plot of the free energy fluctuations $(\Delta F)^2$ as a function of time t at different temperatures $T = 1, \frac{1}{4}, \frac{1}{6}, \frac{1}{8}, \frac{1}{10}, \frac{1}{15}, \frac{1}{40}$ (from bottom to top) in $d = 2+1$ dimensions.

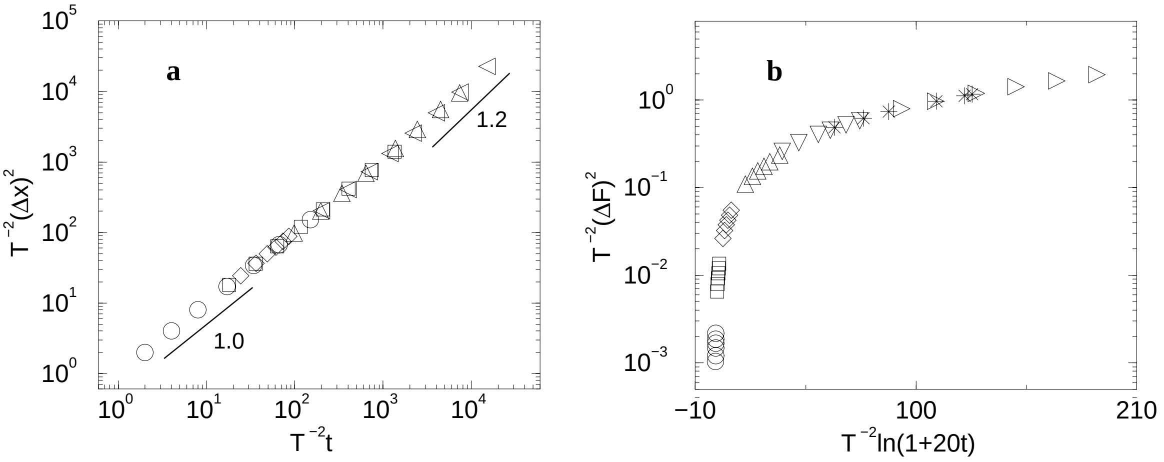

FIG. 4. (a) Scaling plot for the transverse fluctuations $(\Delta x)^2$ in $d = 2+1$ dimension where circle, square, diamond, triangle up, triangle left, correspond to different temperatures $T = 1, \frac{1}{3}, \frac{1}{5}, \frac{1}{7}, \frac{1}{10}$ respectively. (b) Scaling plot for the free energy fluctuations $(\Delta F)^2$ in $d = 2+1$ dimensions where circle, square, diamond, triangle up, triangle down, star, triangle right correspond to different temperatures $T = 5, 1, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}$ respectively.

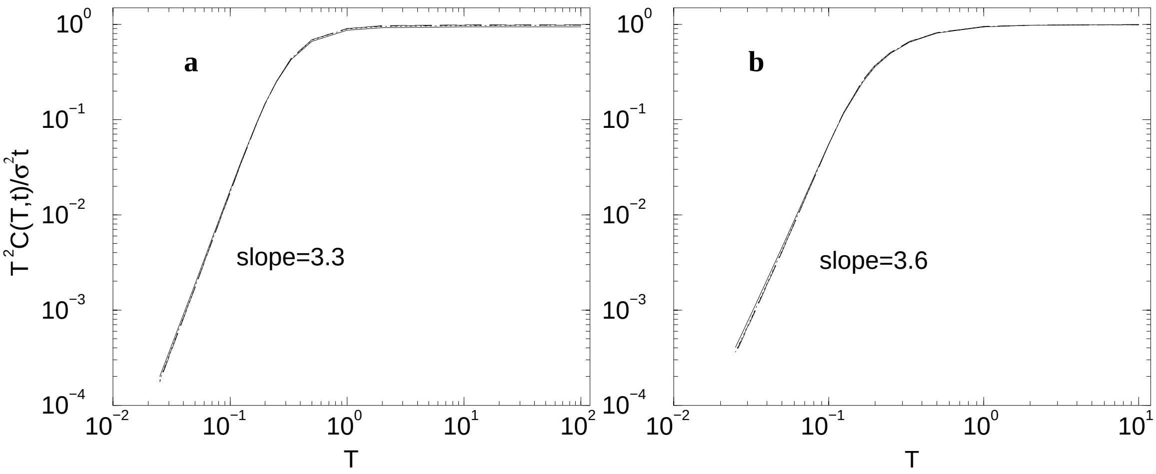

FIG. 5. Plot of the specific heat as a function of temperature, (a) for the different time $t = 100, 500, 1000, 2000$ in $d = 1 + 1$ dimensions and (b) for the different time $t = 50, 100, 120, 150$ in $d = 2 + 1$ dimensions.

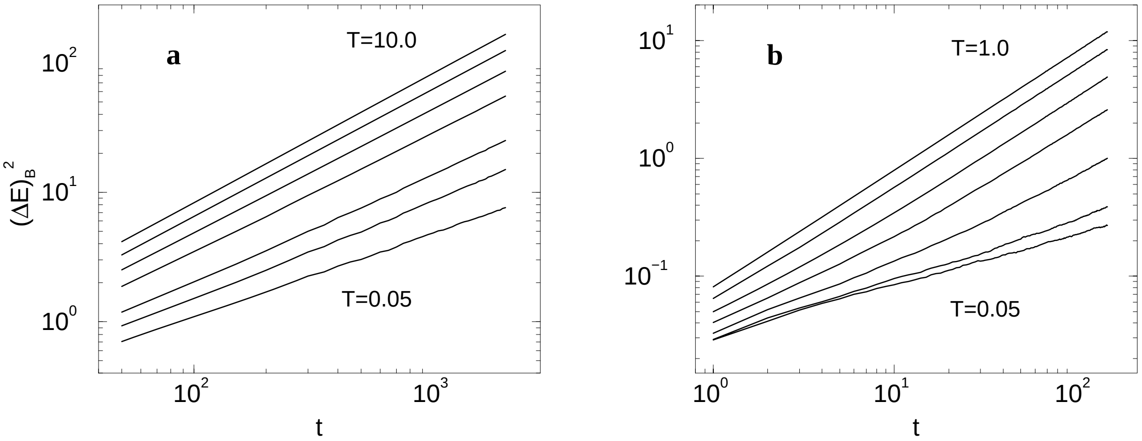

FIG. 6. Plot of the ensemble energy fluctuations $(\Delta E)_B^2$ as a function of time t, (a) for different temperatures $T = 10, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{6}, \frac{1}{8}, \frac{1}{20}$ (from top to bottom) in $d = 1{+}1$ dimensions and (b) for different temperatures $T = 1, \frac{1}{3}, \frac{1}{5}, \frac{1}{7}, \frac{1}{10}, \frac{1}{15}, \frac{1}{20}$ (from top to bottom) in $d = 2 + 1$ dimensions.

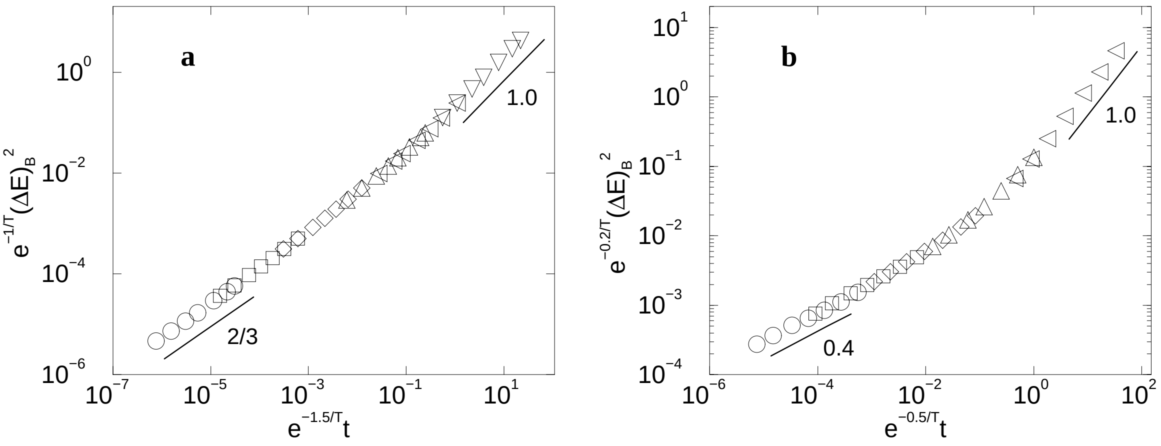

FIG. 7. (a) Scaling plot for the ensemble energy fluctuations $(\Delta E)_B^2$ in $d = 1+1$ dimensions where circle, square, diamond, triangle up, triangle left, triangle down correspond to different temperatures $T = \frac{1}{12}, \frac{1}{10}, \frac{1}{8}, \frac{1}{6}, \frac{1}{5}, \frac{1}{3}$ respectively. (b) Scaling plot in $d = 2+1$ dimensions where circle, square, diamond, triangle up, triangle left correspond to $T = \frac{1}{25}, \frac{1}{20}, \frac{1}{15}, \frac{1}{10}, \frac{1}{3}$ respectively.

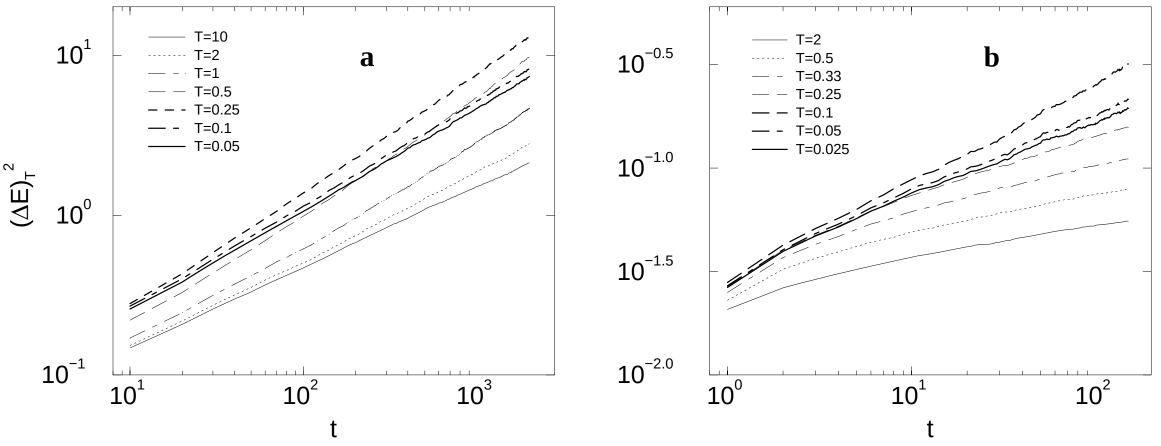

FIG. 8. Plot of the internal energy fluctuations $(\Delta E)_T^2$ as a function of time t, (a) in $d = 1+1$ dimensions and (b) in $d = 2+1$ dimensions.

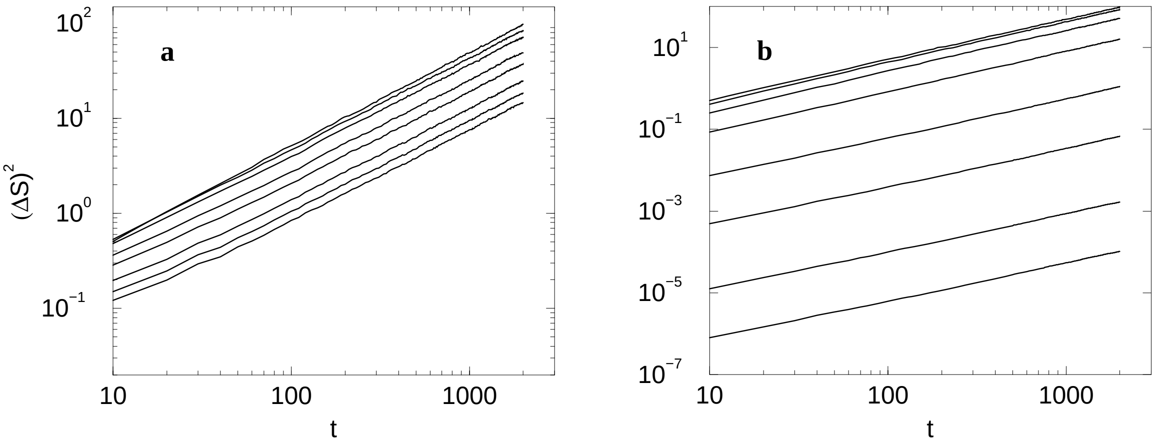

FIG. 9. Plot of entropy fluctuations $(\Delta S)^2$ as a function of time t in $d = 1 + 1$, (a) for different temperatures $T = \frac{1}{5}, \frac{1}{8}, \frac{1}{10}, \frac{1}{15}, \frac{1}{20}, \frac{1}{30}, \frac{1}{40}, \frac{1}{50}$ (from top to bottom) and (b) for different temperatures $T = 10, 5, 2, 1, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}$ (from bottom to top).

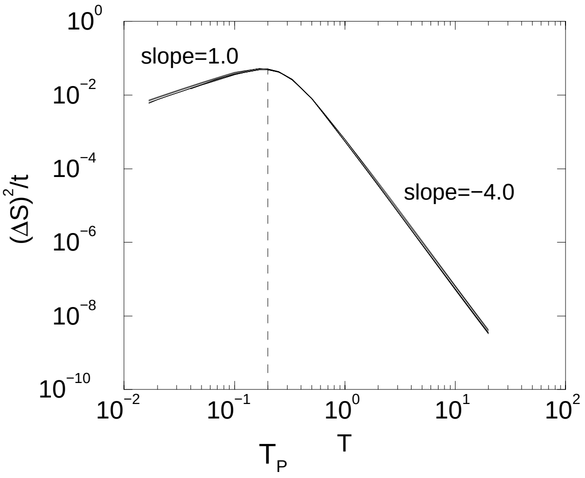

FIG. 10. Plot of entropy fluctuations per unit length of the polymer $(\Delta S)^2/t$ as a function of temperature T for the different time $t = 50, 500, 1000, 2000$ in $d = 1 + 1$ dimensions.

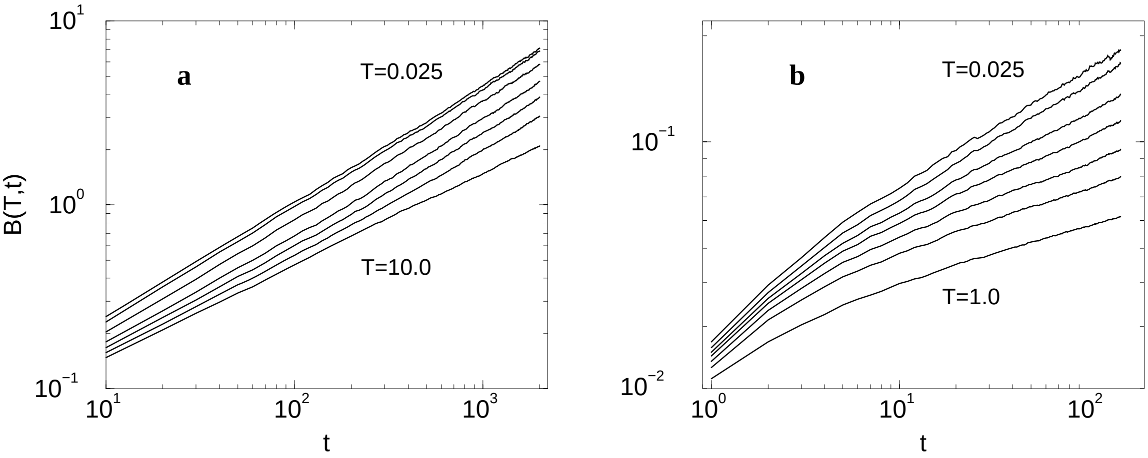

FIG. 11. Plot of the function $B(T,t)$ given in the equation (5) of the text as a function of time t, (a) for different temperatures $T = 10, 1, \frac{2}{3}, \frac{1}{2}, \frac{1}{3}, \frac{1}{5}, \frac{1}{40}$ (from bottom to top) in $d = 1+1$ dimensions and (b) for different temperatures $T = 1, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, \frac{1}{6}, \frac{1}{8}, \frac{1}{40}$ (from bottom to top) in $d = 2+1$ dimensions.