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On the speed of the one-dimensional polymer in the large range regime

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ABSTRACT

We consider a Hamiltonian involving the range of the simple random walk and the Wiener sausage so that the walk tends to stretch itself. This Hamiltonian can be easily extended to the multidimensional cases, since the Wiener sausage is well-defined in any dimension. In dimension one, we give a formula for the speed and the spread of the endpoint of the polymer path. Also, we provide the CLT. It can be easily showed that if the self-repelling strength is stronger, the end point is going away faster. This strict monotonicity of speed has not been proven in the literature for the one-dimensional case.

1. Introduction

1.1. The model and main results

A polymer consists of monomers. Monomers have tendency to repel each other because two monomers cannot occupy the same site. This phenomenon is called the excluded-volume-effect. There is a probabilistic way to model this physical phenomenon (cf. Madras and Slade, 1993, Section 2.2). We use the d-dimensional simple random walk $\{S_n\}_{\mathbb{N}\cup 0}$ under the probability measure P to represent the position of monomers and S_n to represent the end-point of the polymer chain with length n. $S_0 = 0$ and $S_n = \sum_{i=1}^{n} X_i$, where $(X_i)_{i\in\mathbb{N}}$ is a sequence of independent and identically distributed (i.i.d.) random variables. The distribution of X_i's is

$$P(X_1 = x) = \begin{cases} \dfrac{1}{2d}, & x \in \mathbb{Z}^d \text{ with } \|x\| = 1, \\ 0, & \text{otherwise.} \end{cases}$$

The random process $(S_n)_{n\in\mathbb{N}\cup 0}$ is called the *simple random walk* (SRW) on $\mathbb{Z}^d$. Suppose that the end-point has scale α_n, the local density of monomers will be $\frac{n}{\alpha_n^d}$. The self-repelling energy is approximately

$$\exp\left(Energy\right) \approx \exp\left(-\sum_{x\in\mathbb{Z}^d}\left(\frac{n}{\alpha_n^d}\right)^2 \mathbf{1}_{x \text{ is occupied}}\right) \approx \exp\left(-\alpha_n^d \times \left(\frac{n}{\alpha_n^d}\right)^2\right). \tag{1.1}$$

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On the other hand, by the local limit theorem of the simple random walk,

$$P(|S_n| = \alpha_n) \approx \exp(-C\alpha_n^2/n). \tag{1.2}$$

Let

$$\frac{n^2}{\alpha_n^d} = \frac{\alpha_n^2}{n}, \tag{1.3}$$

we get $\alpha_n = n^{\frac{3}{d+2}}$. It is expected that $|S_n| \sim n^{\frac{3}{d+2}}$ for $d = 1, 2, 3$, and $|S_n| \sim n^{1/2}$ for $d \geq 4$ with a logarithmic correction when $d = 4$ under the self-repelling phenomenon.

In this paper, we propose the following Hamiltonian

$$G_n := \frac{n^2}{R_n}, \tag{1.4}$$

where R_n is the number of sites occupied by the walk up to time $n-1$, that is,

$$R_n := \#\{x : \exists i,\ S_i = x,\ 0 \leq i \leq n-1\}. \tag{1.5}$$

Fix $n \in \mathbb{N}$ and a parameter $\beta \in (0, \infty)$, denote

$$Z_n^G := E\left(\exp\left(-\beta G_n\right)\right) \tag{1.6}$$

and

$$Z_n^G(A) := E\left(\mathbf{1}_A \exp\left(-\beta G_n\right)\right). \tag{1.7}$$

The polymer measure is then defined by

$$P_n^G(S) := \frac{e^{-\beta G_n(S)}}{Z_n^G} P(S). \tag{1.8}$$

β is called the strength of the self-repellence. This polymer measure favors the event "the polymer has large range".

Let $I_d(x) := \lim_{n\to\infty} \frac{-1}{n} \log P\{R_n \geq xn\}$ and $I(x) := I_1(x) = \frac{1}{2}(1+x)\log(1+x) + \frac{1}{2}(1-x)\log(1-x)$. The following are our main results for the one-dimensional discrete setting.

Theorem 1.1. (i) *For $\beta > 0$,*

$$\lim_{n\to\infty} \frac{1}{n} \log Z_n^G = g^*(\beta), \tag{1.9}$$

where

$$g^*(\beta) := -\inf_{c\in[\tilde{c}(\beta),1]} \left\{\frac{\beta}{c} + I(c)\right\} \tag{1.10}$$

and $\tilde{c}(\beta) = \frac{\beta}{\beta+\log 2}$.

(ii) *The infimum of (1.10) is obtained at $c^*(\beta)$, where $c^*(\beta)$ is the solution of*

$$\beta = c^2 I'(c) = \frac{c^2}{2}\log\left(\frac{1+c}{1-c}\right). \tag{1.11}$$

Note that c^* is strictly monotone, $\beta^{-1/3}c^*(\beta) \to 1$ as $\beta \to 0$ and $e^{2\beta}(1 - c^*(\beta)) \to 2$ as $\beta \to \infty$. $g^*(\beta)$ can be written as

$$g^*(\beta) = -c^*(\beta)\log\frac{1+c^*(\beta)}{1-c^*(\beta)} - \frac{1}{2}\log(1-c^*(\beta)^2). \tag{1.12}$$

Furthermore, $\beta^{-2/3}g^*(\beta) \to -\frac{3}{2}$ as $\beta \to 0$ and $g^*(\beta) + \beta \to -\log 2$ as $\beta \to \infty$.

Theorem 1.2 (*LLN and LDP*)**.** *For $\beta > 0$, define*

$$P_n^{G,+}(\cdot) = P_n^G(S_n/n \in \cdot | S_n > 0). \tag{1.13}$$

Then $(P_n^{G,+})_{n\in\mathbb{N}}$ satisfies a large deviation principle (LDP) on $[0, 1]$ with rate n and with rate function $I^\beta(\theta)$

$$-I^\beta(\theta) = \begin{cases} -\dfrac{\beta}{\theta} - I(\theta) - g^*(\beta), & c^*\left(\dfrac{\beta}{2}\right) \leq \theta, \\ -\dfrac{\beta}{\tilde{r}} - I(2\tilde{r} - \theta) - g^*(\beta), & \theta < c^*\left(\dfrac{\beta}{2}\right), \end{cases}$$

where $\tilde{r} = \tilde{r}_\beta(\theta)$ is the positive solution of $\beta = 2r^2 I'(2r - \theta)$. Moreover, $I^\beta(\theta)$ has the unique 0 at $c^*(\beta)$.