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## Soft Polymers in Low Dimension

In Chapters 3 and 4 we consider a variation of the SAW in which self-intersections are not forbidden but are penalized. We refer to this as the *soft polymer*. In Chapter 3 will show that the soft polymer has *ballistic* behavior in  $d = 1$ . The proof uses a Markovian representation of the local times of one-dimensional SRW (a powerful technique that is useful also for other models), in combination with large deviation theory, variational calculus and spectral calculus. In Chapter 4 we will show that the soft polymer has *diffusive* behavior in  $d \geq 5$ . The proof there uses a combinatorial expansion technique called the lace expansion, and is based on the idea that in high dimension SAW can be viewed as a “perturbation” of SRW.

The above scaling says that in  $d = 1$  and  $d \geq 5$  the soft polymer is in the *same universality class* as SAW. This is expected to be true also for  $2 \leq d \leq 4$ , but a proof is missing.

In Section 3.1 we define the model, in Section 3.2 we state the main result, a large deviation principle (LDP) for the location of the right endpoint. In Section 3.3 we outline a five-step program to prove the LDP for bridge polymers, i.e., polymers confined between their endpoints. This program is carried out in Section 3.4. In Section 3.5 we remove the bridge condition and prove the full LDP. It will turn out that the rate function has an interesting *critical value strictly below the typical speed*. The main technique that is used is the *method of local times*.

### 3.1 A Polymer with Self-repulsion

The soft polymer on  $\mathbb{Z}^d$  treated in Chapters 3 and 4 is defined by choosing the set of paths and the Hamiltonian in (1.1) as

$$\begin{aligned} \mathcal{W}_n &= \{w = (w_i)_{i=0}^n \in (\mathbb{Z}^d)^{n+1} : w_0 = 0, \|w_{i+1} - w_i\| = 1 \forall 0 \leq i < n\}, \\ H_n(w) &= \beta I_n(w), \end{aligned} \tag{3.1}$$

where  $\beta \in [0, \infty)$  and

$$I_n(w) = \sum_{\substack{i,j=0 \\ i < j}}^n 1_{\{w_i=w_j\}} \quad (3.2)$$

is the *intersection local time* of  $w$ . This model goes under the name of *weakly self-avoiding random walk*: every self-intersection contributes an energy  $\beta$  to the Hamiltonian and is therefore penalized by a factor  $e^{-\beta}$ . Another name used in the literature is Domb-Joyce model. Think of  $\beta$  as a *strength of self-repulsion* parameter.

We write  $P_n^\beta$  to denote the law of the soft polymer of length  $n$  with parameter  $\beta$ , as in (1.2). We add a factor  $(1/2d)^n$  to  $P_n^\beta$  in order to be able to compare it with the law  $P_n$  of SRW, i.e., we put

$$P_n^\beta(w) = \frac{1}{Z_n^\beta} e^{-\beta I_n(w)} P_n(w), \quad w \in \mathcal{W}_n, \quad (3.3)$$

so that we may think of  $P_n^\beta$  as an exponential tilting of  $P_n$ . Thus,  $P_n^\beta$  is the law of a *random process*  $(S_i)_{i=0}^n$  with weak self-repulsion, taking values in  $\mathcal{W}_n$ . Note that, like for SAW in Section 1.2,  $(P_n^\beta)_{n \in \mathbb{N}_0}$  is not (!) a consistent family when  $\beta \in (0, \infty)$ . The case  $\beta = 0$  corresponds to SRW, the case  $\beta = \infty$  to SAW.

In what follows we focus on the case  $d = 1$ . In Chapter 4 we deal with the case  $d \geq 5$ .

## 3.2 Weakly Self-avoiding Walk in Dimension One

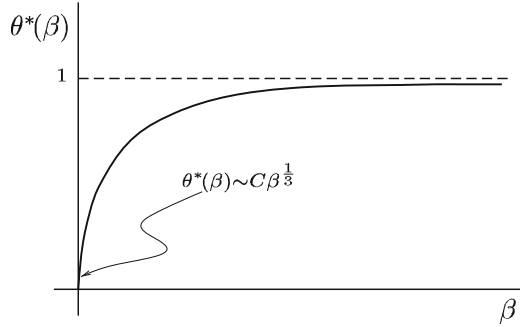
Intuitively, we expect that typical paths under the measure  $P_n^\beta$  hang around the origin for a while and then wander off to infinity at a strictly positive speed because of the self-repulsion (there is a trivial symmetry between moving to the left and moving to the right). Ballistic behavior was first shown by Bolthausen [25], without existence and identification of the speed. Theorems 3.1 and 3.2 below, which are taken from Greven and den Hollander [130], establish existence and identify the speed in terms of a variational problem. See also den Hollander [168], Chapter IX.

**Theorem 3.1.** *For every  $\beta \in (0, \infty)$  there exists a  $\theta^*(\beta) \in (0, 1)$  such that*

$$\lim_{n \rightarrow \infty} P_n^\beta \left( \left| \frac{1}{n} S_n - \theta^*(\beta) \right| \leq \epsilon \mid S_n \geq 0 \right) = 1 \text{ for all } \epsilon > 0. \quad (3.4)$$

**Theorem 3.2.** *The function  $\beta \mapsto \theta^*(\beta)$  can be computed in terms of a variational problem. It follows from the solution of this variational problem that*

$$\begin{aligned} \beta \mapsto \theta^*(\beta) \text{ is analytic on } (0, \infty), \\ \lim_{\beta \downarrow 0} \theta^*(\beta) = 0, \quad \lim_{\beta \rightarrow \infty} \theta^*(\beta) = 1. \end{aligned} \quad (3.5)$$



**Fig. 3.1.** The linear speed of the soft polymer.

The quantity  $\theta^*(\beta)$  is the speed of the soft polymer with strength of repulsion  $\beta$ . In Section 3.6 we will see that  $\beta \mapsto \theta^*(\beta)$  looks like the curve in Fig. 3.1.

Theorems 3.1 and 3.2 will follow from the following *large deviation principle*, which is the main result of the present chapter.

**Theorem 3.3.** For every  $\beta \in (0, \infty)$  the family  $(P_n^{+, \beta})_{n \in \mathbb{N}_0}$  defined by

$$P_n^{+, \beta}(\cdot) = P_n^\beta \left( \frac{1}{n} S_n \in \cdot \mid S_n \geq 0 \right) \quad (3.6)$$

satisfies a large deviation principle (LDP) on  $[0, 1]$  with rate  $n$  and with rate function  $I_\beta$ , identified in (3.66) below, having  $\theta^*(\beta)$  as its unique zero.

The full proof of this LDP will have to wait until Section 3.5 (see Theorem 3.14 and Fig. 3.4). For the definition of LDP, we refer the reader to Dembo and Zeitouni [82], Chapter 1, and den Hollander [168], Chapter III. In essence, Theorem 3.3 says that

$$\lim_{\delta \downarrow 0} \lim_{n \rightarrow \infty} \frac{1}{n} \log P_n^{+, \beta}([\theta - \delta, \theta + \delta]) = -I_\beta(\theta). \quad (3.7)$$

Before we get going on the proof of Theorem 3.3, we first rewrite the definition of  $P_n^\beta$  in (3.3) in a way that is more convenient. Let

$$\widehat{I}_n(w) = \sum_{i, j=0}^n 1_{\{w_i = w_j\}}. \quad (3.8)$$

Then  $\widehat{I}_n(w) = 2I_n(w) + (n + 1)$ . Hence, we may as well put  $\widehat{I}_n(w)$  in the exponential weight factor (which only changes  $\beta$  to  $2\beta$ ). Henceforth we write  $I_n(w)$  again, suppressing the overscript.

The following object is of paramount importance for the argument given below. Define

$$\ell_n(x) = \sum_{i=0}^n 1_{\{w_i = x\}}, \quad x \in \mathbb{Z}, n \in \mathbb{N}_0, \quad (3.9)$$

i.e., the *local time at site  $x$  up to time  $n$* . We can then write

$$I_n(w) = \sum_{x \in \mathbb{Z}} \sum_{i,j=0}^n 1_{\{w_i=w_j=x\}} = \sum_{x \in \mathbb{Z}} \ell_n(x)^2. \quad (3.10)$$

We thus see that the proof of Theorem 3.3 really amounts to understanding the large deviation properties of the random sequence  $\{\ell_n(x)\}_{x \in \mathbb{Z}}$  under the law  $P_n$  of SRW. We will see that this sequence has an underlying *Markovian structure*. Note that  $\sum_{x \in \mathbb{Z}} \ell_n(x) = n + 1$  for all  $n \in \mathbb{N}$ .

In what follows we write  $P, E$  to denote probability and expectation w.r.t. SRW (as in Section 2.1). Recall that  $P_n$  is the projection of  $P$  onto  $\mathcal{W}_n$ .

### 3.3 The Large Deviation Principle for Bridges

In order to obtain the desired LDP for  $P_n^{+, \beta}(\frac{1}{n} S_n \in \cdot)$ , we begin by deriving an LDP under the restriction that the path be a *bridge*, i.e., that it lies between its endpoints. This restriction will be crucial for the proof in Section 3.4, and will only be removed in Section 3.5.

**Folding a path into a bridge.** Our first lemma shows that the bridge condition does not change the normalizing constant.

**Lemma 3.4.** *For  $n \rightarrow \infty$ ,*

$$E(e^{-\beta I_n} 1_{\{S_n \geq 0\}}) = e^{o(n)} E(e^{-\beta I_n} 1_{\otimes_n}), \quad (3.11)$$

with  $I_n = I_n((S_i)_{i=0}^n)$  and

$$\otimes_n = \{S_0 \leq S_i \leq S_n \ \forall 0 \leq i \leq n\}. \quad (3.12)$$

*Proof.* The proof uses a folding argument due to Hammersley and Welsh [143]. Fix  $n$ .

First, suppose that the path is a *half-bridge* to the right, i.e.,  $S_i > S_0 \ \forall 0 < i \leq n$ . We can then do a reflection procedure starting from the left endpoint of the path, as follows. Put  $i_0 = 0$  and, for  $j = 1, 2, \dots$ , define  $(R_j, i_j)$  recursively as

$$\begin{aligned} R_j &= \max_{i_{j-1} < i \leq n} (-1)^j (S_{i_{j-1}} - S_i), \\ i_j &= \text{the largest } i \text{ where the maximum is attained.} \end{aligned}$$

The recursion is stopped at the smallest integer  $k$  such that  $i_k = n$ . What this definition says is that  $R_j$  is the span of the subwalk  $(S_{i_{j-1}}, \dots, S_n)$ . Each subwalk  $(S_{i_{j-1}}, \dots, S_{i_j})$  lies strictly on one side of the point  $S_{i_{j-1}}$ , and

$$R_1 + \dots + R_k \leq n \quad \text{and} \quad R_1 > R_2 > \dots > R_k \geq 1. \quad (3.13)$$

If, for  $j = 1, 2, \dots, k-1$ , we reflect  $(S_{i_j}, \dots, S_n)$  around the point  $S_{i_j}$ , then we end up with a bridge, i.e., a path satisfying  $S_0 < S_i \leq S_n \forall 0 < i \leq n$ . Moreover, this bridge is less penalized than the original path because it has less self-intersections.

Next, we drop the assumption that the path be a half-bridge and only suppose that  $S_n \geq 0$ . Let

$$\begin{aligned} i_- &= \min \left\{ 0 \leq i \leq n : S_i = \min_{0 \leq j \leq n} S_j \right\}, \\ i_+ &= \max \left\{ 0 \leq i \leq n : S_i = \max_{0 \leq j \leq n} S_j \right\}. \end{aligned} \tag{3.14}$$

Then, when  $i_- > 0$  and  $i_+ < n$ , both  $(S_{i_-}, \dots, S_0)$  and  $(S_n, \dots, S_{i_+})$  are half-bridges, and the above reflection procedure applies. If we fold both pieces outwards after the reflection procedure is through, then we end up with a bridge. (The cases  $i_- = 0$  and  $i_+ = n$  need no reflection.) Hence, we conclude that

$$E(e^{-\beta I_n} 1_{\{S_n \geq 0\}}) \leq N_n^2 E(e^{-\beta I_n} 1_{\otimes_n}), \tag{3.15}$$

where  $N_n$  is the number of solutions of (3.13) summed over  $k$  (which is the number of ordered partitions of  $\{1, \dots, n\}$ ). However, it is known that  $N_n = \exp[O(\sqrt{n})]$  (see Madras and Slade [230], Theorem 3.1.4), so this factor is harmless and the claim follows.  $\square$

**The LDP for bridges.** Our main result, whose proof will be given in Section 3.4, is the following LDP for the speed of the bridge soft polymer.

**Theorem 3.5.** *For every  $\beta \in (0, \infty)$  the family  $(P_n^{\beta, \text{bridge}})$ ,  $n \in \mathbb{N}_0$ , defined by*

$$P_n^{\beta, \text{bridge}}(\cdot) = P_n^\beta \left( \frac{1}{n} S_n \in \cdot \mid \otimes_n \right) \tag{3.16}$$

*satisfies the LDP on  $(0, 1]$  with rate  $n$  and with rate function  $J_\beta$  identified in (3.21) and Lemma 3.12 below (see Fig. 3.3 below). The unique zero of  $J_\beta$  is  $\theta^*(\beta)$  in Theorem 3.1.*

To prove Theorem 3.5 we will carry out the following *program*:

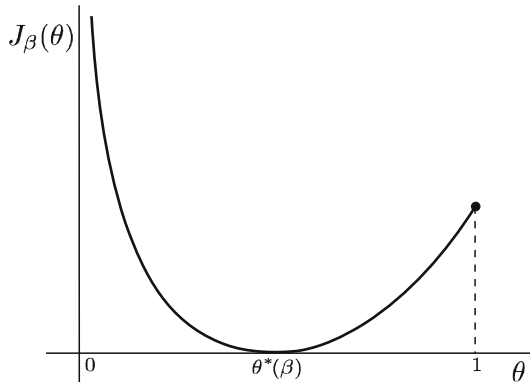
(I) Pick  $\theta \in (0, 1]$  and consider the quantity

$$P_n^\beta(S_n = \lceil \theta n \rceil \mid \otimes_n) = \frac{\widehat{K}_n(\theta)}{\int_{\theta \in (0, 1]} d(\theta n) \widehat{K}_n(\theta)}, \tag{3.17}$$

where

$$\widehat{K}_n(\theta) = E(e^{-\beta I_n} 1_{\{S_n = \lceil \theta n \rceil\}} 1_{\otimes_n}) \tag{3.18}$$

( $\lceil \theta n \rceil$  and  $n$  must have the same parity). The value  $\theta = 0$  is not relevant for bridges.



**Fig. 3.2.** The rate function  $J_\beta$  for bridge soft polymers.

(II) Show that there exists a function  $\widehat{J}_\beta: (0, 1] \rightarrow (0, \infty)$  such that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \widehat{K}_n(\theta) = -\widehat{J}_\beta(\theta), \tag{3.19}$$

with the property that  $\theta \mapsto \widehat{J}_\beta(\theta)$  is continuous, strictly convex and minimal at  $\theta^*(\beta)$ . Identify  $\widehat{J}_\beta$  in terms of a variational problem.

(III) Combine (I) and (II), to obtain

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log P_n^\beta(S_n = \lceil \theta n \rceil \mid \otimes_n) = -J_\beta(\theta), \tag{3.20}$$

with

$$J_\beta(\theta) = \widehat{J}_\beta(\theta) - \inf_{\theta \in (0,1]} \widehat{J}_\beta(\theta). \tag{3.21}$$

Evidently,  $\theta \mapsto J_\beta(\theta)$  is also continuous, strictly convex and minimal at  $\theta^*(\beta)$ , which is its unique zero (see Fig. 3.2).

The argument in Section 3.4 will show that the same results as in (3.19–3.20) apply when  $\theta$  is replaced by  $\theta_n \rightarrow \theta$  as  $n \rightarrow \infty$ , which is why we get Theorem 3.5.

The above *program* will be carried out in Section 3.4, in five steps organized as Sections 3.4.1–3.4.5. The first two steps are a preparation that is needed to get the key quantities in the right format for applying large deviation theory. The actual application of large deviation theory and the analysis of the ensuing variational problem are carried out in the last three steps. The computation is technical but powerful, and can be carried over to other one-dimensional models as well.

After we have completed the proof of Theorem 3.5 we will show how to remove the bridge condition. This is done in Section 3.5 and leads to Theorem 3.3, the LDP we are actually after. It will turn out that the associated rate function is different from  $J_\beta$  but still has  $\theta^*(\beta)$  as its unique zero (see Fig. 3.4 below), which is why Theorems 3.1–3.2 will follow as corollaries.

### 3.4 Program of Five Steps

#### 3.4.1 Step 1: Adding Drift

We begin by going through a number of rewrites of the quantity  $K_n(\theta)$  defined in (3.18).

Fix  $\theta \in (0, 1)$ . (The case  $\theta = 0$  is degenerate, the case  $\theta = 1$  is trivial.) Let  $P_\theta, E_\theta$  denote probability and expectation for the random walk with drift  $\theta$  (i.e., with probabilities  $\frac{1}{2}(1 + \theta)$  and  $\frac{1}{2}(1 - \theta)$  to step to the right and to the left, respectively). Then we can write (3.18) as

$$\widehat{K}_n(\theta) = (1 - \theta)^{-\frac{n - \lceil \theta n \rceil}{2}} (1 + \theta)^{-\frac{n + \lceil \theta n \rceil}{2}} \widetilde{K}_n(\theta), \tag{3.22}$$

with

$$\widetilde{K}_n(\theta) = E_\theta(e^{-\beta I_n} 1_{\{S_n = \lceil \theta n \rceil\}} 1_{\circledast_n}). \tag{3.23}$$

Indeed, every path from 0 to  $\lceil \theta n \rceil$  makes the same number of steps to the left and to the right, so we pick up a simple Radon-Nikodym factor. Thus it suffices to study the asymptotics of  $\widetilde{K}_n(\theta)$ , i.e., *our task now is to relate the soft polymer with drift  $\theta$  to the random walk with drift  $\theta$ .*

The advantage of the reformulation in (3.22–3.23) is that the path does not care to return to  $[0, S_n]$  after time  $n$ .

**Lemma 3.6.** *For every  $\theta \in (0, 1)$  and  $n \in \mathbb{N}_0$ ,*

$$E_\theta(e^{-\beta I_n} 1_{\{S_n = \lceil \theta n \rceil\}} 1_{\circledast_n}) = \frac{1}{\theta} E_\theta(e^{-\beta I_n} 1_{\{S_n = \lceil \theta n \rceil\}} 1_{\circledast_n \cap \circledcirc_n}), \tag{3.24}$$

with

$$\circledcirc_n = \{S_i > S_n \ \forall i > n\}. \tag{3.25}$$

*Proof.* Simply use that  $I_n$  does not depend on  $S_i$  for  $i > n$ , and that  $P_\theta(\circledcirc_n) = \theta$  for all  $n$  (Spitzer [284], Section 1).  $\square$

An important consequence of Lemma 3.6 is that on the event  $\{S_n = \lceil \theta n \rceil\} \cap \circledast_n \cap \circledcirc_n$  we may write

$$I_n = \sum_{x=0}^{\lceil \theta n \rceil} \ell(x)^2, \tag{3.26}$$

where

$$\ell(x) = \sum_{i \in \mathbb{N}_0} 1_{\{S_i = x\}}, \quad x \in \mathbb{Z}, \tag{3.27}$$

is the *total local time at site  $x$* . Indeed, this follows from the observation that on the event  $\{S_n = \lceil \theta n \rceil\} \cap \circledast_n \cap \circledcirc_n$  we have

$$\ell_n(x) = \begin{cases} \ell(x), & \text{if } 0 \leq x \leq \lceil \theta n \rceil, \\ 0, & \text{otherwise.} \end{cases}$$

Therefore we may rewrite (3.23) as

$$\tilde{K}_n(\theta) = \frac{1}{\theta} E_\theta \left( e^{-\beta \sum_{x=0}^{\lceil \theta n \rceil} \ell^2(x)} \mathbf{1}_{\{S_n = \lceil \theta n \rceil\}} \mathbf{1}_{\otimes_n \cap \odot_n} \right). \quad (3.28)$$

Note that time  $n$  has been replaced by space  $\lceil \theta n \rceil$  in (3.28). The total local times turn out to have a nice structure, as we show next.

### 3.4.2 Step 2: Markovian Nature of the Total Local Times

In this section we show that  $\{\ell(x)\}_{x \in \mathbb{N}_0}$  admits a nice Markovian description. This will allow us to deduce the asymptotics of  $\tilde{K}_n(\theta)$  from an LDP for Markov chains. Let

$$m(x) = \sum_{i \in \mathbb{N}_0} \mathbf{1}_{\{S_i = x, S_{i+1} = x+1\}}, \quad x \in \mathbb{Z}, \quad (3.29)$$

be the *total number of jumps from  $x$  to  $x + 1$* . Then, on the event  $\{S_n = \lceil \theta n \rceil\} \cap \otimes_n \cap \odot_n$ , the total number of jumps from  $x + 1$  to  $x$  equals

$$\sum_{i \in \mathbb{N}_0} \mathbf{1}_{\{S_i = x+1, S_{i+1} = x\}} = m(x) - 1, \quad 0 \leq x \leq \lceil \theta n \rceil, \quad (3.30)$$

because the net number of jumps along the edge between  $x$  and  $x + 1$  must be  $+1$ . Since  $\ell(x)$  is the sum of the number of jumps to  $x$  coming from the left and from the right, we have

$$\ell(x) = m(x - 1) + m(x) - \mathbf{1}_{\{x > 0\}}, \quad 0 \leq x \leq \lceil \theta n \rceil. \quad (3.31)$$

Moreover, on the event  $\{S_n = \lceil \theta n \rceil\} \cap \otimes_n \cap \odot_n$ , the total time spent between 0 and  $\lceil \theta n \rceil$  is  $n + 1$ . Therefore

$$\left. \begin{aligned} & \{S_n = \lceil \theta n \rceil\} \cap \otimes_n \cap \odot_n \\ & = \left\{ \sum_{x=0}^{\lceil \theta n \rceil} [m(x - 1) + m(x) - \mathbf{1}_{\{x > 0\}}] = n + 1, m(-1) = 0, m(\lceil \theta n \rceil) = 1 \right\}. \end{aligned} \right\} \quad (3.32)$$

Therefore we may rewrite (3.28) as

$$\begin{aligned} \tilde{K}_n(\theta) &= \frac{1}{\theta} E_\theta \left( e^{-\beta \sum_{x=0}^{\lceil \theta n \rceil} [m(x-1) + m(x) - \mathbf{1}_{\{x > 0\}}]^2} \right. \\ & \quad \left. \times \mathbf{1}_{\left\{ \sum_{x=0}^{\lceil \theta n \rceil} [m(x-1) + m(x) - \mathbf{1}_{\{x > 0\}}] = n + 1 \right\}} \mathbf{1}_{\{m(-1) = 0, m(\lceil \theta n \rceil) = 1\}} \right). \end{aligned} \quad (3.33)$$

The indicator  $\mathbf{1}_{\{x > 0\}}$  and the restrictions  $m(-1) = 0$  and  $m(\lceil \theta n \rceil) = 1$  are to be thought of as harmless boundary terms.

The main reason for the reformulation in (3.33) is the following fact, which goes back to Knight [215].



**Lemma 3.7.** For every  $\theta \in (0, 1)$  under the law  $P_\theta$ ,  $\{m(x)\}_{x \in \mathbb{N}_0}$  is a Markov chain on state space  $\mathbb{N}$  with transition kernel

$$P_\theta(i, j) = \binom{i+j-2}{i-1} \left(\frac{1+\theta}{2}\right)^i \left(\frac{1-\theta}{2}\right)^{j-1}, \quad i, j \in \mathbb{N}. \quad (3.34)$$

*Proof.* Fix  $x$ . If  $m(x) = i$ , then the edge  $(x, x+1)$  receives  $i$  upcrossings and  $i-1$  downcrossings. For  $s = 1, \dots, i-1$ , let  $Z_s$  denote the number of upcrossings of  $(x+1, x+2)$  in between the  $s$ -th upcrossing and the  $s$ -th downcrossing of  $(x, x+1)$ . Let  $Z$  denote the number of upcrossings of  $(x+1, x+2)$  after the  $i$ -th upcrossing of  $(x, x+1)$ , which is different from the others because no further downcrossing of  $(x, x+1)$  is allowed. Since the random walk has drift  $\theta$ , the probability that it makes a loop excursion to the right of  $x+1$  is  $\frac{1-\theta}{2}$ . Hence, we have

$$\begin{aligned} P_\theta(Z_s = k \mid m(x) = i) &= \left(\frac{1+\theta}{1-\theta}\right) \left(\frac{1-\theta}{2}\right)^{k+1}, \quad k \in \mathbb{N}_0, \quad s = 1, \dots, i-1, \\ P_\theta(Z = k \mid m(x) = i) &= \frac{1+\theta}{1-\theta} \left(\frac{1-\theta}{2}\right)^k, \quad k \in \mathbb{N}. \end{aligned} \quad (3.35)$$

Since  $m(x+1) = j$  means that  $Z_1 + \dots + Z_{i-1} + Z = j$ , we see that our process is Markov: it is irrelevant for the outcome of  $m(x+1)$  what the random walk does to the left of  $x$ , only the value of  $m(x)$  matters. Moreover,  $Z_s + 1$ ,  $s = 1, \dots, i-1$ , have the same law as  $Z$ . Since  $(Z_1+1) + \dots + (Z_{i-1}+1) + Z = i+j-1$  and since the number of ways  $i+j-1$  can be divided into  $i$  pieces of length  $\geq 1$  equals the binomial factor in (3.34), we obtain the formula for  $P_\theta(i, j)$  in (3.34).  $\square$

The proof of Lemma 3.7 shows that  $\{m(x)\}_{x \in \mathbb{N}_0}$  is a branching process with one immigrant and with an offspring distribution that has mean smaller than 1. Therefore it is a positive recurrent Markov chain.

### 3.4.3 Step 3: Key Variational Problem

We have now completed our rewrite of  $K_n(\theta)$  in (3.18) and are ready to apply large deviation theory. In this section we derive the key variational problem underlying the LDP for bridges in Theorem 3.5. This can be done along fairly standard lines. However, in order not to get lost in too many technicalities, the reader is asked to make a few small “leaps of faith”.

The nice fact about the representation in (3.33) is that  $\tilde{K}_n(\theta)$  can be expressed in terms of the *pair empirical measure* associated with  $\{m(x)\}_{x \in \mathbb{N}_0}$ . To that end, define

$$L_N^2 = \frac{1}{N} \sum_{x=0}^{N-1} \delta_{(m(x-1), m(x))}, \quad N \in \mathbb{N}, \quad (3.36)$$

with periodic boundary conditions ( $m(-1) = m(N)$ ), and let

$$F_\beta(\nu) = -\beta \sum_{i,j \in \mathbb{N}} (i+j-1)^2 \nu(i,j), \quad (3.37)$$

$$A_\theta = \left\{ \nu \in \widetilde{\mathcal{M}}_1(\mathbb{N} \times \mathbb{N}) : \sum_{i,j \in \mathbb{N}} (i+j-1) \nu(i,j) = \frac{1}{\theta} \right\},$$

where

$$\begin{aligned} \widetilde{\mathcal{M}}_1(\mathbb{N} \times \mathbb{N}) = & \text{the set of probability measures} \\ & \text{on } \mathbb{N} \times \mathbb{N} \text{ with identical marginals.} \end{aligned} \quad (3.38)$$

Then (3.33) becomes

$$\widetilde{K}_n(\theta) = e^{o(n)} E_\theta \left( e^{NF_\beta(L_N^2)} \mathbf{1}_{\{L_N^2 \in A_\theta\}} \right) \text{ with } N = \lceil \theta n \rceil + 1. \quad (3.39)$$

Indeed,

1. The exponential factor in (3.33) equals the one in (3.39), with a negligible error arising from forcing the periodic boundary condition in the definition of  $L_N^2$ .
2. The first constraint in (3.33) is asymptotically the same as the constraint in (3.39), because we replaced  $(n+1)/(\lceil \theta n \rceil + 1)$  by  $1/\theta$ , which will *a posteriori* be justified by the continuity of the function  $\theta \mapsto \widetilde{J}_\beta(\theta)$  appearing in Lemma 3.8 below (see Sections 3.4.4–3.4.5).
3. The second constraint in (3.33) is negligible as  $n \rightarrow \infty$ .

The reason for introducing the representation in (3.39) is that it allows us to use the LDP for the empirical pair measure  $L_N^2$ , based on the Markov property established in Lemma 3.7.

**Lemma 3.8.** *For every  $\theta \in (0, 1)$ ,*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \widetilde{K}_n(\theta) = -\widetilde{J}_\beta(\theta), \quad (3.40)$$

with

$$\widetilde{J}_\beta(\theta) = \theta \inf_{\nu \in A_\theta} \left[ -F_\beta(\nu) + I_{P_\theta}^2(\nu) \right], \quad (3.41)$$

where

$$I_{P_\theta}^2(\nu) = \sum_{i,j \in \mathbb{N}} \nu(i,j) \log \left( \frac{\nu(i,j)}{\bar{\nu}(i) P_\theta(i,j)} \right). \quad (3.42)$$

*Proof.* The formula in (3.42) is the *weak* rate function in the *weak* LDP (see den Hollander [168], Section III.6) for  $(L_N^2)_{N \in \mathbb{N}}$  under the law of the Markov chain  $\{m(x)\}_{x \in \mathbb{N}_0}$  with transition kernel  $P_\theta$ . In order to apply Varadhan's Lemma (see den Hollander [168], Section III.3) we need the LDP, i.e., we need to overcome the technical difficulty that the state space  $\mathbb{N}$  is infinite. This can

be handled via a truncation argument because, as was observed at the end of Section 3.4.2, the Markov chain  $\{m(x)\}_{x \in \mathbb{N}_0}$  has strong recurrence properties (see Greven and den Hollander [130] for more details).

Next we apply Varadhan's Lemma to (3.39), which is an exponential integral restricted to the set  $A_\theta$ . Here another technical difficulty arises: the weak LDP "needs to be transferred from  $\widetilde{\mathcal{M}}_1(\mathbb{N} \times \mathbb{N})$  to  $A_\theta$ " (see Dembo and Zeitouni [82], Lemma 4.1.5). The result of the usual manipulations reads, somewhat informally,

$$\begin{aligned} \widetilde{K}_n(\theta) &= e^{o(n)} E_\theta \left( e^{NF_\beta(L_N^2)} 1_{\{L_N^2 \in A_\theta\}} \right) \\ &= e^{o(n)} \int_{A_\theta} e^{NF_\beta(L_N^2)} P_\theta(L_N^2 \in d\nu) \\ &= e^{o(n)} e^{N \sup_{\nu \in A_\theta} [F_\beta(\nu) - I_{P_\theta}^2(\nu)]}, \quad N \rightarrow \infty, \end{aligned} \quad (3.43)$$

which proves the claim because  $N = \lceil \theta n \rceil + 1$ .  $\square$

At this point we recall (3.22) and (3.23), and rewrite Lemma 3.8 as follows:

**Lemma 3.9.** *For every  $\theta \in (0, 1)$ ,*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \widehat{K}_n(\theta) = -\widehat{J}_\beta(\theta), \quad (3.44)$$

with

$$\widehat{J}_\beta(\theta) = \theta \inf_{\nu \in A_\theta} \left[ -F_\beta(\nu) + I_{P_0}^2(\nu) \right], \quad (3.45)$$

*i.e., the same variational formula as in Lemma 3.8 but with  $P_\theta$  replaced by  $P_0$ , given by (recall Lemma 3.7)*

$$P_0(i, j) = \binom{i+j-2}{i-1} \left(\frac{1}{2}\right)^{i+j-1}, \quad i, j \in \mathbb{N}. \quad (3.46)$$

*Proof.* Simply note that  $\nu \in A_\theta$  implies  $\sum_{i \in \mathbb{N}} i \bar{\nu}(i) = \frac{1+\theta}{2\theta}$ , so that

$$\begin{aligned} I_{P_0}^2(\nu) - I_{P_\theta}^2(\nu) &= \sum_{i, j \in \mathbb{N}} \nu(i, j) \log \left[ (1+\theta)^i (1-\theta)^{j-1} \right] \\ &= \frac{1+\theta}{2\theta} \log(1+\theta) + \frac{1-\theta}{2\theta} \log(1-\theta), \quad \nu \in A_\theta, \end{aligned} \quad (3.47)$$

which makes the prefactor in (3.22) cancel out.  $\square$

Thus we have identified  $\widehat{J}_\beta(\theta)$  for  $\theta \in (0, 1)$ , which is the function we were after in Section 3.3. The same formulas as in (3.44–3.45) apply for the degenerate case  $\theta = 1$ , as is easily checked by direct computation. Finally, (3.21) gives us  $J_\beta$ , the rate function in the LDP for bridge soft polymers in Theorem 3.5.

### 3.4.4 Step 4: Solution of the Variational Problem in Terms of an Eigenvalue Problem

We next proceed to give the solution of the variational problem in (3.45), leading to the qualitative shape of the function  $\theta \mapsto J_\beta(\theta)$  anticipated in Fig. 3.2. The variational problem requires us to minimize a non-linear functional under a linear constraint. It is possible to find the solution in terms of a certain eigenvalue problem that is well-behaved, and we will see that the outcome is relatively simple.

Fix  $\beta \in (0, \infty)$  and  $r \in \mathbb{R}$ , and let  $A_{r,\beta}$  be the  $\mathbb{N} \times \mathbb{N}$  matrix with components

$$A_{r,\beta}(i, j) = e^{r(i+j-1) - \beta(i+j-1)^2} P_0(i, j), \quad i, j \in \mathbb{N}. \quad (3.48)$$

The parameter  $r$  will be seen to play the role of a Lagrange multiplier needed to handle the constraint in (3.45).

**Lemma 3.10.** *Fix  $\beta \in (0, \infty)$ . For every  $r \in \mathbb{R}$ ,  $A_{r,\beta}$  is a self-adjoint operator on  $l^2(\mathbb{N})$  having a unique largest eigenvalue  $\lambda_{r,\beta}$  and corresponding eigenvector  $\tau_{r,\beta}$  (normalized as  $\|\tau_{r,\beta}\|_2 = 1$ ).*

*Proof.* Since  $A_{r,\beta}$  is strictly positive and has rapidly decaying tails, the assertion follows from standard Perron-Frobenius theory. In fact,  $A_{r,\beta}$  has the so-called Hilbert-Schmidt property  $\sum_{i,j \in \mathbb{N}} A_{r,\beta}(i, j)^2 < \infty$  and, consequently, is a compact operator (see Dunford and Schwartz [94], Section XI.6).  $\square$

The eigenvalue  $\lambda_{r,\beta}$  has the following properties:

- Lemma 3.11.** (i)  $(r, \beta) \mapsto \lambda_{r,\beta}$  is analytic on  $\mathbb{R} \times (0, \infty)$ .  
(ii)  $\lim_{r \rightarrow -\infty} \frac{\partial}{\partial r} \log \lambda_{r,\beta} = 1$  and  $\lim_{r \rightarrow \infty} \frac{\partial}{\partial r} \log \lambda_{r,\beta} = \infty$  for all  $\beta \in (0, \infty)$ .  
(iii)  $r \mapsto \log \lambda_{r,\beta}$  is strictly convex for all  $\beta \in (0, \infty)$ .

*Proof.* Here is a quick sketch. For details we refer to Greven and den Hollander [130].

- (i) Analyticity holds because  $\lambda_{r,\beta}$  has multiplicity 1 and all elements of the matrix  $A_{r,\beta}$  are analytic.  
(ii) This follows from straightforward estimates on the eigenvector  $\tau_{r,\beta}$  for  $r \rightarrow -\infty$  and  $r \rightarrow \infty$ , respectively.  
(iii) Convexity follows from the observations:

1.  $\lambda_{r,\beta} = \sup_{x \in l^2(\mathbb{N}): x > 0, \|x\|_2 = 1} \sum_{i,j \in \mathbb{N}} x(i) A_{r,\beta}(i, j) x(j)$ ;
2.  $r \mapsto \log A_{r,\beta}(i, j)$  is linear for all  $i, j \in \mathbb{N}$  and  $\beta \in (0, \infty)$ ;
3. log-convexity is preserved under taking sums and suprema.

Strict convexity follows from convexity in combination with (i) and (ii).  $\square$

With the help of Lemma 3.11 we can express  $\widehat{J}_\beta(\theta)$  in terms of the eigenvalue  $\lambda_{r,\beta}$  for some  $r$  depending on  $\theta$ .

**Lemma 3.12.** Fix  $\beta \in (0, \infty)$ . Then, for every  $\theta \in (0, 1)$ ,

$$\widehat{J}_\beta(\theta) = r - \theta \log \lambda_{r,\beta} \Big|_{r=r_\beta(\theta)}, \tag{3.49}$$

where  $r_\beta(\theta) \in \mathbb{R}$  is the unique solution of the equation

$$\frac{1}{\theta} = \frac{\partial}{\partial r} \log \lambda_{r,\beta}. \tag{3.50}$$

*Proof.* The fact that (3.50) has a solution for all  $\theta \in (0, 1)$  and that this solution is unique follows from Lemma 3.11 (see Fig. 3.3).

Consider the following family of pair probability measures:

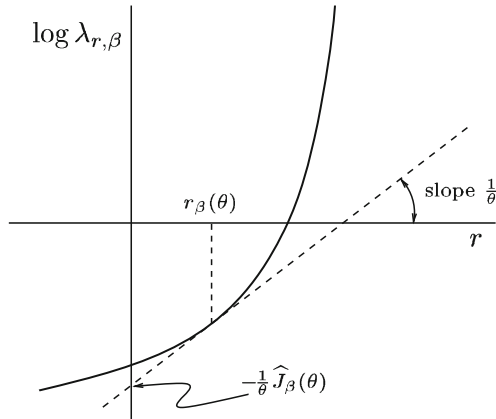
$$\nu_{r,\beta}(i, j) = \frac{1}{\lambda_{r,\beta}} \tau_{r,\beta}(i) A_{r,\beta}(i, j) \tau_{r,\beta}(j), \quad i, j \in \mathbb{N}. \tag{3.51}$$

One easily checks that  $\nu_{r,\beta} \in \widetilde{\mathcal{M}}_1(\mathbb{N} \times \mathbb{N})$ . Compute

$$\begin{aligned} I_{P_0}^2(\nu_{r,\beta}) &= \sum_{i,j} \nu_{r,\beta}(i, j) \log \left( \frac{\nu_{r,\beta}(i, j)}{\bar{\nu}_{r,\beta}(i) P_0(i, j)} \right) \\ &= \sum_{i,j} \nu_{r,\beta}(i, j) \left[ r(i+j-1) - \beta(i+j-1)^2 - \log \lambda_{r,\beta} + \log \frac{\tau_{r,\beta}(j)}{\tau_{r,\beta}(i)} \right], \end{aligned} \tag{3.52}$$

where we use that  $\bar{\nu}_{r,\beta}(i) = \tau_{r,\beta}^2(i)$ . Since  $\nu_{r,\beta}$  has identical marginals, the last term vanishes and we end up with the simple expression

$$I_{P_0}^2(\nu_{r,\beta}) = \frac{r}{\theta} + F_\beta(\nu_{r,\beta}) - \log \lambda_{r,\beta}, \tag{3.53}$$



**Fig. 3.3.** Identification of  $\widehat{J}_\beta(\theta)$ .

provided (!)  $\nu_{r,\beta} \in A_\theta$ . This expression says that

$$-\theta [F_\beta(\nu_{r,\beta}) - I_{P_0}^2(\nu_{r,\beta})] = r - \theta \log \lambda_{r,\beta}. \quad (3.54)$$

We thus see from Lemma 3.9 that the claim in Lemma 3.12 is correct provided (!) we can prove the following two properties:

- (i)  $r = r_\beta(\theta)$  implies  $\nu_{r,\beta} \in A_\theta$ ;
- (ii)  $\nu_{r_\beta(\theta),\beta}$  is a minimizer of the variational problem in (3.45).

Property (i): Compute

$$\begin{aligned} \sum_{i,j} (i+j-1) \nu_{r,\beta}(i,j) &= \frac{1}{\lambda_{r,\beta}} \sum_{i,j} \tau_{r,\beta}(i) \left[ \frac{\partial}{\partial r} A_{r,\beta}(i,j) \right] \tau_{r,\beta}(j) \\ &= \frac{1}{\lambda_{r,\beta}} \frac{\partial}{\partial r} \left[ \sum_{i,j} \tau_{r,\beta}(i) A_{r,\beta}(i,j) \tau_{r,\beta}(j) \right] = \frac{1}{\lambda_{r,\beta}} \frac{\partial}{\partial r} \lambda_{r,\beta} = \frac{\partial}{\partial r} \log \lambda_{r,\beta}. \end{aligned} \quad (3.55)$$

The second equality uses that  $A_{r,\beta} \tau_{r,\beta} = \lambda_{r,\beta} \tau_{r,\beta}$  and  $\|\tau_{r,\beta}\|_2 = 1$  for all  $r, \beta$ . Hence (3.50) indeed guarantees (i).

Property (ii): If  $\nu \in A_\theta$ , then we can write

$$\begin{aligned} &-\theta [F_\beta(\nu) - I_{P_0}^2(\nu)] \\ &= [r - \theta \log \lambda_{r,\beta}] + \theta \sum_{i,j} \nu(i,j) \log \left( \frac{\nu(i,j)}{\bar{\nu}(i) \frac{1}{\lambda_{r,\beta}} A_{r,\beta}(i,j)} \right) \\ &= [r - \theta \log \lambda_{r,\beta}] + \theta \sum_{i,j} \nu(i,j) \log \left( \frac{\nu(i,j)}{\bar{\nu}(i)} \frac{\sqrt{\bar{\nu}_{r,\beta}(i) \bar{\nu}_{r,\beta}(j)}}{\nu_{r,\beta}(i,j)} \right), \end{aligned} \quad (3.56)$$

where we once again use that  $\bar{\nu}_{r,\beta}(i) = \tau_{r,\beta}^2(i)$ . The first term is precisely the value we found when  $\nu = \nu_{r,\beta}$ . Moreover, because  $\nu$  has identical marginals the second term simplifies further to

$$\theta \sum_{i,j} \nu(i,j) \log \left( \frac{\nu(i,j)}{\bar{\nu}(i)} \frac{\bar{\nu}_{r,\beta}(i)}{\nu_{r,\beta}(i,j)} \right) = \theta \sum_i \bar{\nu}(i) H([\nu(i)] \mid [\nu_{r,\beta}(i)]), \quad (3.57)$$

where  $[\nu(i)], [\nu_{r,\beta}(i)] \in \mathcal{M}_1(\mathbb{N})$  (= the set of probability measures of  $\mathbb{N}$ ) are defined by  $[\nu(i)](j) = \nu(i,j)/\nu(i)$  and  $[\nu_{r,\beta}(i)](j) = \nu_{r,\beta}(i,j)/\nu_{r,\beta}(i)$ , while  $H(\cdot \mid \cdot)$  denotes relative entropy, defined as

$$H(\mu_1 \mid \mu_2) = \sum_i \mu_1(i) \log \left( \frac{\mu_1(i)}{\mu_2(i)} \right), \quad \mu_1, \mu_2 \in \mathcal{M}_1(\mathbb{N}). \quad (3.58)$$

Clearly, the r.h.s. of (3.57) is  $\geq 0$  with equality if and only if  $\nu = \nu_{r,\beta}$ .  $\square$

### 3.4.5 Step 5: Identification of the Speed

Lemma 3.12 gives us a nice representation of  $\widehat{J}_\beta(\theta)$ ,  $\theta \in (0, 1)$ , in terms of the family of eigenvalues  $\lambda_{r,\beta}$ ,  $r \in \mathbb{R}$ . As we saw in Fig. 3.2,  $\theta^*(\beta)$  is to be identified as the unique minimum of  $\theta \mapsto \widehat{J}_\beta(\theta)$ .

**Lemma 3.13.** *Fix  $\beta \in (0, \infty)$ . Then*

$$\frac{1}{\theta^*(\beta)} = \frac{\partial}{\partial r} \log \lambda_{r,\beta} \Big|_{r=r^*(\beta)}, \quad (3.59)$$

with  $r^*(\beta) \in (0, \infty)$  the unique solution of the equation

$$\lambda_{r,\beta} = 1. \quad (3.60)$$

*Proof.* The fact that (3.60) has a solution for all  $\beta \in (0, \infty)$  and that this solution is unique follows from Lemma 3.11 (see Fig. 3.3).

Differentiate  $\widehat{J}_\beta(\theta)$  with respect to  $\theta$  to obtain

$$\frac{\partial}{\partial \theta} \widehat{J}_\beta(\theta) = \frac{\partial}{\partial \theta} r_\beta(\theta) - \log \lambda_{r_\beta(\theta),\beta} - \theta \left[ \frac{\partial}{\partial \theta} r_\beta(\theta) \right] \left[ \frac{\partial}{\partial r} \log \lambda_{r,\beta} \right]_{r=r_\beta(\theta)}. \quad (3.61)$$

However, the first and the third term cancel out because of (3.50), so we get

$$\frac{\partial}{\partial \theta} \widehat{J}_\beta(\theta) = -\log \lambda_{r_\beta(\theta),\beta}. \quad (3.62)$$

This is zero if and only if  $\theta$  is such that  $\lambda_{r_\beta(\theta),\beta} = 1$ , i.e., the minimum  $\theta^*(\beta)$  of  $\theta \mapsto \widehat{J}_\beta(\theta)$  is found by solving (3.60). After that we put

$$r_\beta(\theta^*(\beta)) = r^*(\beta) \quad (3.63)$$

and use (3.50). Note that, by Lemma 3.12,

$$\frac{\partial^2}{\partial \theta^2} \widehat{J}_\beta(\theta) = -\frac{1}{\theta} \frac{\partial}{\partial \theta} r_\beta(\theta) > 0 \quad (3.64)$$

(see Fig. 3.3 and note that  $\theta \mapsto r_\beta(\theta)$  has a negative slope), so that  $r_\beta(\theta^*(\beta))$  is indeed the unique minimizer of  $\theta \mapsto \widehat{J}_\beta(\theta)$ .  $\square$

Lemmas 3.11–3.13 yield Fig. 3.3. This finishes our analysis of the rate function  $J_\beta$  for bridge soft polymers, and the proof of Theorem 3.5 is now complete.

Note that  $\theta^*(\beta)$  is the unique minimum of  $\widehat{J}_\beta$  and the unique minimum and zero of  $J_\beta$  (recall (3.21) and Fig. 3.2).

### 3.5 The Large Deviation Principle without the Bridge Condition

In Sections 3.4.1–3.4.5 we have proved Theorem 3.5, the LDP for bridge soft polymers. In this section we give a quick sketch of how to obtain the LDP without the bridge condition, i.e., Theorem 3.3, which implies Theorems 3.1 and 3.2. Remarkably, it turns out that the rate function in this LDP has a linear piece between 0 and a *critical speed*  $\theta^{**}(\beta)$  that is strictly smaller than  $\theta^*(\beta)$  (see Fig. 3.4). What is written below developed out of discussions with W. König.

**Theorem 3.14.** *For every  $\beta \in (0, \infty)$  the family  $(P_n^{+, \beta})_{n \in \mathbb{N}}$  defined by*

$$P_n^{+, \beta}(\cdot) = P_n^\beta \left( \frac{1}{n} S_n \in \cdot \mid S_n \geq 0 \right) \quad (3.65)$$

*satisfies the LDP on  $[0, 1]$  with rate  $n$  and with rate function  $I_\beta$  given by*

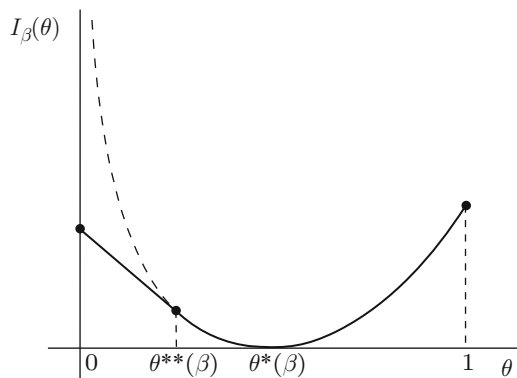
$$I_\beta(\theta) = \begin{cases} J_\beta(\theta), & \text{if } \theta \geq \theta^{**}(\beta), \\ I_\beta(0) + \frac{\theta}{\theta^{**}(\beta)} [J_\beta(\theta^{**}(\beta)) - I_\beta(0)], & \text{if } \theta \leq \theta^{**}(\beta), \end{cases} \quad (3.66)$$

*where  $\theta^{**}(\beta)$  is the unique solution of the equation*

$$J_\beta(\theta) - I_\beta(0) = \theta \frac{\partial}{\partial \theta} J_\beta(\theta), \quad (3.67)$$

*and  $I_\beta(0)$  is identified in Lemma 3.15 below. Moreover,  $\theta^{**}(\beta) \in (0, \theta^*(\beta))$ .*

The linear piece in (3.66) can be understood as follows. If the soft polymer is required to move at a speed  $\theta < \theta^{**}(\beta)$ , then it prefers to violate the bridge condition by moving at speed  $\theta^{**}(\beta)$  between 0 and  $\lceil \theta n \rceil$ , and making two loops, one below 0 and one above  $\lceil \theta n \rceil$ . The penalty for making these loops



**Fig. 3.4.** The rate function  $I_\beta$  (compare with Fig. 3.2).



is less than the penalty for staying locked up like a bridge. The total length of these loops is proportional to  $\theta^{**}(\beta) - \theta$ , i.e., the penalty for not behaving like a bridge grows linearly with  $\theta^{**}(\beta) - \theta$ .

The analogue of Lemmas 3.12 and 3.13 reads as follows (compare (3.46) and (3.48) with (3.69) and (3.68)):

**Lemma 3.15.** *Fix  $\beta \in (0, \infty)$ . For  $r \in \mathbb{R}$ , let  $A_{r,\beta}^\circ$  be the  $\mathbb{N} \times \mathbb{N}$ -matrix with components*

$$A_{r,\beta}^\circ(i, j) = e^{r(i+j) - \beta(i+j)^2} P_0^\circ(i, j), \quad i, j \in \mathbb{N}, \tag{3.68}$$

with

$$P_0^\circ(i, j) = 1_{\{i \neq 0\}} P_0(i, j + 1) + 1_{\{i = j = 0\}}. \tag{3.69}$$

Let  $\lambda_{r,\beta}^\circ$  be the unique largest eigenvalue of  $A_{r,\beta}^\circ$  acting as an operator on  $l^2(\mathbb{N})$ . Then

$$I_\beta(0) = r^{**}(\beta) - r^*(\beta), \tag{3.70}$$

with  $r^{**}(\beta) \in (0, \infty)$  the unique solution of the equation

$$\lambda_{r,\beta}^\circ = 1. \tag{3.71}$$

*Proof.* See den Hollander [168], Chapter IX.  $\square$

It is easy to show that  $r^{**}(\beta) > r^*(\beta)$  for all  $\beta \in (0, \infty)$ . Since (3.67) says that  $r^{**}(\beta) = r_\beta(\theta^{**}(\beta))$ , with  $\theta \mapsto r_\beta(\theta)$  defined in Lemma 3.12, it follows that  $\theta^{**}(\beta) < \theta^*(\beta)$  for all  $\beta \in (0, \infty)$ .

In conclusion, we have proved Theorem 3.3 and identified the rate function  $I_\beta$  in terms of the families of principal eigenvalues  $(r, \beta) \mapsto \lambda_{r,\beta}$  and  $(r, \beta) \mapsto \lambda_{r,\beta}^\circ$  of the operators  $A_{r,\beta}$  and  $A_{r,\beta}^\circ$  defined in (3.48) and (3.68). These families are analytically well-behaved and can also be easily computed numerically (see Greven and den Hollander [130]).

### 3.6 Extensions

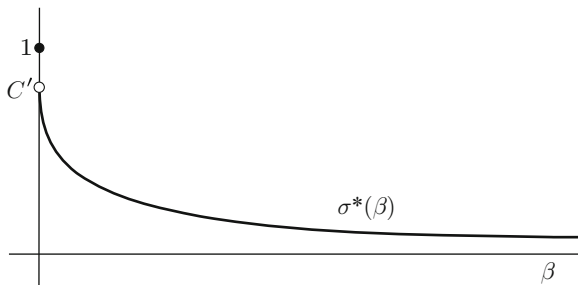
(1) Theorem 3.1 has been extended to a central limit theorem by König [218]. The standard deviation, denoted by  $\sigma^*(\beta)$ , turns out to be given by the formula

$$\frac{1}{\sigma^{*2}(\beta)} = \frac{\partial^2}{\partial \theta^2} J_\beta(\theta) \Big|_{\theta = \theta^*(\beta)} = \frac{\partial^2}{\partial \theta^2} I_\beta(\theta) \Big|_{\theta = \theta^*(\beta)}. \tag{3.72}$$

Numerical computation gives the picture in Fig. 3.5.

(2) Van der Hofstad and den Hollander [157] prove that

$$\lim_{\beta \downarrow 0} \beta^{-\frac{1}{3}} \theta^*(\beta) = C \text{ for some } C > 0 \tag{3.73}$$



**Fig. 3.5.** The spread of the soft polymer.

(recall Fig. 3.1), while van der Hofstad, den Hollander and König [158] prove that

$$\lim_{\beta \downarrow 0} \sigma^*(\beta) = C' \text{ for some } C' \neq 1. \quad (3.74)$$

These asymptotic formulas show that, even in the limit of weak self-repulsion, the behavior of the soft polymer cannot be understood via a perturbation argument around the non-repellent SRW. Van der Hofstad [153] derives rigorous bounds on  $C$  and  $C'$ . Numerically,  $C \approx 1.1$  and  $C' \approx 0.63$ . These constants are related to a Brownian version of the polymer model – called the Edwards model – defined in (3.78) below. We refer to van der Hofstad, den Hollander and König [159] for the analogous law of large numbers (first proved by Westwater [312]) and central limit theorem.

The heuristics behind the scaling in (3.73) is as follows. Suppose that  $S_n \approx \theta n$  and that  $0 \leq S_i \leq S_n$  for all  $0 \leq i \leq n$ . The Hamiltonian  $H_n = \beta \sum_{x \in \mathbb{Z}} \ell_n(x)^2$  is minimal when the local times are constant, i.e., when  $\ell_n(x) \approx n/S_n \approx 1/\theta$  for  $0 \leq x \leq S_n$ , in which case  $H_n \approx \beta(\theta n)(1/\theta)^2 = (\beta/\theta)n$ . The probability under  $P$ , the law of SRW, that  $S_n \approx \theta n$  is roughly  $\exp[-(\theta n)^2/2n]$ . Consequently, the contribution to the partition sum coming from paths with  $S_n \approx \theta n$  is roughly  $\exp[-\{(\beta/\theta) + \frac{1}{2}\theta^2\}n]$ . The term between braces in the exponent is minimal when  $\theta = \beta^{\frac{1}{3}}$ .

(3) Van der Hofstad, den Hollander and König [158] prove that if  $\beta$  is replaced by  $\beta_n$  satisfying

$$\lim_{n \rightarrow \infty} \beta_n = 0 \quad \text{and} \quad \lim_{n \rightarrow \infty} n^{\frac{3}{2}} \beta_n = \infty, \quad (3.75)$$

then the law of large numbers and central limit theorem apply with  $\theta^*(\beta)$  and  $\sigma^*(\beta)$  replaced by

$$\theta^*(\beta_n) \sim C (\beta_n)^{\frac{1}{3}} \quad \text{and} \quad \sigma^*(\beta_n) \sim C'. \quad (3.76)$$

In comparison with (3.73–3.74), this shows that the weak interaction limit has a degree of *universality*. Van der Hofstad, den Hollander and König [161] offer a coarse-graining argument showing that, in one dimension, self-repellent

random walks scale to self-repellent Brownian motions. The proof is based on cutting the path into pieces, controlling the interaction between the different pieces, and applying the invariance principle to the single pieces. The scaling properties are shown to be stable against adding self-attraction, provided the self-repulsion remains dominant. We will return to polymers with self-repulsion and self-attraction in Chapter 6.

(4) König [216], [217] (extending earlier work by Alm and Janson [9]) considers the case where the random walk is “spread out”, e.g., it draws its step uniformly from the set  $\{-L, \dots, L\}$  for some  $L \in \mathbb{N}$ . For this case, the SAW problem is interesting. It is shown that for every  $\beta \in (0, \infty)$  and  $L \in \mathbb{N}$  the self-avoiding polymer has a speed  $\theta^*(\beta, L) \in (0, L)$ . Aldous [3] – assuming that the speed existed – had earlier conjectured that

$$\lim_{L \rightarrow \infty} L^{-\frac{2}{3}} \theta^*(\infty, L) = C'' \text{ for some } C'' \in (0, \infty). \tag{3.77}$$

This conjecture was based on a scaling result for the self-intersection local time of the spread-out random walk in the limit as  $L \rightarrow \infty$ . The conjecture in (3.77) was subsequently proved in van der Hofstad, den Hollander and König [161], where it was shown that  $C'' = C3^{-\frac{1}{3}}$ .

(5) A continuum version of the Domb-Joyce model – called the Edwards model – is analyzed in Kusuoka [224] and van der Hofstad, den Hollander and König [159]. The Hamiltonian for this model is

$$\begin{aligned} H((B_t)_{t \in [0, T]}) \\ = -\beta \int_0^T ds \int_0^T dt \delta(B_s - B_t) = -\beta \int_{\mathbb{R}} L(T, x)^2 dx, \quad T \geq 0, \end{aligned} \tag{3.78}$$

where  $\delta(\cdot)$  is the Dirac delta-function,  $(B_t)_{t \geq 0}$  is standard Brownian motion and  $L(T, x)$  is its local time at position  $x$  up to time  $T$ . The behavior is ballistic, and both a law of large numbers and a central limit theorem apply, with speed  $C\beta^{\frac{1}{3}}$  and spread  $C'$  (which provide the link with the weak interaction limit of the Domb-Joyce model). The corresponding LDP is proved in van der Hofstad, den Hollander and König [160].

### 3.7 Challenges

(1) Prove that  $\beta \mapsto \theta^*(\beta)$  is non-decreasing (see Fig. 3.1). Even though this property seems intuitively plausible, it is actually deep (see Greven and den Hollander [130]) and remains open. Similarly, prove that  $\beta \mapsto \sigma^*(\beta)$  is non-increasing (see Fig. 3.5). It is not hard to compute  $\lambda_{r, \beta}$  numerically and get support for the monotonicity of both quantities. Coupling arguments do not work:  $P_n^\beta$ 's for different values of  $\beta$  are hard to compare, because the normalizing partition sum depends on  $\beta$  (recall (3.3)).

(2) Prove the functional central limit theorem, i.e., show that under the law  $P_n^{+, \beta}$  we have

$$\left( \frac{1}{\sigma^*(\beta)\sqrt{n}} \left[ S_{[tn]} - \theta^*(\beta) [tn] \right] \right)_{0 \leq t \leq 1} \implies (B_t)_{0 \leq t \leq 1} \quad \text{as } n \rightarrow \infty, \quad (3.79)$$

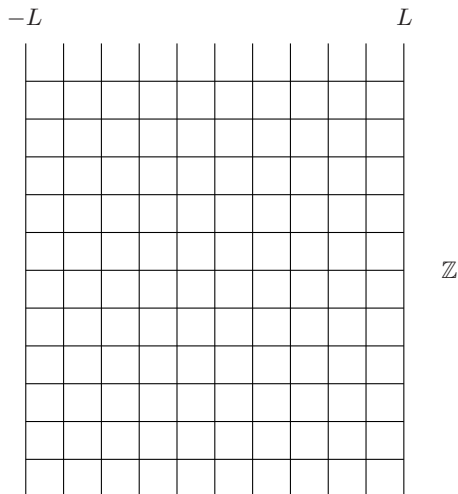
with standard Brownian motion as limit. The proof of (3.79) should not be hard: the method of local times employed in Sections 3.4.1–3.4.3 is very powerful and should allow us to get the multivariate analogues of the law of large numbers and the central limit theorem, together with the appropriate form of tightness.

(3) Derive a functional LDP extending Theorem 3.5.

(4) Van der Hofstad, den Hollander and König [161] have extended the LDP for the speed of the endpoint to the weak interaction limit in (3.75), but only for speeds that are not too small. Extend the proof to all speeds.

(5) Try to put some rigor into the following heuristic observation (put forward in van der Hofstad, den Hollander and König [161]), which argues in favor of the critical exponent  $\nu = \frac{3}{4}$  for the two-dimensional soft polymer (recall (2.26)) based on the result in Section 3.6, Extension (3). Consider simple random walk on the slit  $\{-L, \dots, L\} \times \mathbb{Z}$  with periodic boundary conditions (see Fig. 3.6). Write

$$S = (S_i)_{i=0}^n = (S^{(1)}, S^{(2)}) = (S_i^{(1)}, S_i^{(2)})_{i=0}^n \quad (3.80)$$



**Fig. 3.6.** The slit  $\{-L, \dots, L\} \times \mathbb{Z}$  with periodic boundary conditions.

for its two components, and note that  $S$  makes a self-intersection if and only if both  $S^{(1)}$  and  $S^{(2)}$  make a self-intersection. Under the soft polymer measure  $P_n^\beta$ , we have

$$|S_n^{(1)}| \asymp L \quad \text{and} \quad |S_n^{(2)}| \asymp L^{-\frac{1}{3}} n \quad \text{as } n \rightarrow \infty. \quad (3.81)$$

The first claim is trivial. The second claim comes from the fact that  $S^{(1)}$  self-intersects one out of  $(2L + 1)$  times. Hence, the motion of  $S^{(2)}$  is comparable to that of the one-dimensional soft polymer with self-repulsion parameter  $\beta_n = \beta/(2L + 1)$ . Therefore, according to (3.76),  $S^{(2)}$  moves a distance of order

$$(\beta_n)^{\frac{1}{3}} n \asymp L^{-\frac{1}{3}} n \quad (3.82)$$

in time  $n$ . Now, the two scales in (3.81) coincide when  $L = n^{\frac{3}{4}}$ . Then, the two components run on the same scale, and consequently the slit is wide enough for the motion of  $S$  to be comparable to that of the two-dimensional soft polymer. For  $L = n^{\frac{3}{4}}$ , both  $S_n^{(1)}$  and  $S_n^{(2)}$  run on scale  $n^{\frac{3}{4}}$ , and hence so does  $S_n$ . (Note that  $\beta_n \asymp n^{-\frac{3}{4}}$  when  $L = n^{\frac{3}{4}}$ , which indeed satisfies (3.75).)