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Upper Bounds for Survival Probability of the Contact Process

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A precise description of the nontrivial upper invariant measure for $\lambda > \lambda_c$ is still an open problem for the basic contact process, which is a self-dual, attractive, but nonreversible Markov process of an interacting particle system. By its self-duality, to identify the invariant measure is equivalent to determining the initial-state dependence of the survival probability of the process. A procedure to give rigorous upper bounds for the survival probability is presented based on a lemma given by Harris. Two new bounds are given, improving the simple branching-process bound. In the one-dimensional case, the present procedure can be viewed as a trial to make approximate measures by generalized Markov extensions.

KEY WORDS: Contact process; invariant measure; survival probability; upper bounds; Markov extension; interacting particle systems.

1. INTRODUCTION

We consider the basic contact process of Harris.[1] It is a continuous-time Markov process defined on the d-dimensional hypercubic lattice $\mathbf{Z}^d$. At each site $x \in \mathbf{Z}^d$, a variable $\eta(x)$ takes values 0 and 1. The formal generator of the present Markov semigroup $S(t)$ is given as

$$\Omega f(\eta) = \sum_{x \in \mathbf{Z}^d} c(x, \eta)[f(\eta^x) - f(\eta)] \tag{1.1a}$$

with flip rates

$$c(x, \eta) = \eta(x) + \lambda(1 - \eta(x)) \sum_{y:\, |y-x|=1} \eta(y) \tag{1.1b}$$

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where η^x denotes $\eta^x(y)=\eta(y)$ for $y \neq x$ and $\eta^x(x)=1-\eta(x)$. It is easy to show that there is a unique Markov process η_t on the state space $X=\{0, 1\}^{\mathbf{Z}^d}$ corresponding to $S(t)$.[2] Because this process can be viewed as a simple model for the spread of infection of disease [an individual at $x \in \mathbf{Z}^d$ is infected if $\eta(x)=1$ and healthy if $\eta(x)=0$], the parameter λ is often called an infection rate. In the textbook written by Liggett,[2] for example, Chapter VI is devoted to this process.

In the terminology used for the interacting particle systems,[2-4] the contact process is an attractive spin system. It has a coalescing dual which is the same as the original process (self-duality). However, this process is not a reversible process.

As a result of attractiveness, there exist lower and upper invariant measures;

$$\underline{\mu} = \lim_{t \to \infty} \delta_0 S(t) \tag{1.2a}$$

$$\bar{\mu} = \lim_{t \to \infty} \delta_1 S(t) \tag{1.2b}$$

where δ_0 and δ_1 are point masses on $\eta \equiv 0$ and $\eta \equiv 1$, respectively. Here the lower invariant measure is a trivial point mass δ_0 by the present rule of dynamics (1.1). An important point of the contact process is that there is a finite and positive critical value $\lambda_c(d)$, above which the process has a nontrivial upper invariant measure. In this paper this nontrivial upper invariant measure is denoted by $\nu_{d,\lambda}$ for the d-dimensional contact process with an infection rate λ.

Although the existence is confirmed, neither the exact value of the critical point nor the form of $\nu_{d,\lambda}$ are known yet. Of course, it is an interesting problem from the mathematical point of view; it should be emphasized here that mathematical physicists also have been seeking the precise description of this nontrivial invariant measure. The reason is that processes which are essentially the same as the contact process have appeared in a wide variety of fields of theoretical physics. It is known as a Reggeon quantum spin model for the strong interaction of hadrons.[5-7] The contact process may be considered as a simplified version of Schlögl's first model for some autocatalytic chemical reactions.[8,9] As mentioned above, it can also be viewed as a model of spread of infection.

The purpose of the present paper is to give some approximate measures which bound this nontrivial upper invariant measure. By self-duality, the upper invariant measure $\nu_{d,\lambda}$ of the contact process is completely characterized by the initial-state dependence of the survival probability of the process. In Section 2, a basic lemma of Harris is shown, based on which we derive upper bounds for the survival probability.

Section 3 is devoted to a presentation of our procedure to make approximate measures. In Section 4, three approximate measures are obtained by our procedure; the simple branching-process bound and two new improved bounds. It is proved in Appendices A and B that these approximate measures satisfy the conditions of the basic lemma mentioned in Section 2 and thus they are rigorous upper bounds for the true one. Section 5 is devoted to a summary and concluding remarks.

2. BASIC LEMMA

Let Y be the collection of all finite subsets of $\mathbf{Z}^d$. The finite contact process is the one for which initially, and hence at all times, $\sum_{\mathbf{x}} \eta_t(\mathbf{x}) < \infty$. With the identification $A_t = \{\mathbf{x}: \eta_t(\mathbf{x}) = 1\}$, the finite contact process can be viewed as a Markov chain A_t on Y. This process A_t is the coalescing dual of η_t. Let $\tau = \inf\{t \geqslant 0: A_t = \varnothing\}$, and define a survival probability of the process A_t starting from $A \in Y$ as

$$\sigma_{d,\lambda}(A) = P^A(\tau = \infty) \tag{2.1}$$

for all $A \in Y$ in the d-dimensional contact process.

Remark 2.1. Since the contact process is self-dual, this survival probability can be written in terms of the upper invariant measure $\nu_{d,\lambda}$ as follows[2]:

$$\begin{aligned} \sigma_{d,\lambda}(A) &= \nu_{d,\lambda}\{\eta: \eta(x) = 1 \text{ for some } x \in A\} \\ &= 1 - E_{\nu_{d,\lambda}}\left[\prod_{x \in A} (1 - \eta(x))\right] \end{aligned} \tag{2.2}$$

Thus, to identify the upper invariant measure $\nu_{d,\lambda}$ is equivalent to determining the dependence of the survival probability $\sigma_{d,\lambda}(A)$ on the dimensionality of the system, the infection rate, and initial states.

In order to obtain upper bounds for $\sigma_{d,\lambda}(A)$, here we use the following lemma, which is found in the paper by Harris.[10]

Lemma 2.1. Let $h(\cdot)$ be a $[0, 1]$-valued function defined on Y, where:

(i) $h(\varnothing) = 0$

(ii) $0 < h(A) \leqslant 1$ for all $A \neq \varnothing$

(iii) $\lim_{|A| \to \infty} h(A) = 1$

(iv) $R(h(A)) \leqslant 0$ for all $A \in Y$, with

$$R(h(A)) = -\lambda \sum_{\mathbf{x} \in A} \sum_{\mathbf{y}: |\mathbf{y}-\mathbf{x}|=1, \mathbf{y} \notin A} [h(A) - h(A \cup \mathbf{y})] + \sum_{\mathbf{x} \in A} [h(A \backslash \mathbf{x}) - h(A)] \tag{2.3}$$

Then

$$\sigma(A) \leqslant h(A) \qquad \text{for all} \quad A \in Y \tag{2.4}$$

Remark 2.2. Holley and Liggett used this lemma [with the opposite inequality in the condition (iv)] to give their famous *lower* bound for the survival probability.[11]

This lemma means that if we can correctly choose a function $h(\cdot)$ so that the four conditions of this lemma are satisfied, then we obtain a desired upper bound. As mentioned in Liggett's textbook,[2] it is believed that upper bounds for the survival probability are easier to find than lower bounds. For example, it is well known that some simple branching process gives an upper bound.[12] However, the discrepancy between this branching-process bound and the true one, which has been estimated by some (unfortunately nonrigorous) methods in statistical physics, is rather large.[6,7,13–15] So, here we try to improve this branching-process bound by choosing better functions $h(\cdot)$.

3. OUR CHOICE OF TRIAL FUNCTION $h(\cdot)$

In this section we show our strategy to choose trial functions. Here we write $A \sim B$ when a subset $A \in Y$ can be mapped to a subset $B \in Y$ by some translation, rotation, and reflection. Let $\tilde{Y}$ denote the collection of all equivalence classes determined by this relation. In other words, $\tilde{Y}$ is the collection of all different shapes of finite subsets in Y. We make two remarks before giving our choice of $h(\cdot)$.

Remark 3.1. For every subset A in $\tilde{Y}$ we can determine a number $c_B(A)$ for each subset $B \in \tilde{Y}$ as

$$c_B(A) = \#\{C \in Y: C \subseteq A \text{ and } C \sim B\} \tag{3.1}$$

It denotes the number of subsets included in A, which is equivalent to the subset B. The survival probability should be written as a function of a series of these numbers as

$$\sigma_{d,\lambda}(A) = F(\{c_B(A)\}_{B \in \tilde{Y}}) \tag{3.2}$$

for all $A \in \tilde{Y}$.

Remark 3.2. The survival probability is a stationary solution of the time-evolution equation of the system. Thus, the following equation (harmonicity) should hold for every subset $A \in \tilde{Y}$:

$$R(\sigma_{d,\lambda}(A)) = 0 \tag{3.3}$$

where $R(\cdot)$ is given as (2.3).

Our procedure to choose a trial function is given by the following three steps.

(i) First we choose a finite collection of sets Λ in $\tilde{Y}$.

(ii) We assume a simple form of $h(\cdot)$,

$$h^{(\Lambda)}(A) = 1 - \prod_{B \in \Lambda} (\alpha_B^{(\Lambda)})^{c_B(A)} \qquad \text{for all} \quad A \in \tilde{Y} \tag{3.4}$$

Namely, we introduce some real function $\alpha_B^{(\Lambda)}$ depending on the dimensionality of the system d and the infection rate λ for each subset B belonging to the collection Λ chosen above. Then a simple product is made. Intuitively speaking, we employ a kind of patchwork by using the pieces in Λ.

(iii) The real functions $\alpha_B^{(\Lambda)}$ are determined so that the stationary condition (3.3) is satisfied only for the nonempty subsets included in the collection Λ,

$$R(h^{(\Lambda)}(B)) = 0 \qquad \text{for all} \quad B \in \Lambda, B \neq \varnothing \tag{3.5}$$

In other words, we may say that $\alpha_B^{(\Lambda)}$'s are chosen so that *the partial stationary condition* (3.5) should be satisfied.

4. RESULTS

We give some upper bounds obtained by our procedure. It is shown first that the branching-process bound mentioned at the end of Section 2 is derived following the simplest choice of our trial function $h(\cdot)$. Then two improved bounds are presented.

4.1. Branching-Process Bound

Let Λ be a simple collection of an empty set and a singleton;

$$\Lambda = \Lambda(1) \equiv \{\varnothing, \{x\}\} \subset \tilde{Y} \tag{4.1}$$

Then, the following bound is obtained, which is known as the branching-process bound.

Result 1. For $\lambda > (2d)^{-1}$,

$$\sigma_{d,\lambda}(A) \leqslant h^{(A(1))}(A) \qquad \text{for all} \quad A \in Y$$

with

$$h^{(A(1))}(A) = 1 - (\alpha_{B_1}^{(A(1))})^{c_{B_1}(A)}$$

where $B_1 \equiv \{x\}$ and

$$\alpha_{B_1}^{(A(1))}(d, \lambda) = \frac{1}{2d\lambda}$$

Here the index $c_{B_1}(A)$ is nothing but the cardinality of A; $c_{B_1}(A) = |A|$.

4.2. Pair-Approximation Bound

The first improvement of the branching-process bound is given in arbitrary dimensions, which may be called a pair-approximation bound. Here we let

$$A = A(2) \equiv \{\varnothing, \{x\}, \{x, x+1\}\} \subset \tilde{Y} \tag{4.2}$$

Result 2. For $\lambda > (2d-1)^{-1}$,

$$\sigma_{d,\lambda}(A) \leqslant h^{(A(2))}(A) \qquad \text{for all} \quad A \in Y$$

with

$$h^{(A(2))}(A) = 1 - (\alpha_{B_1}^{(A(2))})^{c_{B_1}(A)} (\alpha_{B_2}^{(A(2))})^{c_{B_2}(A)} \tag{4.3a}$$

where $B_1 \equiv \{x\}$, $B_2 \equiv \{x, x+1\}$, and

$$\alpha_{B_1}^{(A(2))}(d, \lambda) = \frac{2d-1}{2d(2d-1)\lambda - 1}, \qquad \alpha_{B_2}^{(A(2))}(d, \lambda) = \frac{2d(2d-1)\lambda - 1}{(2d-1)^2 \lambda} \tag{4.3b}$$

In this choice the indices $c_{B_1}(A)$ and $c_{B_2}(A)$ are the cardinality of A and the number of neighboring pairs of points included in A, respectively,

$$c_{B_1}(A) = |A|, \qquad c_{B_2}(A) = \tfrac{1}{2} \sum_{x \in A} \sum_{y: |x-y|=1} I_A(x) I_A(y)$$

where $I_A(x)$ is the indicator function of A.

In particular, for the order parameter $\rho_{d,\lambda} \equiv \sigma_{d,\lambda}(\{x\})$, the survival probability of the process starting from a single point, we give

$$\rho_{d,\lambda} \leqslant \frac{2d\{(2d-1)\lambda - 1\}}{2d(2d-1)\lambda - 1} \tag{4.4}$$

Remark 4.1. As desired, this is an improvement of the previous branching-process bound for $\lambda > (2d-1)^{-1}$,

$$\sigma_{d,\lambda}(A) \leqslant h^{(A(2))}(A) \leqslant h^{(A(1))}(A) \qquad \text{for all} \quad A \in Y \tag{4.5}$$

Remark 4.2. This result can be considered as a generalization of the bound found in the monograph by Griffeath (ref. 3, p. 31, Proposition 4.4). His bound is given only for the order parameter in the case of one dimension,

$$\rho_{1,\lambda} \leqslant \frac{2\lambda-2}{2\lambda-1} \qquad \text{for} \quad \lambda > 1 \tag{4.6}$$

Result 2 is a generalization of this bound to the survival probability for all kinds of initial states in arbitrary dimensions.

Remark 4.3. By self-duality of the contact process,[2]

$$\begin{aligned} \lambda_c(d) &\equiv \sup\{\lambda \geqslant 0\text{: process is ergodic}\} \\ &= \inf\{\lambda \geqslant 0\text{: } \rho_{d,\lambda} > 0\} \end{aligned} \tag{4.7}$$

It is proved[2] that $\rho_{d,\lambda}$ is a nondecreasing function of the infection rate λ. Thus this result implies the following lower bound for the critical value, which was first obtained by Harris[1]:

$$\lambda_c(d) \geqslant (2d-1)^{-1} \tag{4.8}$$

Proof of Result 2. See Appendix A.

4.3. Improved Bound and Markov Extension in the One-Dimensional Case

The next result is for the one-dimensional system. In this case we make the finite collection Λ have five sets,

$$\Lambda = \Lambda(3) \equiv \{\varnothing, \{x\}, \{x, x+1\}, \{x, x+1, x+2\}, \{x, x+2\}\} \subset \tilde{Y} \tag{4.9}$$

Here we put $B_1 \equiv \{x\}$, $B_2 \equiv \{x, x+1\}$, $B_3 \equiv \{x, x+1, x+2\}$, and $B_4 \equiv \{x, x+2\}$.

Result 3. For $\lambda > \frac{1}{6}(1+\sqrt{37})$,

$$\sigma_{1,\lambda}(A) \leqslant h^{(\Lambda(3))}(A) \qquad \text{for all} \quad A \in Y$$

with

$$h^{(A(3))}(A) = 1 - \prod_{i=1}^{4} (\alpha_{B_i}^{(A(3))})^{c_{B_i}(A)} \tag{4.10a}$$

where $\alpha_{B_i}^{(A(3))}$ are determined as

$$\begin{aligned}
\alpha_{B_1}^{(A(3))} &= \frac{\lambda(2\lambda+3)+\sqrt{D}}{(2\lambda+1)(6\lambda^2-3\lambda-1)} \\
\alpha_{B_2}^{(A(3))} &= \frac{-(24\lambda^4+16\lambda^3+8\lambda^2+\lambda+1)+(6\lambda-1)(\lambda+1)\sqrt{D}}{2\lambda(\lambda-1)^2} \\
\alpha_{B_3}^{(A(3))} &= \frac{(24\lambda^3+16\lambda^2-2\lambda-3)+(4\lambda+3)\sqrt{D}}{8\lambda(2\lambda+1)^2} \\
\alpha_{B_4}^{(A(3))} &= \frac{(\lambda+1)\{(12\lambda^3-2\lambda^2-\lambda+1)-(3\lambda-1)\sqrt{D}\}}{2\lambda^2(\lambda-1)}
\end{aligned} \tag{4.10b}$$

where $D = 16\lambda^4 + 4\lambda^2 + 4\lambda + 1$. In particular,

$$\rho_{1,\lambda} \leqslant \frac{4\lambda(3\lambda^2-\lambda-3)}{(12\lambda^3-2\lambda^2-8\lambda-1)+(16\lambda^4+4\lambda^2+4\lambda+1)^{1/2}} \tag{4.10c}$$

Remark 4.4. This result implies the following bound for the critical value:

$$\lambda_c(1) \geqslant \tfrac{1}{6}(1+\sqrt{37}) = 1.18046... \tag{4.11}$$

This bound (4.11) was proved in Griffeath.[16] An alternative proof can be found in Section 2 of Chapter VI in the textbook by Liggett.[2] See also ref. 17 for the generalization of this lower bound for λ_c to arbitrary dimensions and an improvement in the one-dimensional system. Ziezold and Grillenberger[18] reported a systematic study of lower bounds on $\lambda_c(1)$. Their best lower bound is $\lambda_c(1) \geqslant 1.539$.

In the one-dimensional case, it should be remarked that our trial function has an interesting feature. As easily verified, it can be given by a generalized Markov extension (see, e.g., ref. 19); a function originally defined only on a small collection A is extended to a function defined on the whole of $\tilde{Y}$. This fact is illustrated below by showing that the function $h^{(A(3))}(\cdot)$ given by (4.10a) and (4.10b) is derived by the three-point Markov extension.

In order to define the three-point Markov extension, we first introduce some sets in Y:

$$W_i^{(2)} = \{i, i+1\} \in Y, \quad W_i^{(3)} = \{i, i+1, i+2\} \in Y \quad \text{for } i \in \mathbf{Z}^1 \tag{4.12}$$

For $A \in Y$, let

$$A_i^{(2)} = A \cap W_i^{(2)}, \qquad A_i^{(3)} = A \cap W_i^{(3)} \tag{4.13}$$

Then, we observe

$$\text{for all} \quad A_i^{(2)}, \qquad {}^{\exists 1}\tilde{A}_i^{(2)} \in \mathcal{A}(3) \quad \text{s.t.} \quad \tilde{A}_i^{(2)} \sim A_i^{(2)} \tag{4.14a}$$

and

$$\text{for all} \quad A_i^{(3)}, \qquad {}^{\exists 1}\tilde{A}_i^{(3)} \in \mathcal{A}(3) \quad \text{s.t.} \quad \tilde{A}_i^{(3)} \sim A_i^{(3)} \tag{4.14b}$$

Now we assume that $\bar{h}^{(3)}(\cdot)$ is defined as a nonzero-valued function on $\mathcal{A}(3)$ with normalization $\bar{h}^{(3)}(\varnothing) = 1$. Then the Markov extension is defined as the following procedure which extends it to a function on Y. For $A \in Y \backslash \mathcal{A}(3)$, define

$$l_A = \min\{x: x \in A\}, \qquad r_A = \max\{x: x \in A\} \tag{4.15}$$

Then, put

$$\bar{h}^{(3)}(A) \equiv \frac{\prod_{i=l_A}^{r_A-2} \bar{h}^{(3)}(\tilde{A}_i^{(3)})}{\prod_{i=l_A+1}^{r_A-2} \bar{h}^{(3)}(\tilde{A}_i^{(2)})} \tag{4.16}$$

and define

$$h^{(3)}(A) \equiv 1 - \bar{h}^{(3)}(A) \tag{4.17}$$

It is easily verified that if we define $\bar{h}^{(3)}(\cdot)$ on the finite collection $\mathcal{A}(3)$ so that the following relations with the functions $\{\alpha_B^{(\mathcal{A}(3))}\}$ defined by (4.10b) should hold,

$$\begin{aligned} \alpha_{B_1}^{(\mathcal{A}(3))} &= \bar{h}^{(3)}(B_1), \qquad & \alpha_{B_2}^{(\mathcal{A}(3))} &= \frac{\bar{h}^{(3)}(B_2)}{(\bar{h}^{(3)}(B_1))^2} \\ \alpha_{B_3}^{(\mathcal{A}(3))} &= \frac{\bar{h}^{(3)}(B_3)\,\bar{h}^{(3)}(B_1)}{(\bar{h}^{(3)}(B_2))^2}, \qquad & \alpha_{B_4}^{(\mathcal{A}(3))} &= \frac{\bar{h}^{(3)}(B_4)}{(\bar{h}^{(3)}(B_1))^2} \end{aligned} \tag{4.18}$$

then the function $h^{(3)}(\cdot)$ extended to Y by (4.16) and (4.17) is equivalent to the function $h^{(\mathcal{A}(3))}(\cdot)$ defined by (4.10a).

A sketch of the proof of Result 3 is given in Appendix B, where properties derived from the form (4.16) of the Markov extension are fully used. Complete proof for the lemmas in Appendix B is reported in ref. 20.

5. SUMMARY AND CONCLUDING REMARKS

As summary, we give in Fig. 1 a numerical comparison of the various bounds for the order parameter in the one-dimensional contact process.

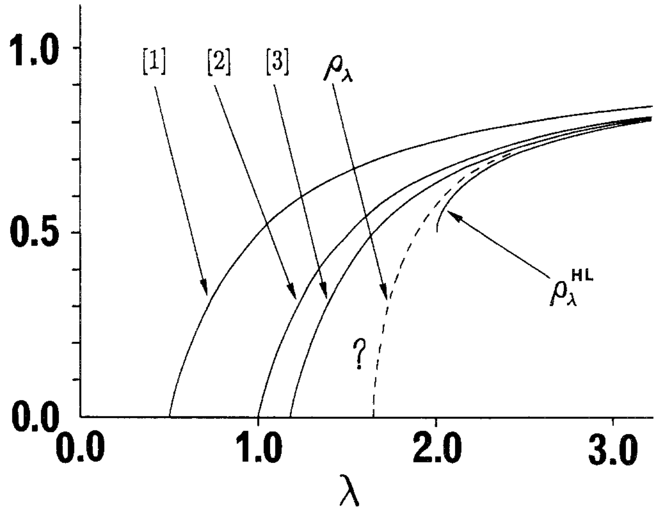

Fig. 1. Three upper bounds for $\rho_{1,\lambda}$ are shown for the one-dimensional contact process: [1] $h^{(\Lambda(1))}(\{x\}) = (2\lambda - 1)/2\lambda (\lambda > 1/2)$; [2] $h^{(\Lambda(2))}(\{x\}) = (2\lambda - 2)/(2\lambda - 1)(\lambda > 1)$; and [3] $h^{(\Lambda(3))}(\{x\})$, which is given as the right-hand side of (4.10c) for $\lambda > \frac{1}{6}(1 + \sqrt{37})$. The line denoted by $\rho_\lambda^{\rm HL}$ is the Holley–Liggett lower bound for $\rho_{1,\lambda}$,[11] $\rho_\lambda^{\rm HL} = 1/2 + [(\lambda - 2)/4\lambda]^{1/2}$ $(\lambda \geq 2)$.

We have some numerical data which suggest the convergence of the bounds obtained by the present procedure to the exact one as the limit $\Lambda \to \tilde{Y}$ with some assumptions on the convergence rate as reported in ref. 15. At this stage, however, we can give no rigorous arguments on this convergence problem for the d-dimensional contact process.

Finally, it is remarked that an alternative method to improve upper bounds for $\rho_{d,\lambda}$ can be constructed by using the Harris–FKG inequalities, which is reported in a separate paper.[21]

APPENDIX A. PROOF OF RESULT 2

In this Appendix we prove the fact that $h^{(\Lambda(2))}(\cdot)$ given by (4.3) in Result 2 satisfies the four conditions (i)–(iv) of Lemma 2.1 presented in Section 2, when $\lambda > (2d-1)^{-1}$.

Hereafter, we omit the superscript $\Lambda(2)$ in $\alpha_{B_i}^{(\Lambda(2))}$ for simplicity. The following lemmas are verified by direct computation using the expressions (4.3b) for α_{B_1} and α_{B_2}.

Lemma A.1. The function α_{B_1} is a monotonically decreasing function of λ. When $\lambda = (2d-1)^{-1}$, α_{B_1} takes the value 1. It goes to zero as $\lambda \to \infty$.

Lemma A.2. The function α_{B_2} is a monotonically increasing function of λ. When $\lambda=(2d-1)^{-1}$, $\alpha_{B_2}=1$. And $\lim_{\lambda\to\infty}\alpha_{B_2}=2d/(2d-1)$. Thus, if $\lambda>(2d-1)^{-1}$, $1<\alpha_{B_2}\leqslant 2d/(2d-1)$.

Lemma A.3. When $\lambda>(2d-1)^{-1}$, $0<\alpha_{B_1}\alpha_{B_2}^k<1$ for $1\leqslant k\leqslant 2d$.

The condition (i) and the right inequality in (ii) of Lemma 2.1 follow the definition of $h^{(A(2))}(\cdot)$ and Lemmas A.1 and A.2. For any nonempty $A\in Y$, $c_{B_2}(A)\leqslant d\cdot|A|$, where $|A|=c_{B_1}(A)$. Thus, by Lemma A.2,

$$h^{(A(2))}(A)\geqslant 1-(\alpha_{B_1}\alpha_{B_2}^d)^{|A|}>0 \qquad \text{for all} \quad A\in Y \tag{A.1}$$

where the positivity of $h^{(A(2))}(A)$ is assured by Lemma A.3. Since $h^{(A(2))}(A)\leqslant 1$ and Lemma A.3 holds, (A.1) gives the condition (iii) of Lemma 2.1.

To prove the fourth condition is the hardest part. Fix $A\in Y$, and write $A=\bigcup_{k=0}^{2d}A_k$, where $A_k=\{\mathbf{x}\in A\colon \sum_{\mathbf{y}:|\mathbf{y}-\mathbf{x}|=1}I_A(\mathbf{y})=k\}$. Then $R_{d,\lambda}(h^{(A(2))}(A))=\sum_{k=0}^{2d}R_k$, with

$$\begin{aligned} R_k= {}&-\lambda\sum_{\mathbf{x}\in A_k}\ \sum_{\mathbf{y}:|\mathbf{y}-\mathbf{x}|=1,\mathbf{y}\notin A}[h^{(A(2))}(A)-h^{(A(2))}(A\cup\mathbf{y})]\\ &+\sum_{\mathbf{x}\in A_k}[h^{(A(2))}(A\backslash\mathbf{x})-h^{(A(2))}(A)] \end{aligned}\tag{A.2}$$

For $0\leqslant k\leqslant 2d-1$, (A.2) is written as

$$R_k=\alpha_{B_1}^{c_{B_1}(A)}\alpha_{B_2}^{c_{B_2}(A)}\sum_{\mathbf{x}\in A_k}\left\{\lambda\sum_{\mathbf{y}:|\mathbf{y}-\mathbf{x}|=1,\mathbf{y}\notin A}[1-\alpha_{B_1}\alpha_{B_2}^{\gamma(A,\mathbf{y})}]-[\alpha_{B_1}^{-1}\alpha_{B_2}^{-k}-1]\right\} \tag{A.3}$$

where

$$\gamma(A,\mathbf{y})=\sum_{\mathbf{z}:|\mathbf{z}-\mathbf{y}|=1}I_A(\mathbf{z}) \tag{A.4}$$

Since $1\leqslant\gamma(A,\mathbf{y})\leqslant 2d$, $[1-\alpha_{B_1}\alpha_{B_2}^{\gamma(A,\mathbf{y})}]\leqslant[1-\alpha_{B_1}\alpha_{B_2}]$ for $\lambda>(2d-1)^{-1}$ by Lemma A.2. Then

$$R_k\leqslant\alpha_{B_1}^{c_{B_1}(A)}\alpha_{B_2}^{c_{B_2}(A)}\,|A_k|\,M_k \tag{A.5}$$

with

$$M_k=(2d-k)\,\lambda[1-\alpha_{B_1}\alpha_{B_2}]-[\alpha_{B_1}^{-1}\alpha_{B_2}^{-k}-1] \tag{A.6}$$

for $0\leqslant k\leqslant 2d-1$ and for $\lambda>(2d-1)^{-1}$. It is easy to show by using (4.3b) that

$$\begin{aligned} &M_0=M_1=0\\ &M_k=-\frac{(2d-1)\,\lambda-1}{2d-1}\sum_{p=1}^{k-1}(1-\alpha_{B_2}^{-p}) \quad \text{for } 2\leqslant k\leqslant 2d-1 \end{aligned}\tag{A.7}$$

Lemma A.2 implies that $M_k \leqslant 0$ for $0 \leqslant k \leqslant 2d-1$ if $\lambda \geqslant (2d-1)^{-1}$. On the other hand,

$$R_{2d} = -\alpha_{B_1}^{c_{B_1}(A)-1} \alpha_{B_2}^{c_{B_2}(A)-2d} |A_{2d}| \cdot (1 - \alpha_{B_1} \alpha_{B_2}^{2d})$$

Lemma A.3 ensures that $R_{2d} \leqslant 0$ for $\lambda > (2d-1)^{-1}$.

APPENDIX B. PROOF OF RESULT 3

In the present Appendix, we give a sketch of proof for the Result 3 given in Section 4. The complete proof is found in ref. 20.

Now we show how to verify the fact that the four conditions in Lemma 2.1 are satisfied by the function $h^{(A(3))}(\cdot)$ given by (4.10a) for $\lambda > \lambda^{(3)} \equiv \frac{1}{6}(1+\sqrt{37})$. To describe our proof, it is convenient to use the expressions (4.16) and (4.17) obtained by the three-point Markov extension with (4.18) rather than to use the expression (4.10a). The three conditions (i)–(iii) of Lemma 2.1 are guaranteed by the following lemma, which can be verified by direct calculation.

Lemma B.1. For $\lambda > \lambda^{(3)}$,

(i) $0 < \bar{h}^{(3)}(B_1) < 1$

(ii) $\bar{h}^{(3)}(B_2) > (\bar{h}^{(3)}(B_1))^2$

(iii) $\bar{h}^{(3)}(B_3) > \dfrac{(\bar{h}^{(3)}(B_2))^2}{\bar{h}^{(3)}(B_1)}$

(iv) $\bar{h}^{(3)}(B_4) > (\bar{h}^{(3)}(B_1))^2$

(v) $\dfrac{\bar{h}^{(3)}(B_3)}{\bar{h}^{(3)}(B_4)} > \dfrac{\bar{h}^{(3)}(B_2)}{\bar{h}^{(3)}(B_1)}$

(vi) $0 < \dfrac{\bar{h}^{(3)}(B_3)\,\bar{h}^{(3)}(B_4)}{\bar{h}^{(3)}(B_2)(\bar{h}^{(3)}(B_1))^2} < 1$

In order to prove the last condition (iv) of Lemma 2.1, we reduce a subset $A \in Y$ to obtain some subsets A^{R_1} and $A^{R_2} \in Y$ and compare the value of $R(h^{(3)}(A))$ with that of $R(h^{(3)}(A^{R_2}))$. Now we define the three kinds of reduction. Here, τ_n means a translation of a set in Y on $\mathbf{Z}^1$ to the right by n lattice spacings and τ_{-n} means a translation to the left by n.

Reduction I. If there is a point $x \in \mathbf{Z}^1$ such that $\{x, x+1, x+2, x+3\} \subset A$, replace A by the following reduced set:

$$\{A \cap (-\infty, x-1]\} \cup \{x, x+1, x+2\} \cup \tau_{-1}\{A \cap [x+4, \infty)\}$$

Reduction II. If there is a point $x \in \mathbf{Z}^1$ such that $x \notin A$, $x+2k \notin A$, and $x+(2k-1) \in A$ for $k=1, 2, 3$, replace A by the following reduced set:

$$\{A \cap (-\infty, x-1]\} \cup \{x+1, x+3\} \cup \tau_{-2}\{A \cap [x+7, \infty)\}$$

We define A^{R_1} as the set obtained from A by operating with the above two reductions as many times as possible, and write $A^{R_1} = \bigcup_i A_i^{R_1}$, where $A_i^{R_1} = [l_i^{R_1}, r_i^{R_1}]$ are the ordered maximal connected components of A^{R_1}. By the definition of A^{R_1}, $|A_i^{R_1}| = r_i^{R_1} - l_i^{R_1} + 1 \leqslant 3$ for all i. Then we define the third reduction.

Reduction III. If there are $A_i^{R_1}$ and $A_{i+1}^{R_1}$ in A^{R_1} such that $r_i^{R_1} + 1 = l_{i+1}^{R_1} - 1$ and that $|A_i^{R_1}| + |A_{i+1}^{R_1}| \geqslant 3$, replace A^{R_1} by the following reduced set:

$$\{A^{R_1} \cap (-\infty, r_i^{R_1}]\} \cup \tau_2\{A^{R_1} \cap [l_{i+1}^{R_1}, \infty)\}$$

We define A^{R_2} as the set obtained from A^{R_1} by operating with Reduction III as many times as possible.

We notice that $R(h^{(3)}(A))$ can be rewritten to the following form for the one-dimensional system:

$$R(h^{(3)}(A)) = \sum_{x \in \mathbf{Z}^1} R_x(A) \tag{B.1}$$

with

$$R_x(A) = c(A, x)\left[1 - \frac{\bar{h}^{(3)}(A^x)}{\bar{h}^{(3)}(A)}\right]\bar{h}^{(3)}(A) \tag{B.2}$$

where

$$c(A, x) = \lambda(1 - I_A(x))(I_A(x-1) + I_A(x+1)) + I_A(x) \tag{B.3}$$

and

$$A^x = \begin{cases} A \cup x, & \text{if } x \notin A \\ A \backslash x, & \text{if } x \in A \end{cases} \tag{B.4}$$

To compare the value of $R(h^{(3)}(A))$ with that of $R(h^{(3)}(A^{R_2}))$, the following significant property of the three-point Markov extension should be noticed.

Lemma B.2. When $A \in Y$, for all $x \in \mathbf{Z}^1$,

$$\frac{\bar{h}^{(3)}(A^x)}{\bar{h}^{(3)}(A)} = \frac{\bar{h}^{(3)}(A^x \cap \{x-2, x-1, x\})\, \bar{h}^{(3)}(A^x \cap \{x-1, x, x+1\}) \times \bar{h}^{(3)}(A^x \cap \{x, x+1, x+2\})}{\bar{h}^{(3)}(A \cap \{x-2, x-1, x\})\, \bar{h}^{(3)}(A \cap \{x-1, x, x+1\}) \times \bar{h}^{(3)}(A \cap \{x, x+1, x+2\})} \times \frac{\bar{h}^{(3)}(A \cap \{x-1, x\})\, \bar{h}^{(3)}(A \cap \{x, x+1\})}{\bar{h}^{(3)}(A^x \cap \{x-1, x\})\, \bar{h}^{(3)}(A^x \cap \{x, x+1\})}$$

By using this property and Lemma B.1, we obtain the following.

Lemma B.3. For $A \in Y$, when $\lambda > \lambda^{(3)}$,

$$R(h^{(3)}(A)) \leqslant f_A \cdot R(h^{(3)}(A^{R_2}))$$

with

$$f_A = \left(\frac{\bar{h}^{(3)}(B_3)}{\bar{h}^{(3)}(B_2)}\right)^{n_1(A)} \left(\frac{\bar{h}^{(3)}(B_4)}{\bar{h}^{(3)}(B_1)}\right)^{n_2(A)} \left(\frac{\bar{h}^{(3)}(B_4)}{(\bar{h}^{(3)}(B_1))^2}\right)^{n_3(A)}$$

where $n_1(A)$, $n_2(A)$, and $n_3(A)$ denote the numbers of procedures of Reductions I, II, and III in the map $A \to A^{R_2}$, respectively.

Since $f_A \geqslant 0$ for $\lambda > \lambda^{(3)}$, this lemma means that it is sufficient to show $R(h^{(3)}(A^{R_2})) \leqslant 0$ to prove the condition (iv) of Lemma 2.1.

Next we decompose A^{R_2} at the places where we find points which are not included in A^{R_2} more than twice in succession and write

$$A^{R_2} = \bigcup_j \hat{A}_j^{R_2} \tag{B.5}$$

Let $\hat{l}_j = \min\{x: x \in \hat{A}_j^{R_2}\}$ and $\hat{r}_j = \max\{x: x \in \hat{A}_j^{R_2}\}$. The above decomposition (B.5) means that $\hat{l}_{j+1} - \hat{r}_j - 1 \geqslant 2$, and that if $x \in [\hat{l}_j, \hat{r}_j]$, but $x \notin \hat{A}_j^{R_2}$, then $x-1 \in \hat{A}_j^{R_2}$ and $x+1 \in \hat{A}_j^{R_2}$. Following (B.5), we write

$$R(h^{(3)}(A^{R_2})) = \sum_j R^{(j)}(h^{(3)}(A^{R_2})) \tag{B.6a}$$

with

$$R^{(j)}(h^{(3)}(A^{R_2})) = \sum_{\hat{l}_j - 1 \leqslant x \leqslant \hat{r}_j + 1} R_x(A^{R_2}) \tag{B.6b}$$

where $R_x(\cdot)$ is given by (B.2).

It should be noticed that each segment $\hat{A}_j^{R_2}$ can be mapped to a non-empty set in $\Lambda(3)$ by appropriate translation and reflection; $^{\exists 1}B \in \Lambda(3)$, s.t. $B \neq \varnothing$, $B \sim \hat{A}_j^{R_2}$. By using Lemma B.2 successively, and noticing the inequality (iv) in Lemma B.1, we obtain for each j with $\hat{A}_j^{R_2} \sim B \in \Lambda(3)$, $B \neq \varnothing$, that

$$R^{(j)}(h^{(3)}(A^{R_2})) \leqslant \frac{\bar{h}^{(3)}(A^{R_2})}{\bar{h}^{(3)}(B)} R(h^{(3)}(B)) \tag{B.7}$$

for $\lambda > \lambda^{(3)}$. Let $n(A^{R_2}, B) = \#\{j: \hat{A}_j^{R_2} \sim B\}$ for $B \in \Lambda(3)$, $B \neq \varnothing$, then (B.6) and (B.7) give

$$R(h^{(3)}(A^{R_2})) \leqslant \sum_{B \in \Lambda(3), B \neq \varnothing} n(A^{R_2}, B) \frac{\bar{h}^{(3)}(A^{R_2})}{\bar{h}^{(3)}(B)} R(h^{(3)}(B)) \tag{B.8}$$

for $\lambda > \lambda^{(3)}$. Since $R(h^{(3)}(B)) = 0$ for $B \in A(3)$ by the partial stationary condition (3.5), the proof is completed.

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