Distribution of domain sizes in the zero temperature Glauber dynamics of the one-dimensional Potts model

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For the zero temperature Glauber dynamics of the q-state Potts model, we calculate the exact distribution of domain sizes by mapping the problem on an exactly soluble one-species coagulation model ($A+A\rightarrow A$). In the long time limit, this distribution is universal and, from its (complicated) exact expression, we extract its behavior in various regimes. Our results are tested in a simulation and compared to the predictions of a simple approximation proposed recently. Considering the dynamics of domain walls as a reaction-diffusion model $A+A\rightarrow A$ with probability $(q-2)/(q-1)$ and $A+A\rightarrow\phi$ with probability $1/(q-1)$, we calculate the pair correlation function in the long time regime. [S1063-651X(96)12809-9]

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I. INTRODUCTION

When a ferromagnetic system is quenched from the high temperature phase to a temperature below its Curie temperature, one observes a pattern of growing domains. In the long time limit, when the typical size of domains becomes much larger than the lattice spacing (or the correlation length) but is still small compared to the system size, the domains at different times form a (statistically) self similar structure (see [1] and references therein). For a nonconserved order parameter, it is well established that the size of the domains grows with time t like $t^{1/2}$. Much less is known about the distribution of domain sizes.

The purpose of the present paper is to give the exact distribution of domain sizes in the case of the one-dimensional (1D) q-state Potts model evolving according to zero temperature Glauber dynamics [2] (in 1D, the low temperature phase reduces only to zero temperature). As [3,4] the average domain size grows with time like $t^{1/2}$, the distribution of domain sizes can only be determined up to a change of scale, and we will rescale the length x of the domains so that, for the distribution $g(x;q)$, the average domain size is unity ($\int xg(x;q)dx=1$). So far, this distribution has been calculated only for $q=\infty$ [5,6] because it is related to the probability that two walkers do not meet up to time t. Our goal, here, is to extend this result to arbitrary $q>1$.

Our approach is a generalization of a calculation done recently [7,8] to obtain the fraction of permanent spins (i.e., spins which never flip up to time t). We calculate the probability $Q(N)$ that N given consecutive spins are parallel at time t, and explain how $g(x;q)$ can be extracted from $Q(N)$. As for the number of persistent spins, the full expression of $Q(N)$ is rather complicated, but it can be used to write explicit formulas in various limits.

It has been known for a long time that the zero temperature Glauber dynamics of the 1D Potts model is fully equivalent to a single-species reaction-diffusion model [4,5,6,9,10]. If one represents each domain wall by a particle A, and if the initial spin configuration is random with no correlation, it is easy to show that the particles A diffuse along the line, and that whenever two particles sit on the same bond, they instantaneously react according to

$$A+A\rightarrow\begin{cases} A & \text{with probability } (q-2)/(q-1) \\ \phi & \text{with probability } 1/(q-1). \end{cases} \tag{1}$$

We will see that several of our results can be reinterpreted as properties of this 1D reaction-diffusion problem.

An easy way to implement the zero temperature dynamics of the 1D q-state Potts model is to say that, during every infinitesimal time interval dt, each spin $S_i(t)$ is updated according to

$$S_i(t+dt)=\begin{cases} S_i(t) & \text{with probability } 1-2dt \\ S_{i-1}(t) & \text{with probability } dt \\ S_{i+1}(t) & \text{with probability } dt. \end{cases}$$

This shows the close analogy with random walk problems [11]. As in [7,8,12], this analogy will be the basis of our calculation.

The paper is organized as follows. In Sec. II, we recall several properties of random walks which are used in the following sections and the relation between random walks and the zero temperature Glauber dynamics of a spin chain. In Sec. III, we obtain, using several relations derived in [8], the probability $Q(N)$ that, at time t, N given consecutive spins are parallel, and we show how the distribution of domain sizes follows from the knowledge of the $Q(N)$. In Sec. IV, we give more explicit expressions in various limits, and in Sec. V we compare our predictions with the results of simulations. In Sec. VI, we calculate the pair correlation for the reaction diffusion model (1).

II. PROPERTIES OF RANDOM WALKS IN ONE DIMENSION AND THE $q=\infty$ CASE

Let us first recall some properties of random walks in one dimension. Several of these properties are well known (in particular they can be obtained by representing the walkers as free fermions [13–15]), but we spend some time discuss-

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ing them because they are essential to an understanding of the following sections. These properties will include the probability $c_{i,j}$ that two walkers starting at positions $x_i<x_j$ do not meet up to time t, and the probability $c^{(n)}_{1,2,\ldots,2n}$ that no pair meets up to time t between $2n$ walkers starting at positions $x_1<x_2<\cdots x_{2n}$.

Consider a random walker on a 1D lattice which hops, during each infinitesimal time interval to its right with probability dt, to its left with probability dt (and of course remains at the same position with probability $1-2dt$). The probability $p_t(y,x)$ of finding the walker at position y at time t, given that it was initially (at time 0) at position x, evolves according to

$$\frac{d}{dt}p_t(y,x)=p_t(y+1,x)+p_t(y-1,x)-2p_t(y,x)$$
$$=p_t(y,x+1)+p_t(y,x-1)-2p_t(y,x), \quad (2)$$

and the solution is

$$p_t(y,x)=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta\,\cos(x-y)\theta e^{-2(1-\cos\theta)t}. \quad (3)$$

Consider now two walkers on this 1D lattice starting at positions x_i and x_j with $x_i<x_j$. The probability $C_t(x_i,x_j)\equiv c_{i,j}$ that these two walkers never meet up to time t evolves according to

$$\frac{d}{dt}C_t(x,x')=C_t(x+1,x')+C_t(x-1,x')+C_t(x,x'+1)$$
$$+C_t(x,x'-1)-4C_t(x,x'), \quad (4)$$

with the boundary conditions that $C_t(x,x)=0$ at any time t and that $C_0(x,x')=1$ if $x<x'$. It is easy to check that the expression

$$c_{i,j}=C_t(x_i,x_j)=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta\,\frac{\sin\theta\,\sin(x_j-x_i)\theta}{1-\cos\theta}\,e^{-4(1-\cos\theta)t} \quad (5)$$

satisfies (4). It is remarkable [8] that the probabilities of all the meeting events of N coalescing random walkers starting at positions $x_1\leqslant x_2\leqslant\cdots\leqslant x_N$ can be expressed in terms of the matrix $c_{i,j}$. For example, for three walkers starting at positions $x_1\leqslant x_2\leqslant x_3$, the probability that none of them meets any of the other two up to time t is given by

$$c_{1,2}+c_{2,3}-c_{1,3}.$$

For four walkers starting at $x_1\leqslant x_2\leqslant x_3\leqslant x_4$, the probability that no pair meets up to time t is given by

$$c^{(2)}_{1,2,3,4}=c_{1,2}c_{3,4}+c_{1,4}c_{2,3}-c_{1,3}c_{2,4}. \quad (6)$$

Below, we will use the fact that [8] the probability that, up to time t, no pair meets among $2n$ walkers starting at positions $x_1\leqslant x_2\leqslant\cdots x_{2n}$, is given by the Pfaffian of the $2n\times 2n$ matrix $c_{i,j}$

$$c^{(n)}_{1,2,\ldots,2n-1,2n}=\frac{1}{2^n n!}\sum_{\sigma}\epsilon(\sigma)c_{\sigma(1),\sigma(2)}\cdots c_{\sigma(2n-1),\sigma(2n)}, \quad (7)$$

where the sum runs over all the permutations σ of the indices $\{1,2,...,2n\}$, $\epsilon(\sigma)$ is the signature of the permutation σ, and the matrix $c_{i,j}$ is antisymmetrized,

$$c_{i,j}=-c_{j,i}<0 \quad \text{when} \quad i>j.$$

There are several ways of deriving (6) and (7), for example by considering the walkers as free fermions [13,14,15,8] or by using the method of images. One can also simply write equations similar to (4) which govern the evolution of these probabilities, and check that (6) and (7) do satisfy these equations with the right boundary conditions when $c_{i,j}$ is the solution of (4). (Note that the above relations would not be valid in dimensions higher than 1: it is only in 1D that whenever 1 and 2 do not meet, it implies that 1 and 3 do not meet because of the order of the walkers along the line.)

Apart the probabilities that the walkers never meet, the knowledge of the matrix $c_{i,j}$ allows one to calculate all the meeting probabilities between coalescing random walkers [8]. For example, when four walkers start at positions $x_1<x_2<x_3<x_4$, one finds for the probability $\psi_{12,34}$ that walkers 1 and 2 coalesce, walkers 3 and 4 coalesce, but walkers 2 and 3 do not coalesce before time t,

$$\psi_{12,34}=c_{1,3}+c_{2,4}+c^{(2)}_{1,2,3,4}-c_{1,2}-c_{2,3}-c_{3,4}, \quad (8)$$

and for the probability $\psi_{1,23,4}+\psi_{1,2,3,4}$ that walkers 1 and 2 and walkers 3 and 4 do not meet (without saying whether walkers 2 and 3 meet or not)

$$\psi_{1,23,4}+\psi_{1,2,3,4}=c_{1,3}+c_{2,4}+c^{(2)}_{1,2,3,4}-c_{1,4}-c_{2,3}. \quad (9)$$

In the long time limit, all the above expressions (6), (7), (8), and (9) remain valid, with $c_{i,j}$ replaced by the asymptotic expression of (5),

$$c_{i,j}=C_t(x_i,x_j)=f\left(\frac{x_j-x_i}{\sqrt{8t}}\right), \quad (10)$$

$$f(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-u^2}du. \quad (11)$$

A. Relation between random walks and the dynamics of the spin chain

As in [12,7,8], we are going to use the close analogy between the problem of coalescing random walkers and the properties of a spin chain evolving according to zero temperature dynamics: assume that we want to calculate, for a Potts chain with no correlation in the initial condition, the probability that spins at position $x_1<x_2<\cdots<x_N$ are equal at time t. One can consider N coalescing random walkers starting at positions $x_1<x_2<\cdots<x_N$, and if $P(m,t)$ denotes the probability that, at time t, there are m walkers left in the system, one has [7,8]

$$\text{Probability}\{S_{x_1}(t)=S_{x_2}(t)=\cdots S_{x_N}(t)\} = \sum_{m=1}^{N} P(m,t)\,\frac{1}{q^{m-1}}. \tag{12}$$

This expression can be understood by noticing that initially the spins are random, and that the probability that m spins have the same color in the initial condition is just $1/q^{m-1}$.

B. Case $q=\infty$

In the limit $q\to\infty$ only the first term of the sum contributes, and one finds that

$$\text{Probability}\{S_{x_1}(t)=S_{x_2}(t)=\cdots S_{x_N}(t)\}=1-C_t(x_1,x_N). \tag{13}$$

This expression can easily be understood: for $q=\infty$, all spins in the initial configuration are different; if $S_{x_1}(t)=S_{x_N}(t)$, this means that the two walkers starting at x_1 and x_N have met before time t and, therefore, at time t, all the spins located between x_1 and x_N are equal. This can be used to calculate the distribution of domain sizes in the $q\to\infty$ limit: if $p_1(l)$ is the density of domains of length l, one has

$$\text{Probability}\{S_{x_1}(t)=S_{x_2}(t)=\cdots S_{x_N}(t)\} = \sum_{l\geqslant x_N-x_1} (l-x_N+x_1)p_1(l). \tag{14}$$

This leads to

$$p_1(l)=2C_t(0,l)-C_t(0,l+1)-C_t(0,l-1), \tag{15}$$

and, in the long time limit

$$p_1(l)=-\frac{1}{8t}\,f''\left(\frac{1}{\sqrt{8t}}\right). \tag{16}$$

For $q=\infty$, this allows one to calculate the average domain size at time t,

$$\langle l\rangle_\infty=\frac{\sum_l l p_1(l)}{\sum_l p_1(l)}\simeq\frac{\sqrt{8t}}{f'(0)}=\sqrt{2\pi t} \tag{17}$$

and the distribution $g(x;\infty)$ of domain sizes [6] (normalized such that the average size is 1)

$$g(x;\infty)=\langle l\rangle\,\frac{p_1(\langle l\rangle x)}{\sum_{l'} p_1(l')}=\frac{\pi}{2}\,xe^{-x^2\pi/4}. \tag{18}$$

This expression had been obtained up to a factor in [17].

For similar reasons, it is easy to see that, for $q=\infty$, the probability that $S_{x_1}(t)=S_{x_2}(t)\neq S_{x_3}(t)=S_{x_4}(t)$ is given by

$$\text{Probability}\{S_{x_1}(t)=S_{x_2}(t)\neq S_{x_3}(t)=S_{x_4}(t)\}=\psi_{12,34}. \tag{19}$$

This can be used to obtain $p_2(l_1,l_2)$, the density of domains of length l_1 followed by a domain of length l_2 (because for $q=\infty$, whenever two spins have a certain color, all the spins between them have the same color),

$$\text{Probability}\{S_{x_1}(t)=S_{x_2}(t)\neq S_{x_2+1}(t)=S_{x_4}(t)\} = \sum_{l_1\geqslant x_2-x_1}\ \sum_{l_2\geqslant x_4-x_2-1} p_2(l_1,l_2). \tag{20}$$

and consequently (8)–(11), the (normalized) distribution $g_2(x,y;\infty)$ of neighboring domain sizes is given by

$$g_2(x,y;\infty)=\langle l\rangle^2\,\frac{p_2(\langle l\rangle x,\langle l\rangle y)}{\sum_{l'}p_1(l')}=\frac{\pi}{2}\,(x+y)[e^{-(x^2+y^2)\pi/4} - e^{-(x+y)^2\pi/4}]. \tag{21}$$

This means that the lengths of consecutive domains in the limit $q\to\infty$ are correlated. In particular, if l_1 and l_2 are the lengths of two consecutive domains, one has

$$\frac{\langle l_1 l_2\rangle}{\langle l\rangle^2}=\int_0^\infty dx\int_0^\infty dy\ g_2(x,y;\infty)xy=\frac{3}{\pi}\neq 1. \tag{22}$$

Remark 1: The knowledge of the distribution of domain sizes and of all the correlations between consecutive domain sizes for $q=\infty$ gives the distribution of domain sizes for arbitrary q. If $l_1,l_2,\ldots,l_n,\ldots$ are the lengths of consecutive domains when $q=\infty$, one can obtain the length l of a typical domain for finite q by

$$l=\begin{cases} l_1 & \text{with probability } \dfrac{q-1}{q} \\ l_1+l_2 & \text{with probability } \dfrac{q-1}{q^2} \\ \cdots & \\ l_1+l_2+\cdots+l_n & \text{with probability } \dfrac{q-1}{q^n}\,. \\ \cdots & \end{cases} \tag{23}$$

This is because one way of performing the dynamics at finite q is first to make the system evolve with all spins different in the initial condition (as in the case $q=\infty$), and then suppress the domain walls with probability $1/q$. This is due to the fact that, for finite q, two initial values are identical with probability $1/q$.

A consequence of (23) is that, in the long time limit, the average length for finite q is given by (17)

$$\langle l\rangle_q=\frac{q}{q-1}\langle l\rangle_\infty\simeq\frac{q}{q-1}\sqrt{2\pi t}\ . \tag{24}$$

It is clear also from (23) that the calculation of any other moment $\langle l^n\rangle$ of the length would require the knowledge of all the correlations between the l_i.

Remark 2: If these correlations between successive domain sizes for $q=\infty$ were absent, the calculation of the normalized distribution $g(x;q)$ for arbitrary q would be straightforward: neglecting the correlations in (23) would give, for the generating function of $g(x;q)$,

$$\int_0^\infty dx\ g(x;q)e^{\alpha qx/(q-1)}dx=\frac{(q-1)\int_0^\infty dx\ g(x;\infty)e^{\alpha x}dx}{q-\int_0^\infty dx\ g(x;\infty)e^{\alpha x}dx}. \tag{25}$$

Then using expression (18), one would find (by analyzing the limit $\alpha\to-\infty$)

$$g(x;q)=\frac{\pi}{2}\frac{q}{q-1}x-\frac{\pi^2}{24}\frac{(3q-1)q^2}{(q-1)^3}x^3+\frac{\pi^3}{960}\frac{(15q^2-6q+1)q^3}{(q-1)^5}x^5+O(x^7) \tag{26}$$

and (by analyzing the pole in α)

$$g(x;q)\simeq\exp[-A(q)x+B(q)]\quad\text{for large } x, \tag{27}$$

where $A(q)$ is the root of

$$\frac{\pi}{2}\int_0^\infty dx\ x\ \exp\left[-\frac{\pi x^2}{4}+\frac{(q-1)x}{q}A(q)\right]=q, \tag{28}$$

and $B(q)$ is given by

$$B(q)=\ln\left\{\frac{q^2\pi A(q)}{q\pi+2(q-1)A(q)^2}\right\}. \tag{29}$$

For $q=2$, this is precisely the prediction recently given in [16], based on the assumption that the intervals $l_1,l_2,\ldots$ are uncorrelated. We have already seen [(21) and (22)] that this assumption is not valid. Our goal in the following sections is to obtain the true distribution $g(x;q)$ where these correlations have been taken into account. We will see that the exact expression of $g(x;q)$ differs from (26), (28), and (29).

III. ARBITRARY CORRELATION FUNCTIONS

Our solution for the distribution of size of domains is based on our ability to write exact expressions for all correlation functions (valid at an arbitrary time) when the initial condition is random with no correlation (i.e., each spin initially takes one of the q possible colors with equal probability). These exact expressions involve the probabilities $c^{(n)}$ given by (5)–(7). One can show in particular that the probability that N spins located at positions $x_1\leqslant x_2\leqslant\cdots x_N$ are identical at time t is given by

$$\begin{aligned}\text{Prob}\{S_{x_1}(t)=\cdots S_{x_N}(t)\}&=1-\mu\sum_{i=1}^{N-1}c_{i,i+1}+\mu^2\sum_{i<j}c^{(2)}_{i,i+1,j,j+1}\\&-\mu^3\sum_{i<j<k}c^{(3)}_{i,i+1,j,j+1,k,k+1}\\&+\cdots-\lambda\Big\{\mu c_{1,N}-\mu^2\sum_i c^{(2)}_{1,i,i+1,N}\\&+\mu^3\sum_{i<j}c^{(3)}_{1,i,i+1,j,j+1,N}-\cdots\Big\},\end{aligned} \tag{30}$$

where

$$\lambda=q-1, \tag{31}$$

$$\mu=\frac{q-1}{q^2}. \tag{32}$$

[Note that as long as N is finite, (30) is the sum of a finite number of terms and is therefore a polynomial in the variable μ.]

The proof of (30) is exactly the same as the one given in [7]: one shows that (30) is equivalent to (12) for N coalescing random walkers starting at positions $x_1\leqslant x_2\leqslant\cdots x_N$ by considering all possible coalescing events between the N walkers. The weight a_m in (30) of an event where at time t the N walkers have merged into m walkers is given by

$$\begin{aligned}a_m&=1-(m-1)\mu+\frac{(m-2)(m-3)}{2!}\mu^2\\&-\frac{(m-3)(m-4)(m-5)}{3!}\mu^3\ldots-\lambda\Big(\mu-(m-3)\mu^2\\&+\frac{(m-4)(m-5)}{2!}\mu^3\ldots\Big),\end{aligned} \tag{33}$$

which is just $a_m=1/q^{m-1}$ [see (31) and (32)]. This therefore proves that (30) is equivalent to (12).

In [8], several ways of rewriting (30) were given. In particular it was shown that (30) can be rewritten as the square root of a determinant

$$\mathrm{Prob}\ \{S_{x_1}(t)=\cdots S_{x_N}(t)\}=\left\|\begin{pmatrix}1&0&0&0&&\\0&1&0&0&&\\0&0&\cdot&&&\\&&&\cdot&&\\&&&&\cdot&\\&&&&&1\end{pmatrix}+\mu\begin{pmatrix}0&1&0&&0&\lambda\\-1&0&1&0&&0\\0&-1&0&1&0&\\1&&\cdot&&\cdot&\\0&&&\cdot&&1\\-\lambda&0&&&-1&0\end{pmatrix}\begin{pmatrix}&&\\&c_{i,j}&\\&&\end{pmatrix}\right\|^{1/2}. \tag{34}$$

By choosing N consecutive sites for $x_1\leqslant x_2\leqslant\cdots x_N$, expressions (30) and (34) give the probability $Q(N)$ that N consecutive spins are parallel and the density $p_1(l)$ of domains of length l follows from a relation similar to (14),

$$Q(N)=\sum_{l\geqslant N}(l-N+1)p_1(l).$$

Long time regime

In the long time limit, $c_{i,j}$ varies slowly with the positions x_i and x_j of the sites, and becomes a continuous function $c(x_i,x_j)$ of these two positions. Moreover, for large N, all the sums in the expression (30) become integrals. As in [8], one can show that in this continuum limit, (30) or (34) can be rewritten as

$$Q(N)=[\sqrt{1-\mu\tilde{c}(N,N)}-\lambda\sqrt{-\mu\tilde{c}(N,N)}]\exp[\tfrac{1}{2}\mathrm{tr}\ \ln M], \tag{35}$$

where this time $c(x,y)=f[(y-x)/\sqrt{8t}]$ as in (10) and (11); the matrix M is defined by

$$M(x,y)=\delta(x-y)+2\mu\frac{d}{dx}c(x,y),$$

and the quantities appearing in (35) are given by

$$\mathrm{tr}\ \ln M=-\sum_{n=1}^{\infty}\frac{(-2\mu)^n}{n}\int_0^N dx_1\ldots\times\int_0^N dx_n\frac{d}{dx}c(x_1,x_2)\ldots\frac{d}{dx}c(x_n,x_1) \tag{36}$$

and

$$\tilde{c}(N,N)\equiv\int_0^N dy\ c(N,y)M^{-1}(y,N)=\sum_{n=1}^{\infty}(-2\mu)^n\int_0^N dx_1\ldots\int_0^N dx_n c(N,x_1)\times\frac{d}{dx}c(x_1,x_2)\ldots\frac{d}{dx}c(x_n,N). \tag{37}$$

If one normalizes all the distances on the lattice to make the average domain size become 1, one defines x by

$$N=\sqrt{2\pi t}\,\frac{q}{q-1}\,x, \tag{38}$$

and the distribution of domain sizes $g(x;q)$ is then given by

$$Q(N)=\int_x^{\infty}dy(y-x)g(y;q),$$

so that, in the long time limit, one ends up with

$$\int_x^{\infty}dy(y-x)g(y;q)=[\sqrt{1-\mu A_1(x)}-\lambda\sqrt{-\mu A_1(x)}]e^{A_2(x)}, \tag{39}$$

where

$$A_1(z)=\sum_{n=1}^{\infty}(-2\mu)^n\int_0^z dx_1\ldots\int_0^z dx_n\gamma(z,x_1)\times\frac{d}{dx}\gamma(x_1,x_2)\ldots\frac{d}{dx}\gamma(x_n,z) \tag{40}$$

and

$$A_2(z)=-\frac{1}{2}\sum_{n=1}^{\infty}\frac{(-2\mu)^n}{n}\int_0^z dx_1\ldots\int_0^z dx_n\,\frac{d}{dx}\,\gamma(x_1,x_2)\ldots\times\frac{d}{dx}\,\gamma(x_n,x_1), \tag{41}$$

where

$$\gamma(x,y)=F(y-x)=\frac{2}{\sqrt{\pi}}\int_0^{\sqrt{\pi}(y-x)q/2(q-1)}e^{-u^2}du \tag{42}$$

and

$$\frac{d}{dx}\,\gamma(x,y)=-\frac{q}{q-1}\,\exp\left[\frac{-\pi(y-x)^2q^2}{4(q-1)^2}\right].$$

Differentiating (39) twice with respect to x leads to the exact expression of $g(x;q)$.

IV. EXPANSIONS FOR THE DISTRIBUTION OF DOMAIN SIZES

The exact expression (39) for $g(x;q)$ requires the calculation of A_1 and A_2, which we did not succeed in doing explicitly for general q and x. However, it can be used to expand to arbitrary orders in various limits: small x, large x, and large q.

A. Small *x*

The small x expansion is straightforward. One just needs to expand $\gamma(x,y)$ in (42) in powers of $y-x$,

$$\gamma(x,y)=F(y-x)=\frac{q}{q-1}\,(y-x)-\frac{\pi}{12}\left(\frac{q}{q\text{-}1}\right)^3(y-x)^3+\frac{\pi^2}{160}\left(\frac{q}{q-1}\right)^5(y-x)^5\ldots,$$

and to replace γ by its expansion in (39), (40), and (41). MATHEMATICA performs this to high order, and we found, for $g(x;q)$ up to order x^{13},

$$\begin{aligned}g(x;q)=&\frac{\pi}{2}\,\frac{q}{q-1}\,x-\frac{\pi^2}{8}\,\frac{q^3}{(q-1)^3}\,x^3+\frac{\pi^2}{24}\,\frac{q^3}{(q-1)^4}\,x^4+\frac{\pi^3}{64}\,\frac{q^5}{(q-1)^5}\,x^5-\frac{\pi^3}{120}\,\frac{q^5}{(q-1)^6}\,x^6-\frac{\pi^4}{768}\,\frac{q^7}{(q-1)^7}\,x^7\\&+\frac{\pi^4}{26\,880}\,\frac{q^6(3+23q)}{(q-1)^8}\,x^8+\frac{\pi^5}{12\,288}\,\frac{q^9}{(q-1)^9}\,x^9-\frac{\pi^5}{483\,840}\,\frac{q^8(11+29q)}{(q-1)^{10}}\,x^{10}-\frac{\pi^6}{245\,760}\,\frac{q^{11}}{(q-1)^{11}}\,x^{11}\\&+\frac{\pi^6}{170\,311\,680}\,\frac{q^{10}(429+547q)}{(q-1)^{12}}\,x^{12}+\frac{\pi^6}{1\,857\,945\,600}\,\frac{q^{10}(64-64q+315\pi q^3)}{(q-1)^{13}}\,x^{13}+O(x^{14}).\end{aligned} \tag{43}$$

This expression is clearly different from the one obtained (26) in the uncorrelated approximation [16]. Note that only the first term in both expansions is identical.

B. Large *x*

For domains much larger than the average size, we expect that, for finite q, $g(x;q)$ decays exponentially:

$$g(x;q)\simeq\exp[-A(q)x+B(q)]. \tag{44}$$

This can be understood by recalling that a large domain of size L at finite q is created (23) by combining n domains at $q=\infty$ with n typically $L/\langle l\rangle_{q=\infty}$. The probability of this is exponentially small in n. If the domains at $q=\infty$ were not correlated, the constants $A(q)$ and $B(q)$ would be given by (28) and (29). The existence of correlations between the lengths of domains (22) alters the coefficients of the decay, but not the exponential decay itself.

The large x behavior of $g(x;q)$ is directly connected (39) to the large N behavior of $Q(N)$,

$$Q(N)=\int_x^{\infty}dy(y-x)g(y;q)\simeq\exp[-A(q)x+B(q)-2\ln A(q)]. \tag{45}$$

Therefore, we need the large x behavior of $A_1(x)$ and $A_2(x)$ given by (40) and (41). It turns out that (as in [8]) the prefactor $\sqrt{1-\mu A_1(x)}-\lambda\sqrt{-\mu A_1(x)}$ vanishes as $x\to\infty$, when $q>2$ but has a nonzero finite limit when $q<2$. One has therefore to examine these two cases separately.

(i) For $q<2$, the prefactor (which has been calculated in equation (35) of [8]) has the following limit:

$$\sqrt{1-\mu A_1(x)}-\lambda\sqrt{-\mu A_1(x)}\to\sqrt{q(2-q)}\quad\text{for }x\to\infty. \tag{46}$$

To evaluate the large x behavior of $A_2(x)$, one can use well known results on Toeplitz determinants [18–20], namely, that for an even function $a(u)$ which decays as $u\to\pm\infty$,

$$-\sum_{n=1}^{\infty}\frac{(-2\mu)^n}{n}\int_0^x du_1\ldots\int_0^x du_n a(u_1-u_2)\ldots a(u_n-u_1)$$
$$\simeq \frac{x}{2\pi}\int_{-\infty}^{\infty}\ln[1+2\mu\tilde{a}(k)]dk$$
$$+\int_0^{\infty}u\ du\ \frac{1}{4\pi^2}\left|\int_{-\infty}^{\infty}e^{-iku}\ln[1+2\mu\tilde{a}(k)]dk\right|^2, \tag{47}$$

where

$$\tilde{a}(k)=\int_{-\infty}^{\infty}e^{iku}a(u)du.$$

When this is used in the case of $A_2(x)$ given by (41) and (42), one finds that

$$a(u)=-\frac{q}{q-1}\exp\left\{\frac{-\pi u^2q^2}{4(q-1)^2}\right\}$$

and

$$\tilde{a}(k)=-2\exp\left\{\frac{-k^2(q-1)^2}{\pi q^2}\right\}. \tag{48}$$

This leads to the following expressions in terms of $\mu=(q-1)/q^2$:

$$A(q)=\frac{1}{4}\frac{q}{q-1}\sum_{n=1}^{\infty}\frac{(4\mu)^n}{n^{3/2}}, \tag{49}$$

$$B(q)-2\ln A(q)=\tfrac{1}{2}\ln q(2-q)+\frac{1}{4\pi}\sum_{n=2}^{\infty}\frac{(4\mu)^n}{n}\sum_{p=1}^{n-1}\frac{1}{\sqrt{p(n-p)}}, \tag{50}$$

which can be rewritten in order to make each term have a finite limit in the previous expression when $q\to 2$,

$$B(q)-2\ln A(q)=\ln q-\frac{q-1}{q^2}+\frac{1}{4\pi}\sum_{n=2}^{\infty}\frac{(4\mu)^n}{n}\times\left\{-\pi+\sum_{p=1}^{n-1}\frac{1}{\sqrt{p(n-p)}}\right\}. \tag{51}$$

In (49) and (51), the series are convergent for all values of q [since $(q-1)/q^2=\mu\leqslant\frac{1}{4}$], and so these expressions can be used to calculate numerically $A(q)$ and $B(q)$. In Sec. V, we will compare the values predicted by (49) and (51) to those [(28) and (29)] of the approximation where the domains are uncorrelated.

Remark 1: The radius of convergence of the sums which appear in (49) and (51) is $\mu=\frac{1}{4}$. So as $\mu\to\frac{1}{4}$, that is $q\to 2$, these expressions could become singular. As $\mu<\frac{1}{4}$ when $q>2$, (49) and (51) can be computed for both for $q<2$ and $q>2$. However, it is easy to see that these expressions as a function of q are not analytic at $q=2$ (for example, it is possible to show that $(d/dq)/(q-1/q)A(q)\to\sqrt{\pi}/4$ as $q\to 2$, so that $A(q)$ given by (49) has a cusp at $q=2$). We will argue below, that for $q>2$, expressions (49) and (51) are no longer valid as they are, but should be replaced by their analytic continuation from the range $q<2$.

Remark 2: A priori, in the Potts model, q is an integer and so the case $q<2$ is of little interest. However, Fortuin and Kasteleyn [21] showed a long time ago that noninteger values of q have physical realizations as cluster models. Here it is very easy to check that, if one considers the zero temperature dynamics of an Ising chain where the spins are initially uncorrelated, but a nonzero magnetization m, the distribution of the sizes of domains of + spins is exactly the same as for the q-state Potts model when

$$q=\frac{2}{1+m}.$$

In particular, $q\to\infty$ corresponds to an initial condition where the + spins are very rare, whereas $q\to 1$ corresponds to very few − spins. So m can take any value between −1 and 1, and q can vary continuously between 1 and ∞. Also, for $q>2$, the reaction diffusion model (1) makes sense for a noninteger q.

(ii) For $q>2$, the large x behavior of $A_2(x)$ is exactly the same as for $q<2$. However the prefactor in (39) vanishes as $x\to\infty$. The evaluation of this prefactor for large x is not simple. A similar calculation was done in [8], and the result for $q>2$ turned out to be simply the analytic continuation of the result obtained for $q<2$. Here we assume that this property remains true for $g(x;q)$ (in the small x expansion, at least, one can easily check that all the coefficients can be analytically continued at $q=2$), and that $A(q)$ and $B(q)$ in the range $q>2$ are given by the analytic continuation $\overline{A(q)},\overline{B(q)}$ of their expressions (49) and (51) for $q<2$.

In the Appendix, we give a way of deriving the following expressions of $\overline{A(q)}$ and $\overline{B(q)}$:

$$\overline{A(q)}=\frac{q\sqrt{\pi}}{q-1}\sqrt{-\ln 4\mu}+\frac{1}{4}\frac{q}{q-1}\sum_{n=1}^{\infty}\frac{(4\mu)^n}{n^{3/2}}, \tag{52}$$

$$\overline{B(q)}-2\ln\overline{A(q)}=\tfrac{1}{2}\ln q(q-2)-\ln 4-\ln(-\ln 4\mu)+\frac{1}{4\pi}\sum_{n=2}^{\infty}\frac{(4\mu)^n}{n}\sum_{p=1}^{n-1}\frac{1}{\sqrt{p(n-p)}}-2\sum_{n=1}^{\infty}\frac{1}{n\sqrt{\pi}}\int_{\sqrt{-n\ln 4\mu}}^{\infty}dv\ e^{-v^2}. \tag{53}$$

C. Large q expansion

In the large q limit, μ, λ and $\gamma(x,y)$ can be expanded in powers of $1/q$ [see (31), (32), and (42)]. This leads to

$$A_1(z)=-\mu\gamma^2(0,z)+4\mu^2\gamma(0,z)\int_0^z dx\ \gamma(0,x)\ \frac{d\gamma(x,z)}{dx}+O\left(\frac{1}{q^3}\right),$$

$$A_2(z)=-\frac{x}{q}+O\left(\frac{1}{q^2}\right),$$

and to

$$Q(N)=1-\int_0^x du\ e^{-\pi u^2/4}+\frac{1}{q}\left\{-x\left(1-\int_0^x du\ e^{-\pi u^2/4}\right)+2\int_0^x du\ e^{-\pi u^2/4}-xe^{-\pi x^2/4}-2\int_0^x dy\int_0^y dz\ e^{-\pi/4[z^2+(x-y)^2]}\right\}+O\left(\frac{1}{q^2}\right), \quad (54)$$

which, using (39), becomes

$$g(x;q)=\frac{\pi}{2}\,xe^{-x^2\pi/4}+\frac{1}{q}\left\{-\frac{\pi^2}{4}\,x^3e^{-x^2\pi/4}-\frac{\pi}{2}\,x^2e^{-x^2\pi/4}+\frac{\pi}{2}\,xe^{-x^2\pi/4}+\frac{\pi}{2}\,x\int_0^x dze^{-[(x-z)^2+z^2]\pi/4}\right\}+O\left(\frac{1}{q^2}\right). \quad (55)$$

For the moments of distribution $g(x;q)$, this gives

$$\langle x^n\rangle=\left(\frac{2}{\sqrt{\pi}}\right)^n\left[\Gamma\left(\frac{n}{2}+1\right)+\frac{1}{q}\left\{-(n+1)\Gamma\left(\frac{n}{2}+1\right)-\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{n+1}{2}+1\right)+\frac{2}{\sqrt{\pi}}\sum_{p=0}^{n}\binom{n}{p}\Gamma\left(\frac{p+1}{2}\right)\Gamma\left(\frac{n-p+2}{2}\right)\right\}\right]+O\left(\frac{1}{q^2}\right). \quad (56)$$

and, in particular,

$$\langle x^2\rangle=\frac{4}{\pi}\left(1+\frac{1}{2q}\right)+O\left(\frac{1}{q^2}\right).$$

Remark: Because of (23), all the results to order $1/q$ can be recovered from the knowledge [(18) and (21)] of $g(x;\infty)$ and $g_2(x,x';\infty)$, and it is easy to check that

$$g(x;q)=\left(1+\frac{1}{q}\right)\left\{\left(1-\frac{1}{q}\right)g\left[\left(1+\frac{1}{q}\right)x;\infty\right]+\frac{1}{q}\int_0^{[1+1/q]x}dz\ g_2\left[\left(1+\frac{1}{q}\right)x-z,z;\infty\right]\right\}+O\left(\frac{1}{q^2}\right)$$

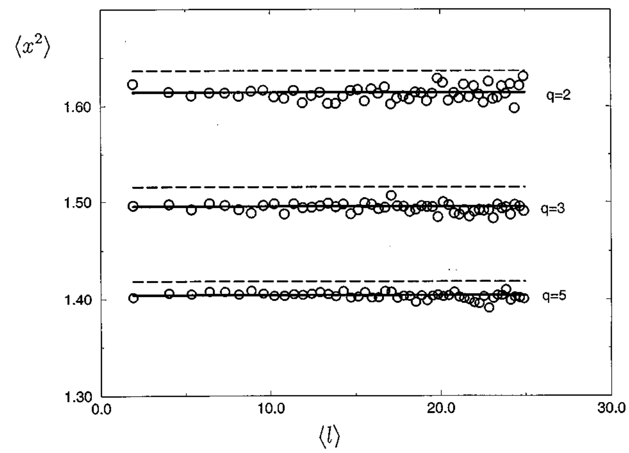

FIG. 1. The second moment $\langle x^2\rangle$ vs $\langle l\rangle_\infty$ for $q=2$, 3, and 5 for a system of 10^6 spins. The plain lines indicate the values predicted by the improved approximation (58), and the dashed lines those of the independent approximation (57).

is equivalent to (55). It is straightforward in principle to generate higher order terms in $1/q$, but the expressions become quite complicated.

V. SIMULATIONS

In order to check the validity of our results against the predictions of the independent interval approximation [16], we made a simulation. Because of (23), the distribution of domain sizes for all values of q can be extracted from a single simulation done at $q=\infty$. One starts with a random initial condition at $q=\infty$ (this is done by choosing initially each spin with a different value: for example, spin i is given color i) and let the system coarsen according to zero temperature Glauber dynamics. Once the system at $q=\infty$ has evolved for a certain time, one obtains a system for an arbitrary value (integer or noninteger) of q by removing each domain wall with probability $1/q$.

The easiest properties one can measure are the moments of the distribution of domain sizes. Our data (for a system of 10^6 spins) for the second moment $\langle x^2\rangle$ of the distribution $g(x;q)$ of domain sizes for $q=2$, 3, and 5 are shown in Fig. 1 as a function of the average size $\langle l\rangle_\infty$ of the domains for $q=\infty$. For Glauber dynamics, this average $\langle l\rangle_\infty$ increases with time like $t^{1/2}$. The larger $\langle l\rangle_\infty$ is, the closer we are from the asymptotic regime. However, as the simulation is done for a finite system, the results become noisy if one waits too long, simply because the number of domains is too small to allow good statistics.

These numerical results can be compared to the approximation where the correlations are neglected (25),

$$\langle x^2\rangle_{\text{independent}}=\frac{q-1}{q}\,\frac{4}{\pi}+\frac{2}{q}. \quad (57)$$

We see in Fig. 1 that our numerical data seem stable and accurate enough to show a clear discrepancy from the approximation. Unfortunately, our exact expression (39) is complicated, and we were unable to obtain closed expressions of the moments for the whole range of q. However, we

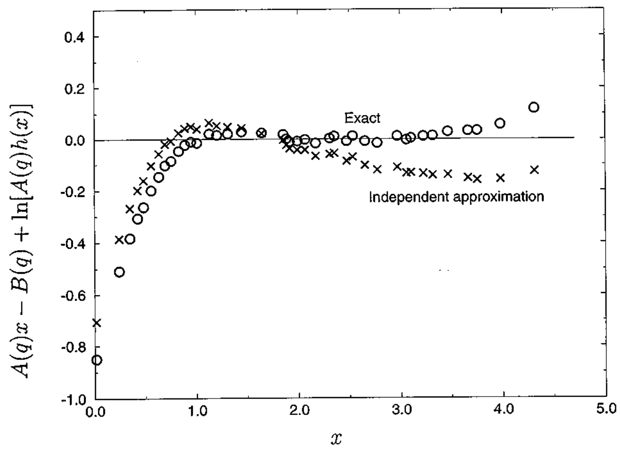

FIG. 2. The logarithm of the (measured) integrated distribution $h(x;q)$ divided by its predicted asymptotic form $A(q)x-B(q)+\ln A(q)+\ln h(x;q)$ for a system of 2×10^6 spins after 1000 updatings per spin. When the exact expressions of $A(q)$ and $B(q)$ are used (circles), the agreement is very satisfactory in the range $1<x<3.5$, where x is large enough but the data are not yet too noisy, whereas, when one takes $A(q)$ and $B(q)$ of the independent domain approximation (crosses), there is no range where the data are consistent with the limiting value 0.

could test our conviction that correlations between the domains at $q=\infty$ have an effect. If in the calculation of $\langle x^2\rangle$, we neglect the correlations between all pairs of domains except for nearest neighbor domains (22), we find an improved estimate

$$\langle x^2\rangle_{\text{improved}}=\frac{q-1}{q}\,\frac{4}{\pi}+\frac{2}{q}+2\,\frac{q-1}{q^2}\left(\frac{3}{\pi}-1\right), \qquad (58)$$

which, although not exact, seems to be in much better agreement with the results of the simulations.

As we could not calculate the moments from (39), we tried to test our results by measuring the exponential tail of the distribution $g(x;q)$. It is always difficult to measure a probability distribution numerically, because one has to use bins: if they are too narrow, the data are noisy, and if they are too broad, all the details of the distribution are smoothened out. To avoid this difficulty, we measured the integrated distribution $h(x;q)$,

$$h(x;q)=\int_x^\infty g(y;q)dy$$

and we compared it to our prediction (44) for the tail [(49) and (51)] for $q<2$ and [(52) and (53)] for $q>2$. We also compared the results of our simulations to the prediction of the independent domains approximation (28) and (29). In Fig. 2, we plot the logarithm of the integrated distribution divided by its predicted form $[A(q)x-B(q)+\ln A(q)]+\ln h(x;q)$ versus x for $q=5$ for a system of two millions spins, after 1000 updatings per spin. We see that the agreement is very good when (52) and (53) are used, whereas, for (28) and (29), there is a small but visible discrepancy. Of course, for an x that is too large, our data are too noisy, and for an x that is too small, the asymptotic form has no reason to be valid, so that the range where the agreement is the best is $1<x<3.5$. In that range, the independent interval approximation presents a nonvanishing slope, indicating that (28) is not correct. Moreover, if one considers that the data (in the independent case) flatten for $x>3.5$ (where the data start to be noisy), the fact that the limit in Fig. 2 is below zero indicates that prediction (29) for $B(q)$ is not correct.

TABLE I. The exact values of $A(q)$ and $B(q)$ obtained from (49) and (51) for $q<2$, and (52) and (53) for $q>2$, are compared to those coming from the independent domain approximations (28) and (29).

q	Exact $A(q)$	Exact $B(q)$	Approximate $A(q)$	Approximate $B(q)$
1.2	1.0769	0.153	1.0675	0.133
1.5	1.1748	0.344	1.1532	0.299
2.0	1.3062	0.597	1.2685	0.517
3.0	1.4998	0.963	1.4370	0.832
5.0	1.7537	1.439	1.6630	1.239
10.0	2.1066	2.101	1.9777	1.809
100.0	3.2273	4.369	3.0065	3.804

In Table I, the exact values of $A(q)$ and $B(q)$ obtained from (49) and (51) for $q<2$ and from (52) and (53) for $q>2$ are compared to those coming from the independent domains approximation (28) and (29). We see that, although different, they are very close.

We tried also to see whether one could distinguish by numerical simulations our exact results from the independent interval approximation for small x, but we found that this was even more difficult than in the large x limit.

As we did not obtain a closed form for the distribution $g(x;q)$, we used Padé approximants based on the expansion (43) to draw the shapes of $g(x;q)$ shown in Fig. 3. We see that as $q\to 1$, the shape becomes an exponential.

VI. REACTION-DIFFUSION MODEL

The relation between the spin dynamics and the reaction-diffusion model (1) can be used to calculate all kinds of properties of the reaction-diffusion model. For the zero tem-

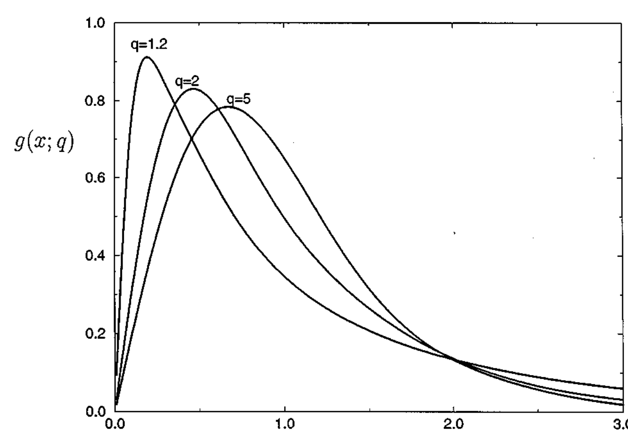

FIG. 3. The shapes of the distribution $g(x;q)$ of the interval lengths obtained from a Padé analysis of expansion (43).

perature Glauber dynamics of the Potts chain, it results from the analogy to random walks (Sec. II) that

$$\text{Prob}\{S_{x_1}(t)\neq S_{x_2}(t)\}=\left(\frac{q-1}{q}\right)c_{1,2}$$

and that [Eq. (9)] for $x_1<x_2<x_3<x_4$:

$$\text{Probability}\{S_{x_1}(t)\neq S_{x_2}(t) \text{ and } S_{x_3}(t)\neq S_{x_4}(t)\}$$
$$=\left(\frac{q-1}{q}\right)^2[c_{1,3}+c_{2,4}-c_{2,3}-c_{1,4}+c^{(2)}_{1,2,3,4}].$$

In the long time regime, using (10) and (11) for $x_1=0$, $x_2=1$, $x_3=r$, and $x_4=r+1$, this becomes

$$\text{Probability}\{S_0(t)\neq S_1(t)\}\simeq H'(0),$$

$$\text{Probability}\{S_0(t)\neq S_1(t) \text{ and } S_r(t)\neq S_{r+1}(t)\}$$
$$\simeq\left(\frac{q-1}{q}\right)^2[-H''(r)+H''(r)H(r)-(H'(r))^2+(H'(0))^2],$$

where

$$H(r)=\frac{2}{\sqrt{\pi}}\int_0^{r/\sqrt{8t}}e^{-u^2}du.$$

If these expressions are interpreted in terms of domain walls (i.e., of particles in the reaction-diffusion model), one obtains that the density ρ of particles and the probability $\rho_2(0,r)$ of finding a pair of particles at 0 and at r are given by

$$\rho\simeq\frac{q-1}{q}H'(0)=\frac{q-1}{q}\frac{1}{\sqrt{2\pi t}},$$

$$\rho_2(0,r)\simeq\left(\frac{q-1}{q}\right)^2[-H''(r)+H''(r)H(r)-(H'(r))^2+(H'(0))^2].$$

By eliminating the time t between these two equations, one finds that, in the long time limit, the probability of finding a particle at 0 and r is given by

$$\rho_2(0,r)=\rho^2\left[1-e^{-2z^2}+2ze^{-z^2}\int_z^\infty e^{-u^2}du\right] \quad (59)$$

and

$$z=\frac{q}{q-1}\frac{\sqrt{\pi}}{2}\rho r.$$

We see in particular that the correlations decay like a Gaussian instead of the ‘‘usual’’ exponential.

Remark: It has already been noted [22–26] that several properties of reaction-diffusion models can be calculated exactly, by writing closed equations for the probability that an interval of length l is empty (or two intervals are empty). This method (which is rather close in spirit to our approach, as it essentially considers that walkers which do not meet in one dimension are free fermions) could also be used to recover (59).

VII. CONCLUSION

The long time regime of domain growth phenomena is in many respects analogous to what happens near a critical point in a second order phase transition: this regime is characterized both by universal exponents and by universal scaling functions. In the present paper, we have determined the distribution of domain sizes in this regime, for the q-state Potts model in one dimension. This distribution is universal, in the sense that, at least, it would remain the same for short ranged correlations in the initial condition.

The exact expression we found is rather complicated [39–42], but it can be simplified in several limits (Sec. IV). Our exact results are different from (although rather close to) the predictions of a simple approximation proposed recently [16]. However, with sufficient numerical effort, we think that the simulations of Sec. V indicate the validity of our results against those [(28) and (29)] of that approximation.

The present work has a lot in common with [8], where the exponent characteristic of the persistent spins has been calculated exactly for the same system. Here we are concerned with space properties, whereas [8] was devoted to time properties. The existence of nontrivial exponents for the number of persistent spins [27–31] in $d>1$ certainly has its counterpart in terms of distribution of domain sizes. However, in $d>1$, size is one among many ways of characterizing a domain (its volume, its perimeter, its shape [32], its number of neighboring domains, etc.). It would be interesting to know whether the probability distributions of all these characteristics of domains are universal in $d>1$. Another open question for systems in $d>1$ is how to define the domains in the presence of thermal noise (i.e., at nonzero temperature), and how to distinguish them from thermal fluctuations. When the typical size of domains is much larger than the equilibrium correlation length, it seems intuitively easy to make this distinction, but, to our knowledge, a clean way of measuring the size of domains (in presence of noise) has not yet been proposed.

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APPENDIX: ANALYTIC CONTINUATIONS

In this appendix we show how to continue analytically expressions (49) and (51) of $A(q)$ and $B(q)$ obtained in the large x expansion for $q<2$ to the range $q>2$. It is easier to start with the expressions coming from (45)–(47); that is,

$$A(q)=\frac{-1}{4\pi}\int_{-\infty}^{\infty}dk\,\ln[1+2\mu\tilde{a}(k)] \quad (A1)$$

$$B(q)-2\ln A(q)=\tfrac{1}{2}\ln q(2-q)+\frac{1}{8\pi^2}\int_0^\infty y\,dy \times\left|\int_{-\infty}^{\infty}dk\,e^{iky}\ln[1+2\mu\tilde{a}(k)]\right|^2, \tag{A2}$$

where $\tilde{a}(k)$ is given by [Eq. (48)]

$$\tilde{a}(k)=-2\exp\left\{\frac{-k^2(q-1)^2}{\pi q^2}\right\}. \tag{A3}$$

As $q\to 2$, that is $\mu\to\frac{1}{4}$, the integrands in (A1) and (A2) become singular at $k=0$: two complex zeros in the complex plane of the variable k approach $k=0$ as $q\to 2$, and the exchange of these two zeros is at the origin of the analytic continuation.

A generic example: To make an analytic continuation of (A1) and (A2) simpler to understand, we first treat a case where expression (A3) for $\tilde{a}(k)$ would be replaced by

$$\tilde{a}(k)=\frac{-2}{1+Q(k)} \tag{A4}$$

where $Q(k)$ is a real polynomial of degree $2n$ with $[Q(k)\sim k^2$ as $k\to 0$, and such that $Q(k)+1$ and $Q(k)+1-4\mu$ have both only complex zeros]. One can therefore write

$$1+2\mu\tilde{a}(k)=1-\frac{4\mu}{1+Q(k)}=\prod_{j=1}^{n}\frac{(z_j-k)(z_j^*-k)}{(y_j-k)(y_j^*-k)}, \tag{A5}$$

where y_j are the n zeros of $1+Q(k)$ with positive imaginary parts, and z_j are the n zeros of $1-4\mu+Q(k)$ with positive imaginary parts. One can rewrite (A1) and (A2) as

$$A(q)=\frac{1}{4\pi}\int_{-\infty}^{\infty}dk\,\frac{2\mu k\tilde{a}'(k)}{1+2\mu\tilde{a}(k)} =\frac{1}{4\pi}\int_{-\infty}^{\infty}dk\,\frac{4\mu kQ'(k)}{[1+Q(k)][1-4\mu+Q(k)]}, \tag{A6}$$

$$B(q)-2\ln A(q) =\tfrac{1}{2}\ln q(2-q)+\frac{1}{8\pi^2}\int_0^\infty\frac{dy}{y} \times\left|\int_{-\infty}^{\infty}dk\,e^{iky}\frac{4\mu Q'(k)}{[1+Q(k)][1-4\mu+Q(k)]}\right|^2, \tag{A7}$$

and find, using the theorem of residues,

$$A(q)=\frac{i}{2}\sum_{j=1}^{n}z_j-y_j \tag{A8}$$

and

$$B(q)-2\ln A(q) =\frac{1}{2}\ln q(2-q)+\frac{1}{2}\sum_{j=1}^{n}\sum_{j'=1}^{n}\ln\left\{\left(\frac{iy_{j'}^*-iz_j}{iy_{j'}^*-iy_j}\right)\times\left(\frac{iz_{j'}^*-iy_j}{iz_{j'}^*-iz_j}\right)\right\}. \tag{A9}$$

Expressions (A8) and (A9) are valid for $q<2$. To obtain their analytic continuation $\overline{A(q)},\overline{B(q)}$ to the range $q>2$, we have essentially to exchange the role of z_1 and z_1^*, the two zeros of $1-4\mu+Q(k)$, which go through $k=0$ when $q=2$. So, for $q>2$,

$$\overline{A(q)}=\frac{i}{2}(z_1^*-z_1)+\frac{i}{2}\sum_{j=1}^{n}z_j-y_j \tag{A10}$$

and

$$\overline{B(q)}-2\ln\overline{A(q)}=\left[\frac{1}{2}\ln q(q-2)-i\frac{\pi}{2}\right] +\left[\frac{1}{2}\ln\left|\frac{iz_1^*-iz_1}{iz_1-iz_1^*}\right|+i\frac{\pi}{2}\right] +\frac{1}{2}\sum_{j=1}^{n}\ln\left\{\left(\frac{iy_j^*-iz_1^*}{iy_j^*-iz_1}\right)\left(\frac{iz_1-iy_j}{iz_1^*-iy_j}\right)\right\} +\frac{1}{2}\sum_{j=2}^{N}\ln\left\{\left(\frac{iz_j^*-iz_1}{iz_j^*-iz_1^*}\right)\left(\frac{iz_1^*-iz_j}{iz_1-iz_j}\right)\right\} +\frac{1}{2}\sum_{j=1}^{n}\sum_{j'=1}^{n}\ln\left\{\left(\frac{iy_{j'}^*-iz_j}{iy_{j'}^*-iy_j}\right)\times\left(\frac{iz_{j'}^*-iy_j}{iz_{j'}^*-iz_j}\right)\right\} \tag{A11}$$

where we have added an infinitesimal imaginary part to q to define the analytic continuation $\ln(iz_1-iz_1^*)$ and $\ln q(2-q)$.

Using the fact that

$$\prod_{j=1}^{n}(z_1-y_j)(z_1-y_j^*)=1+Q(z_1)=4\mu,$$

and that

$$\prod_{j=2}^{n}(z_1-z_j)(z_1-z_j^*)=\frac{Q'(z_1)}{z_1-z_1^*},$$

(A11) becomes

$$\overline{B(q)}-2\mathrm{h}\quad \overline{A(q)}=\tfrac{1}{2}\ \ln q(q-2)+\ln 4\mu-\ln|Q'(z_1)| +\ln|z_1-z_1^*| -\sum_{j=1}^{n}\ln\{(z_1^*-y_j)(z_1-y_j^*)\} +\sum_{j=2}^{N}\ln\{(z_1-z_j^*)(z_1^*-z_j)\} +\frac{1}{2}\sum_{j=1}^{n}\sum_{j'=1}^{n}\ \ln\left\{\left(\frac{iy_{j'}^*-iz_j}{iy_{j'}^*-iy_j}\right)\times\left(\frac{iz_{j'}^*-iy_j}{iz_{j'}^*-iz_j}\right)\right\}. \tag{A12}$$

This can be further transformed using the identity

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}dk\left(\frac{1}{k-z_1}-\frac{1}{k-z_1^*}\right)\ln\left(\frac{(k-z_j)(k-z_j^*)}{(k-y_j)(k-y_j^*)}\right) =\ln\left(\frac{(z_1-z_j^*)(z_1^*-z_j)}{(z_1-y_j^*)(z_1^*-y_j)}\right),$$

to become

$$\overline{B(q)}-2\ln\overline{A(q)}=\tfrac{1}{2}\ \ln q(q-2)+\ln 4\mu-\ln|Q'(z_1)| -\ln|z_1-z_1^*|+\frac{1}{2\pi i} \times\int_{-\infty}^{\infty}dk\left(\frac{1}{k-z_1}-\frac{1}{k-z_1^*}\right) \times\ln\left(1-\frac{4\mu}{1+Q(k)}\right) +\frac{1}{2}\sum_{j=1}^{n}\sum_{j'=1}^{n}\ \ln\left\{\left(\frac{iy_{j'}^*-iz_j}{iy_{j'}^*-iy_j}\right)\times\left(\frac{iz_{j'}^*-iy_j}{iz_{j'}^*-iz_j}\right)\right\}. \tag{A13}$$

Finally, using the identity

$$2\mu\widetilde{a}'(z_1)=\frac{4\mu Q'(z_1)}{[1+Q(z_1)]^2}=\frac{Q'(z_1)}{4\mu},$$

one finds, for $q>2$,

$$\overline{B(q)}-2\ln\overline{A(q)}=\tfrac{1}{2}\ \ln q(q-2)-\ln|2\mu\widetilde{a}'(z_1)| -\ln|z_1-z_1^*|+\frac{1}{2\pi i} \times\int_{-\infty}^{\infty}dk\left(\frac{1}{k-z_1}-\frac{1}{k-z_1^*}\right) \times\ln[1+2\mu\widetilde{a}(k)]+\frac{1}{8\pi^2}\int_0^{\infty}y\ dy\left| \times\int_{-\infty}^{\infty}dk\ e^{iky}\ \ln[1+2\mu\widetilde{a}(k)]\right|^2. \tag{A14}$$

This expression together with [Eq. (A10)]

$$\overline{A(q)}=\frac{i}{2}\ (z_1^*-z_1)-\frac{1}{4\pi}\int_{-\infty}^{\infty}dk\ \ln[1+2\mu\widetilde{a}(k)] \tag{A15}$$

give, for the generic example (A3), the analytic continuation $\overline{A(q)},\overline{B(q)}$ of $A(q)$ and $B(q)$ to the range $q>2$.

Although (A14) and (A15) were derived for $\widetilde{a}(k)$ of the form (A3), they should remain valid for a broader class of functions, probably as long as $\widetilde{a}(k)$ is such that only a pair of zeros of $1+2\mu\widetilde{a}(k)$ exchange as q crosses 2.

We believe that (A14) and (A15) remain valid for $\widetilde{a}(k)$ given by (48), so that

$$z_1=i\ \frac{q\sqrt{\pi}}{q-1}\ \sqrt{-\ln 4\mu},$$

$$\overline{A(q)}=\frac{q\sqrt{\pi}}{q-1}\ \sqrt{-\ln 4\mu}+\frac{1}{4}\ \frac{q}{q-1}\sum_{n=1}^{\infty}\ \frac{(4\mu)^n}{n^{3/2}}, \tag{A16}$$

$$\overline{B(q)}-2\ln\overline{A(q)}=\tfrac{1}{2}\ \ln q(q-2)-\ln 4-\ln(-\ln 4\mu) +\frac{1}{4\pi}\sum_{n=2}^{\infty}\ \frac{(4\mu)^n}{n}\sum_{p=1}^{n-1}\ \frac{1}{\sqrt{p(n-p)}} -2\sum_{n=1}^{\infty}\ \frac{1}{n\sqrt{\pi}}\int_{\sqrt{-n\ \ln 4\mu}}^{\infty}dv\ e^{-v^2}. \tag{A17}$$

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