Exponents appearing in the zero-temperature dynamics of the 1D Potts model

B Derrida

Laboratoire de Physique Statistique, ENS, 24 rue Lhomond, 75005 Paris, France
and
Service de Physique Théorique, CE Saclay, F91191 Gif sur Yvette, France

Abstract. For the Glauber dynamics of the one-dimensional q-state Potts model at zero temperature, the fraction of spins which have never flipped up to time t decreases as $t^{-\theta(q)}$ where the exponent $\theta(q)$ varies continuously with q. The calculation of the q dependence of this exponent can be reduced to the study of a simple reaction–diffusion model. Using finite-size scaling, this allows one to obtain accurate estimates of $\theta(q)$ for all values of q. One can also show that for $q = 1 + \epsilon$, the expansion of $\theta(q)$ is given by $\theta(q) = (2/\pi)\epsilon + O(\epsilon^2)$.

1. Introduction

The zero-temperature dynamics of one-dimensional classical spin models such as the Ising or q-state Potts model are known as well understood problems [1–5]. If a random initial spin configuration is quenched at zero temperature, one observes a coarsening phenomenon, with a characteristic domain size growing with $t^{1/2}$. It was shown [6], however, that, even for such simple systems, some dynamical properties are more difficult to understand. For example, the fraction $r(q, t)$ of spin which has never flipped [6] up to time t decays with a power law

$$r(q, t) \simeq t^{-\theta(q)} \tag{1}$$

where the exponent $\theta(q)$ varies with q. Monte Carlo simulations [6–8] give $\theta(2) \simeq 0.376$, $\theta(3) \simeq 0.53$ $\theta(5) \simeq 0.70$, $\theta(10) \simeq 0.82$ and so far, $q = \infty$ is the only case [6] for which the exponent is known exactly ($\theta(\infty) = 1$).

In the present work, the problem of calculating the fraction $r(q, t)$ of spins which have never flipped for all values of q is reduced to a single (and simple) reaction–diffusion problem: particles diffuse and aggregate ($A + A \rightarrow A$) on a one-dimensional chain with a source of particles at the origin. If the reaction–diffusion problem starts at $t = 0$ with no particle in the system (except at the origin) and if one calls $P(m, t)$, the probability that at time t there are exactly m particles in the system (including the one at the origin which is always present), we shall see that $r(q, t)$ is given by

$$r(q, t) = \sum_{m=1}^{\infty} P(m, t) q^{1-m}. \tag{2}$$

This relationship with the reaction–diffusion problem will allow us:

(i) to obtain the estimates in table 1 for the exponent $\theta(q)$ for integer and non-integer values of q;

Table 1. Numerical values of $\theta(q)$ obtained in section 4 using finite-size scaling.

q	0.5	1.01	1.5	2	3	5	10	100	∞
$\theta(q)$	−0.513	0.006 320 3	0.2350	0.3750	0.5379	0.6928	0.8310	0.9815	1.0000
Error	0.001	0.000 000 2	0.0001	0.0001	0.0002	0.0003	0.0005	0.0010	0.0005
Monte Carlo				0.376	0.53	0.70	0.82		1.0
Exact									1

(ii) to find the first term of the expansion of $\theta(q)$ in powers of $q - 1$

$$\theta(q) = \frac{2}{\pi}(q - 1) + O((q - 1)^2).$$ (3)

(iii) to obtain bounds on the exponent $\theta(q)$: for $q_1 < q_2$

$$\theta(q_2) \leqslant \theta(q_1)\frac{\log q_2}{\log q_1}$$ (4)

which combined with (3) gives, for $q > 1$,

$$\theta(q) \leqslant \frac{2}{\pi}\log q.$$ (5)

The paper is organized as follows. In section 2, the problem of finding the fraction $r(q, t)$ of spins which have never flipped is reduced to a simple reaction–diffusion model and (2) is derived. In section 3, the steady-state properties of the reaction–diffusion model for finite system sizes are presented. In section 4, these results are analysed, assuming finite-size scaling to obtain accurate predictions (of table 1) for the exponent $\theta(q)$ for arbitrary values of q. Analytic expressions for some of the properties of the reaction–diffusion model can be obtained for arbitrary system sizes and this will be the way, in section 5, of deriving the first term in the expansion of $\theta(q)$. Finally the bounds (4), (5) are obtained using (2) and Jensen's inequality.

2. Relation to a reaction–diffusion model

One can implement the Glauber dynamics of a one-dimensional q-state Potts model at zero temperature as follows: during any infinitesimal time interval dt, each spin $S_i(t)$ has a probability $dt/2$ of becoming equal to its left neighbour, $dt/2$ of becoming equal to its right neighbour, and a probability $1 - dt$ of keeping its own value. The only difference between the different values of q is in the random initial condition: at $t = 0$, each spin $S_i(0)$ is assigned a random integer between 1 and q.

There is a very direct way [2, 4, 5, 8–11] of relating this coarsening phenomenon to reaction–diffusion models [12–22]: one considers that the domain walls perform random walks and when two of these random walkers meet, they either annihilate $(A+A \rightarrow \emptyset)$ with probability $1/(q-1)$ or they aggregate $(A+A \rightarrow A)$ with probability $(q-2)/(q-1)$. These rates are easy to understand by considering what happens when two domain walls meet, i.e. when a domain disappears: either, the two neighbours of the domain which disappears are in the same state and the two domain walls annihilate; or they are in different states and the two domain walls merge into a single domain wall. This reaction–diffusion model with the fact that in the initial condition, each bond is occupied by a domain wall with probability $(q - 1)/q$ is completely equivalent to the initial spin problem. Then the density $r(q, t)$ of spins which have never flipped up to time t is just the fraction of sites which have never

been jumped over by a domain wall [6, 8, 9]. This domain wall description is a useful one, but the model changes when q varies and difficulties arise if one tries to consider non-integer values of q (for example for q close to 1, one has to work with negative probabilities).

In this paper, a different reasoning is used to relate the calculation of the fraction $r(q, t)$ to a reaction–diffusion model. It is useful to think of the dynamics of the spin model in terms of random walks. We have seen that the value of $S_i(t)$ at time t is equal to $S_{i-1}(t-dt)$, $S_i(t-dt)$ or $S_{i+1}(t-dt)$ with probabilities $dt/2$, $1-dt$ and $dt/2$. These spin values, in turn, depend on $S_{i-2}(t-2dt)$, $S_{i-1}(t-2dt)$, $S_i(t-2dt)$, $S_{i+1}(t-2dt)$, $S_{i+2}(t-2dt)$ and so on. Tracing back in time the sequence of spins responsible for the value of $S_i(t)$ defines a random walk. Thus the value of spin $S_i(t)$ at time t is equal to the value of another spin $S_j(0)$ at time 0 with a probability $p(j-i, t)$ where $p(j-i, t)$ is the probability for a random walk to go from i to j during time t, given that during each time interval dt, the random walk moves to its left with probability $dt/2$, to its right with probability $dt/2$ or does not move with probability $1-dt$. So to know the value of $S_0(t)$, one just needs to look at the position at time t of a random walk starting at $t=0$ at the origin.

Assume that one wants to know the values of $S_0(t)$ and $S_0(t')$ with $t > t'$. Then one has to consider the positions at time t of two random walkers, the first one starting at the origin at time $t=0$ and the second one starting at the origin at time $t-t'$. Clearly, if the two walkers occupy the same site at a given time, they follow, at any later time, the same trajectory. So the two walkers are like two diffusing particles which aggregate when they meet.

Let us call $p(1; t, t')$ the probability that the two walkers aggregate before time t and $p(2; t, t')$ the probability that they do not. Then the probability that $S_0(t) = S_0(t')$ is given by $p(1, t; t') + p(2, t, t')/q$. This reasoning can easily be extended to obtain the probability that $S_0(t) = S_0(t') = S_0(t'') = \cdots$. It follows that, to calculate the probability $r(q, t)$ that the spin at the origin has never flipped up to time t, one needs to consider the following reaction–diffusion problem: the system consists of random walkers which diffuse and aggregate; moreover the origin is always occupied (i.e. whenever the walker which is at the origin jumps to one of its neighbours, a new walker is produced at the origin). If initially the system is empty (except for the origin) and if one calls $P(m, t)$ the probability of having m walkers in the system at time t, the same argument as above (when comparing $S_0(t)$ and $S_0(t')$) leads to

$$r(q, t) = \sum_{m=1}^{\infty} P(m, t) q^{1-m}. \tag{6}$$

This is the origin of the equation (2) which is the starting point of the present work. Reaction–diffusion models with sources have already been studied in the literature [2, 11–13, 15]. A number of results are known, but, to my knowledge, the exact expression for $P(m, t)$ has not yet been given.

3. Steady-state properties of a finite system

Let us consider the reaction–diffusion problem on a ring of L sites. One site (which we call the origin) is always occupied and all the other sites are either occupied by one particle or empty. The particles diffuse and when two particles meet, they aggregate ($A + A \rightarrow A$). The effect of the aggregation is to reduce the number of particles in the system whereas the source at the origin increases this number. The result is a steady state with a probablity $\psi(m, L)$ of finding m sites occupied on a ring of L sites.

Clearly, a ring of L sites has 2^{L-1} possible configurations (each site is either occupied or empty except for the origin which is always occupied). If $W(C', C) \, dt$ is the probability during time dt to go from a configuration C to a configuration C', the weights $p(C)$ in the steady state are solutions of

$$\sum_{C'} W(C', C) p(C) = \sum_{C'} W(C, C') p(C'). \tag{7}$$

For L not too large, the matrix $W(C', C)$ can be constructed explicitly by enumerating all possible configurations and all possible moves and it is then easy to find numerically the weights $p(C)$ by solving equations (7). For example for $L = 4$, and if the origin (i.e. the source of particles) is at position 4, one finds the following weights in the steady state for the 2^3 possible configurations

$$p(0001) = \tfrac{8}{44} \qquad p(1001) = p(0011) = \tfrac{8}{44} \qquad p(0101) = \tfrac{7}{44}$$
$$p(1011) = \tfrac{6}{44} \qquad p(1101) = p(0111) = \tfrac{3}{44} \qquad p(1111) = \tfrac{1}{44}$$

and therefore

$$\psi(1, 4) = \tfrac{8}{44} \qquad \psi(2, 4) = \tfrac{23}{44} \qquad \psi(3, 4) = \tfrac{12}{44} \qquad \psi(4, 4) = \tfrac{1}{44}.$$

Table 2 gives all the $\psi(m, L)$ for $L \leqslant 14$.

One finds that the $\psi(m, L)$ are rational numbers which are listed in table 2 (for each m, the numerators of $\psi(m, L)$ are given in table 2 and at the end of each list, the sum of all the numerators gives the denominator).

Remark 1. So far, there are two properties of the $\psi(m, L)$ which could be obtained analytically for all L: first, the exact expression for $\psi(1, L)$ is

$$\psi(1, L) = \frac{16}{(L + 1)^2} \sum_{k \text{ even}} \sum_{k' \text{ odd}} \frac{\sin^2 k\alpha \sin^2 k'\alpha}{(\cos k'\alpha - \cos k\alpha)(2 - \cos k\alpha - \cos k'\alpha)} \tag{8}$$

second, one can also show that

$$\sum_{m=1}^{L} (m - 1) \psi(m, L) = \frac{8}{(L + 1)^2} \sum_{k \text{ even}} \sum_{k' \text{ odd}} \frac{\sin^2 k\alpha (1 + \cos k'\alpha)}{(\cos k'\alpha - \cos k\alpha)(2 - \cos k\alpha - \cos k'\alpha)} \tag{9}$$

where the range of the sums over k and k' are

$$2 \leqslant k \leqslant L \qquad 1 \leqslant k' \leqslant L$$

and

$$\alpha = \frac{\pi}{L + 1}.$$

The derivation of these two expressions is explained in the appendix.

Remark 2. Except for these two expressions, the general expression for $\psi(m, L)$ is not known. In particular, simple observations, such as the fact that the numerator of $\psi(L, L)$ is always 1, are not yet understood. As we shall see in section 4, knowledge of all the $\psi(m, L)$ would lead to an exact expression for the exponent $\theta(q)$ for all q.

From the knowledge of the steady-state properties of the reaction–diffusion problem, one can predict some properties of the spin system. Namely, one can show that for the zero-temperature dynamics of the Potts chain, the probablity $\rho(q, L)$ that starting, with a random initial configuration, a given spin never flips (from $t = 0$ until $t = \infty$) is

$$\rho(q, L) = \sum_{m=1}^{L} \psi(m, L) \frac{1}{q^{m-1}}. \tag{10}$$

Table 2. The probabilities $\psi(m, L)$ of finding m particles on a lattice of L sites in the steady state of the reaction–diffusion model.

m	$\psi(m, 2)$
1	1
2	1
sum	2

m	$\psi(m, 3)$
1	2
2	1
3	1
sum	7

m	$\psi(m, 4)$
1	8
2	23
3	12
4	1
sum	44

m	$\psi(m, 5)$
1	62
2	224
3	176
4	32
5	1
sum	495

m	$\psi(m, 6)$
1	912
2	3864
3	3983
4	1135
5	81
6	1
sum	9976

m	$\psi(m, 7)$
1	25086
2	119732
3	150210
4	58176
5	6756
6	200
7	1
sum	360161

m	$\psi(m, 8)$
1	1277408
2	6695536
3	9762824
4	4746233
5	773400
6	38718
7	488
8	1
sum	23291608

m	$\psi(m, 9)$
1	119576386
2	676517512
3	1112007236
4	645394088
5	135690378
6	9838624
7	218160
8	1184
9	1
sum	2699243569

m	$\psi(m, 10)$
1	20474137792
2	123496972192
3	223393771328
4	149999841000
5	38560644737
6	3705492761
7	122922478
8	1221342
9	2865
10	1
sum	560355006496

m	$\psi(m, 11)$
1	6388684874754
2	40708419909844
3	80209940784610
4	60481733418936
5	18319389302802
6	2202781988876
7	99517558822
8	1528827648
9	6828422
10	6924
11	1
sum	208412003501639

m	$\psi(m, 12)$
1	3622889653916496
2	24211360923970368
3	51221197561172352
4	42707471805322080
5	11837097911823344
6	2144816831398223
7	121110019690236
8	2669867444891
9	19055991456
10	38215653
11	16724
12	1
sum	138874633672261824

m	$\psi(m, 13)$
1	3725652928914581886
2	25973574563856969936
3	58445552881310138984
4	53139445247340801901
5	20750614440790945780
6	3502168958728517856
7	248619865303718416
8	7015761751464736
9	72121835757780
10	238763471424
11	214295200
12	40384
13	1
sum	16579271700881070471287

m	$\psi(m, 14)$
1	6936113120455343354112
2	50209936705293228575104
3	119310287438547969062272
4	117003747981700514417952
5	50555756326565866257120
6	9742994699891535651248
7	822037265003972734943
8	29055474859170269599
9	401461517708733251
10	1968774404275827
11	30105379022909
12	1201356189
13	97505
14	1
sum	354610332445621455708032

This expression can be understood by using the same argument which was used in section 2 to derive expression (2): the equivalence between the spin model and the reaction–diffusion model. Assume that one starts the dynamics of the reaction–diffusion model at $t = 0$ and call $P(m, t)$ the probability that there are m particles in the system at time t. For a finite system of L sites, $P(m, t) \rightarrow \psi(m, L)$ as $t \rightarrow \infty$. Therefore in the infinite time limit, (2) becomes (10).

Remark 3. For an infinite system, the probability $r(q, t)$ that a given spin has never flipped

up to time t decreases to zero as $t \rightarrow \infty$. This is not the case for a finite system: for a finite system there is a finite probability (q^{1-L}) that initially all spins are in the same state and obviously $\rho(q, L) \geqslant q^{1-L}$.

Using the results given in table 2 for $\psi(m, L)$, one finds for the probability $\rho(q, L)$ that, for a random initial condition, a spin never flips between $t = 0$ and $t = \infty$,

$$\rho(q, 1) = 1$$

$$\rho(q, 2) = \frac{q+1}{2q}$$

$$\rho(q, 3) = \frac{2q^2 + 4q + 1}{7q^2}$$

$$\rho(q, 4) = \frac{8q^3 + 23q^2 + 12q + 1}{44q^3}$$

$$\rho(q, 5) = \frac{62q^4 + 224q^3 + 176q^2 + 32q + 1}{495q^4}$$

$$\rho(q, 6) = \frac{912q^5 + 3864q^4 + 3983q^3 + 1135q^2 + 81q + 1}{9976q^5}$$

and so on.

Clearly, for $q = 1$, one has $\rho(1, L) = 1$ for all L: the 'random' initial configuration is the configuration where all spins are the same. Thus the dynamics is trivial and nothing ever moves.

4. Finite-size scaling

Finite-size scaling is a well known method to obtain accurate estimates of critical exponents by calculating exactly the properties of finite systems and by analysing their size dependence [23–25, 20, 21]. Using the analogy with the reaction–diffusion model, the $\rho(q, L)$ are exactly known for arbitrary q up to size $L = 14$. (One could certainly do better as the size of the transfer matrix is 2^{L-1} and the matrix is sparse.) Let us assume that $\rho(q, L)$ decays algebraically for large L:

$$\rho(q, L) \sim L^{-\theta'(q)}. \tag{11}$$

This defines an exponent $\theta'(q)$ which is, in principle, related to the exponent $\theta(q)$ of (1) by [6]

$$\theta'(q) = 2\theta(q). \tag{12}$$

This relation can be justified by the fact that there is a characteristic length $l(t)$ growing with $t^{1/2}$ and that the dynamics stops when $l(t)$ becomes comparable to the system size as there is a single domain left in the system.

The first estimate of $\theta(q)$ one can make based on (11) and (12) is

$$\theta(q) = -\frac{1}{2} \frac{\log[\rho(q, L+1)/\rho(q, L)]}{\log[(L+1)/L]}. \tag{13}$$

The results of these estimates for $q = 2$ and $q = \infty$ are given for $1 \leqslant L \leqslant 13$ in column 0 of tables 3 and 4. The convergence is rather slow but looks regular and one can try to extrapolate the data of column 0. If one makes a polynomial extrapolation of the data of column 0 by taking k consecutive values $x_L, x_{L+1}, \ldots, x_{L+k-1}$ of column zero and by using

Table 3. Estimates of the exponent $\theta(q)$ for $q = 2$. The column 0 is obtained using the finite-size scaling expression (12). Columns 1–6 are polynomial extrapolations of degree 1–6 of the data of column 0.

				$q = 2$			
L	0	1	2	3	4	5	6
1	0.207 519	0.313 634	0.360 881	0.371 070	0.371 517	0.373 260	0.374 975
2	0.260 576	0.345 132	0.368 523	0.371 428	0.372 970	0.374 730	0.375 187
3	0.288 761	0.356 827	0.370 266	0.372 456	0.374 227	0.375 073	0.375 037
4	0.305 778	0.362 203	0.371 361	0.373 468	0.374 756	0.375 049	0.374 983
5	0.317 063	0.365 255	0.372 264	0.374 112	0.374 918	0.375 009	0.374 989
6	0.325 095	0.367 258	0.372 957	0.374 470	0.374 964	0.374 998	0.375 000
7	0.331 118	0.368 683	0.373 461	0.374 668	0.374 980	0.374 999	0.375 004
8	0.335 814	0.369 744	0.373 823	0.374 781	0.374 988	0.375 001	
9	0.339 584	0.370 560	0.374 084	0.374 850	0.374 993		
10	0.342 681	0.371 201	0.374 276	0.374 894			
11	0.345 274	0.371 713	0.374 418				
12	0.347 477	0.372 130					
13	0.349 374						

Table 4. Estimates of the exponent $\theta(q)$ for $q = \infty$. The column 0 is obtained using the finite-size scaling expression (12). Columns 1–6 are polynomial extrapolations of degree 1–6 of the data of column 0.

				$q = \infty$			
L	0	1	2	3	4	5	6
1	0.500 000	0.880 182	1.024 671	0.979 200	0.946 464	0.988 116	1.016 309
2	0.690 091	0.976 508	0.990 568	0.953 012	0.981 174	1.012 281	1.004 275
3	0.785 564	0.983 538	0.968 034	0.971 786	1.003 393	1.006 277	0.996 287
4	0.835 057	0.977 337	0.969 910	0.989 848	1.005 196	0.999 617	0.997 456
5	0.863 513	0.974 861	0.978 455	0.997 522	1.002 096	0.998 321	0.999 578
6	0.882 071	0.975 888	0.985 605	0.999 555	1.000 209	0.999 007	1.000 297
7	0.895 474	0.978 317	0.990 255	0.999 816	0.999 662	0.999 652	1.000 272
8	0.905 829	0.980 970	0.993 123	0.999 760	0.999 658	0.999 938	
9	0.914 178	0.983 401	0.994 933	0.999 726	0.999 766		
10	0.921 100	0.985 498	0.996 132	0.999 738			
11	0.926 955	0.987 270	0.996 964				
12	0.931 981	0.988 761					
13	0.936 349						

the polynomial P of degree k which satisfies $x_{L+i} = P(1/(L + i))$ for $0 \leqslant i \leqslant k - 1$, one obtains the data of column k.

We see that for $q = 2$ and $q = \infty$, the convergence is greatly improved and leads to accurate estimates of $\theta(q)$. However, one cannot choose polynomials of too high a degree because, as the degree of the extrapolation increases, the value obtained is more and more sensitive to rounding errors. This is probably why one cannot see much improvement for $k > 4$.

From the data of tables 3 and 4, one can estimate that

$$\theta(2) = 0.3750 \pm 0.0001$$

and

$$\theta(\infty) = 1.0000 \pm 0.0005.$$

For $q = \infty$, one recovers the exact prediction [6] that $\theta(\infty) = 1$ and the results of table 4 serve as a test of the accuracy of the extrapolation procedure.

As the $\rho(q, L)$ are known for arbitrary q, it is, of course, no problem to repeat these calculations for other choices of q. They lead to the estimates given in table 1 for $\theta(q)$.

5. ϵ expansion and bounds

One can exploit some of the results which are known exactly on finite systems to calculate the exponent $\theta(q)$ for q close to 1:

$$q = 1 + \epsilon. \tag{14}$$

Equation (10) then becomes

$$\rho(1 + \epsilon, L) = 1 - \epsilon \sum_{m=1}^{L} (m - 1)\psi(m, L) + O(\epsilon^2) \tag{15}$$

and one can use the exact result (9) of section 3. The large L dependence of the expression (9) is dominated by small values of k and k' and one finds that for large L

$$\sum_{m=1}^{L} (m - 1)\psi(m, L) \simeq \frac{4}{\pi} \log L.$$

Then using (11) and (12), one gets

$$\theta(q) = (2/\pi)\epsilon + O(\epsilon^2). \tag{16}$$

Therefore for small ϵ, one has $\theta(q) \simeq 0.6366\epsilon$ and this agrees rather well with the estimate for $\epsilon = 0.01$ reported in table 1 (the small discrepancy being due to the order ϵ^2).

Remark 4. There is a situation in which exponents corresponding to non-integer values of q could be measured directly in simulations. Assume that one considers the Ising model with a non-zero average magnetization μ in the initial condition. Initially each spin is either up with a probability $\frac{1}{2}(1 + \mu)$ and down with a probability $\frac{1}{2}(1 - \mu)$. Let us call $r_+(t)$ the probability that a spin initially up never flips between time 0 and time t and $r_-(t)$ the same quantity if the spin is initially down. By the same reasoning as for equation (10), one can show that

$$r_\pm(t) = \sum_{m=1}^{L} P(m, t) \left(\frac{1 \pm \mu}{2} \right)^{m-1}.$$

Comparing this with (10) leads to $r_\pm(t) = r(q_\pm, t)$ with

$$q_\pm = \frac{2}{1 \pm \mu}.$$

Clearly $\mu \to 1$ corresponds to an initial situation in which almost all spins are identical to the one at the origin, that is q close to 1, and $\mu \to -1$ corresponds to $q \to \infty$ as almost all spins in the system are different from the one at the origin.

Relation (10) also gives rigorous bounds for the exponent $\theta(q)$. If one chooses two values q_1 and q_2 with $q_1 < q_2$, one can write

$$q_2 \rho(q_2, L) = \sum_{m=1}^{L} \psi(m, L) q_2^{-m} = \sum_{m=1}^{L} \psi(m, L) [q_1^{-m}]^{\log q_2 / \log q_1}.$$

Then using Jensen's inequality (for a positive random variable x, one has $\langle x^\gamma \rangle \geqslant \langle x \rangle^\gamma$ when $\gamma \geqslant 1$), one finds

$$q_2 \rho(q_2, L) \geqslant [q_1 \rho(q_1, L)]^{\log q_2 / \log q_1}.$$

This obviously leads to

$$\theta'(q_2) \leqslant \theta'(q_1) \frac{\log q_2}{\log q_1}$$

and therefore to (4). As $\theta(q)$ is known for q close to 1, this leads for $q > 1$ to

$$\theta(q) \leqslant \frac{2}{\pi} \log q.$$

For example this bound predicts $\theta(2) < 0.441\,27$ which is clearly satisfied by the estimate $\theta(2) \simeq 0.3750$ of table 1.

6. Conclusion

In this paper, the calculation of the fraction of spins which have never flipped in the zero-temperature dynamics of the one-dimensional Potts model has been related to the properties of a simple reaction–diffusion model. This analogy has been used to obtain accurate estimates for the exponent $\theta(q)$ for any q, the first term of an ϵ-expansion for q close to 1 and bounds on this exponent.

The numerical estimate indicates $\theta(q)$ is very close to $3/8$ for $q = 2$ and it would certainly be of interest to see whether this prediction is exact. More generally, we have seen that some properties (8), (9) of the reaction–diffusion model can be obtained exactly. With more work, one could try to push further the ϵ expansion or to obtain a large q expansion (this would require an exact expression of $\psi(2, L)$ for all L). One can even hope to find a complete analytic solution of the reaction–diffusion model. This would automatically lead to the exact expression of $\theta(q)$ for all q.

Appendix A.

In this appendix some of the steady-state properties of the reaction–diffusion model are calculated exactly. These properties give, as special cases, the results (8), (9). We consider the reaction–diffusion model on a ring of L sites with the origin located at position L, i.e. the site 0 ($\equiv$ site L) is always occupied. Then during any time interval dt, each particle in the system jumps with probability $dt/2$ to its left and $dt/2$ to its right. When two particles

occupy the same site, they instantaneously coalesce $A + A \rightarrow A$. Also if the particle at the origin jumps to one of its neighbours, the origin is instantaneously filled by a new particle.

Let us call $f(i, j)$ the probability that in the steady state, all the sites k between i and j are empty ($i \leqslant k \leqslant j$). Clearly with this definition, the probability that site i is empty is just $f(i, i)$. Moreover as the origin is always occupied, one has for all i and j

$$f(0, j) = f(i, L) = 0. \tag{A1}$$

During each time interval dt, it is possible to write a steady-state equation for $i < j$:

$$\frac{dt}{2}[f(i+1, j) - f(i, j)] + \frac{dt}{2}[f(i, j-1) - f(i, j)]$$

$$= \frac{dt}{2}[f(i, j) - f(i-1, j)] + \frac{dt}{2}[f(i, j) - f(i, j+1)]. \tag{A2}$$

The left-hand side of this equation is the probablility of entering into a configuration where all sites between i and j are empty. This happens either if all sites between $i + 1$ and j are empty with a particle present at site i (first term) or if all sites between i and $j - 1$ are empty with a particle present at site j (second term). The right-hand side can be understood as the probability of leaving the configuration. The case $i = j$ has to be treated separately, and one finds that (A2) is replaced by

$$dt[1 - f(i, i)] = \frac{dt}{2}[f(i, i) - f(i-1, i)] + \frac{dt}{2}[f(i, i) - f(i, i+1)]. \tag{A3}$$

Clearly (A2) and (A3) are equivalent to

$$4f(i, j) = f(i-1, j) + f(i+1, j) + f(i, j-1) + f(i, j+1) \tag{A4}$$

and

$$4f(i, i) = 2 + f(i-1, i) + f(i, i+1). \tag{A5}$$

The solution for $f(i, j)$ is then

$$f(i, j) = \sum_{k \text{ even}} \sum_{k' \text{ odd}} \frac{8 \sin k\alpha \sin k'\alpha[\sin ki\alpha \sin k'(j+1)\alpha - \sin k'i\alpha \sin k(j+1)\alpha]}{(L+1)^2(\cos k'\alpha - \cos k\alpha)(2 - \cos k\alpha - \cos k'\alpha)} \tag{A6}$$

where

$$\alpha = \frac{\pi}{L+1} \qquad 2 \leqslant k \leqslant L \qquad 1 \leqslant k' \leqslant L. \tag{A7}$$

Then (8) and (9) follow as

$$\psi(1, L) = f(1, L-1)$$

and

$$L - 1 - \sum_{i=1}^{L-1} f(i, i) = \sum_{m=1}^{L}(m-1)\psi(m, L)$$

(this last expression just means that the average occupation of site i is just $1 - f(i, i)$).

The easiest way to check that (A6) is the solution of (A4)–(A5) is numerically on a computer. It is also possible to derive a proof based on the following trigonometric identities:

$$\frac{\sin x \sin y[\sin ix \sin(j+1)y - \sin iy \sin(j+1)x]}{\cos y - \cos x}$$

$$= \sum_{p=0}^{j-i} \sum_{q=0}^{j+i} \sin(p+q-j)x \sin x \sin(q-p-i)y \sin y \tag{A8}$$

and for $-L \leqslant n \leqslant L$

$$\sum_{k \text{ even}} \sin k\alpha \sin nk\alpha = \frac{L+1}{4}[\delta_{n,-L} - \delta_{n,-1} + \delta_{n,1} - \delta_{n,L}] \tag{A9}$$

$$\sum_{k' \text{ odd}} \sin k'\alpha \sin nk'\alpha = \frac{L+1}{4}[-\delta_{n,-L} - \delta_{n,-1} + \delta_{n,1} + \delta_{n,L}] \tag{A10}$$

where k, k' and α satisfy (A7).

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