Exact relations between damage spreading and thermodynamic functions for the $\mathcal{N}$-color Ashkin–Teller model

A S dos Anjos$^1$, I S Queiroz$^2$, A M Mariz$^1$ and F A da Costa$^{1,3}$

$^1$ Departamento de Física Teórica e Experimental, Universidade Federal do Rio Grande do Norte, Caixa Posta 1641, 59072-970 Natal–Rio Grande do Norte, Brazil
$^2$ Departamento de Ciências Ambientais, Universidade Federal Rural do Semi-Árido—UFERSA, BR 110-Km 47, Bairro Presidente Costa e Silva, CEP 59.625-900 Mossoró–Rio Grande do Norte, Brazil
E-mail: asafilho@dfte.ufrn.br, idalmirjr@hotmail.com, ananias@dfte.ufrn.br and fcosta@dfte.ufrn.br

Received 29 April 2009
Accepted 15 July 2009
Published 4 August 2009

Online at stacks.iop.org/JSTAT/2009/P08002
doi:10.1088/1742-5468/2009/08/P08002

Abstract. Some exact results are derived relating quantities computable by the so-called damage spreading method and thermodynamic functions for the $\mathcal{N}$-color Ashkin–Teller model. The results are valid for any ergodic dynamics. Since we restrict our analysis to the ferromagnetic case, the results are also valid for any translationally invariant lattice. The relations derived can be used in order to determine the $\mathcal{N}$-color Ashkin–Teller critical exponents numerically, providing better accuracy and requiring less computational effort than standard Monte Carlo simulations.

Keywords: classical Monte Carlo simulations, correlation functions (theory), other numerical approaches

$^3$ Author to whom any correspondence should be addressed.
Since its introduction, the damage spreading (DS) method has become a powerful tool in the study of phase transitions and critical phenomena [1, 2]. Basically it consists in following the time evolution of two initially identical copies of a given system, each subject to the same dynamical rules and to the same thermal noise, after the introduction of a small perturbation (called damage) in one of them at a given time. This method presents some advantages over the traditional Monte Carlo (MC) method where the time evolution of a single copy of the system is investigated [3]. For instance, in the DS method the fluctuations are substantially reduced as compared to the conventional MC method case. A recent review of the DS method can be found in [4].

In statistical mechanics, the most important question when performing a simulation is that of how to obtain the equilibrium thermal properties of the system under investigation. Thus it is very important to establish exact relations relating measurable quantities obtained in a DS simulation to the thermodynamical properties of the system. Such relations were first obtained for the ferromagnetic Ising model for a square lattice and the numerical results showed a prominent reduction of fluctuations and finite-size effects [5]. In the wake of those findings the exact relations between damage spreading computable quantities such as magnetization and spin–spin correlation functions and thermal equilibrium quantities have been obtained for several systems, e.g., the Potts [6], Ashkin–Teller [6], discrete $N$-vector [7], $(N_{\alpha}, N_{\beta})$ [8], and spin-1 [9] models. These relations are valid for any translationally invariant system which evolves in time under any ergodic dynamics. Recently, such relations were applied to numerically investigate the Potts [10], two-color Ashkin–Teller [11] and spin-1 [9] models. In all these cases the computed critical exponents were in agreement with the exact known results to within four decimal places, revealing the accuracy of the DS method.

The Ashkin–Teller (AT) model was introduced to investigate cooperative phenomena in quaternary alloys [12]. It was shown to be equivalent to a two-layer Ising model with a four-spin coupling between the two layers [13]. In two dimensions the AT model can be mapped onto a staggered eight-vertex model at the critical point and shows non-universal critical behavior along a self-dual line where the exponents vary continuously [14]. In general, despite its simplicity, the two-color AT model displays a wide variety of critical and multicritical phenomena already in two dimensions, as has been shown in studies based on duality arguments [15], real-space renormalization group [16]–[18] and mean-field renormalization group approaches [19]–[21], finite-size scaling [22]–[24], and conventional Monte Carlo simulations [22], [25]–[28].

The $N$-color Ashkin–Teller ($N$-AT) model consists of $N$ Ising models coupled pairwise through a four-spin interaction [29]. When $N = 2$ it becomes the usual AT model discussed above (also known as the two-color AT model). It was argued that for $N > 2$ the model has a first-order transition as long as the four-spin coupling is ferromagnetic [29]. In [29] the phase diagram was investigated using mean-field analysis and Monte Carlo simulation for $N = 3$ and by several other techniques for $N > 2$ [30]–[37]. Recently there has been renewed interest in this model mainly due to the richness of its phase diagram and its relation to other systems [38]–[41]. However, it still needs a lot of work in order to fully understand the main features of the $N$-AT for $N > 2$ in any dimension. We believe that the DS simulations are quite suitable for giving us more information about this model.

The purpose of the present note is to determine exact relations involving thermodynamic quantities and some specific combinations of damage for the $N$-color...
Ashkin–Teller model. The model is defined by the Hamiltonian

$$\mathcal{H} = -J_2 \sum_{(ij)} \sum_{a=1}^{N} \sigma_i^a \sigma_j^a - \frac{1}{2} J_4 \sum_{(ij)} \sum_{a \neq b} \sigma_i^a \sigma_j^a \sigma_i^b \sigma_j^b,$$

(1)

where $\sigma_i^a = \pm 1$, $a$ and $b$ label different Ising spins (distinguished by their ‘color’) at a site $i$ and $\langle ij \rangle$ indicates that the sum is performed over all distinct pairs of sites on a given lattice. For $N = 1$ we recover the Ising model, whereas for $N = 2$ we have the usual Ashkin–Teller model. In what follows, our treatment is valid for any value of $N$, and for $(J_2, J_4)$ in the ferromagnetic range, in order to take into account the translational invariance of the lattice.

According to the usual mean-field procedure we can write a single-site effective Hamiltonian

$$\beta \mathcal{H}_{\text{eff}} = \sum_{a=1}^{N} h_i^a \sigma_i^a + \frac{1}{2} \sum_{a \neq b} h_{ib} \sigma_i^a \sigma_i^b,$$

(2)

where $h_i^a = K_2 \sum_{j \neq i} \langle \sigma_j^a \rangle$ and $h_{ib} = K_4 \sum_{j \neq i} \langle \sigma_j^a \sigma_j^b \rangle$. In the above equation $\langle \cdots \rangle$ denotes the thermal average and we have introduced the new variables $K_n = J_n / k_B T$ ($n = 2, 4$). The structure of the effective fields acting on $\sigma_i^a$ and $\sigma_i^a \sigma_i^b$ implies that the order parameters are given by

$$m^a = \langle \sigma_i^a \rangle, \quad a = 1, \ldots, N,$$

(3)

and

$$M^{ab} = \langle \sigma_i^a \sigma_i^b \rangle, \quad a \neq b,$$

(4)

while the correlation functions are expressed by

$$\Gamma_{ij}^a = \langle \sigma_i^a \sigma_j^a \rangle - \langle \sigma_i^a \rangle \langle \sigma_j^a \rangle, \quad a = 1, \ldots, N,$$

(5)

and

$$\Gamma_{ij}^{ab} = \langle \sigma_i^a \sigma_i^b \sigma_j^a \sigma_j^b \rangle - \langle \sigma_i^a \sigma_i^b \rangle \langle \sigma_j^a \sigma_j^b \rangle, \quad a \neq b.$$

(6)

To implement the damage spreading technique it is convenient to introduce the following binary variables:

$$\Pi_i^a = \frac{1}{2} (1 + \sigma_i^a),$$

(7)

$$\Pi_i^{ab} = \frac{1}{2} (1 + \sigma_i^a \sigma_i^b), \quad a \neq b.$$

(8)

Let us consider two configurations (referred to as $A$ and $B$) on a regular, translational invariant, lattice evolving in time according to the same (and ergodic) dynamics such as Metropolis, heat-bath or Glauber ones [3]. We define damage combinations of four
different types:

(1) \( \Pi_i^a(A) = 1 \) and \( \Pi_i^a(B) = 0 \),

(2) \( \Pi_i^a(A) = 0 \) and \( \Pi_i^a(B) = 1 \),

(3) \( \Pi_i^{ab}(A) = 1 \) and \( \Pi_i^{ab}(B) = 0 \), \( a \neq b \),

(4) \( \Pi_i^{ab}(A) = 0 \) and \( \Pi_i^{ab}(B) = 1 \), \( a \neq b \).

It is known that after a long time the system eventually reaches thermal equilibrium. In this regime, the above-defined damage types occur with probabilities given, respectively, by

\[
p_1 = \langle \Pi_i^a(A)[1 - \Pi_i^a(B)] \rangle_t, \quad (13)
\]

\[
p_2 = \langle [1 - \Pi_i^a(A)]\Pi_i^a(B) \rangle_t, \quad (14)
\]

\[
p_3 = \langle \Pi_i^{ab}(A)[1 - \Pi_i^{ab}(B)] \rangle_t, \quad (15)
\]

\[
p_4 = \langle [1 - \Pi_i^{ab}(B)]\Pi_i^{ab}(B) \rangle_t, \quad (16)
\]

where \( \langle \cdots \rangle_t \) means the time average over the trajectory followed by the copies of the system in their phase space. In what follows it is convenient to introduce differences between such probabilities:

\[
F = p_1 - p_2 = \langle \Pi_i^a(A) \rangle_t - \langle \Pi_i^a(B) \rangle_t, \quad a = 1, \ldots, N, \quad (17)
\]

and

\[
G = p_3 - p_4 = \langle \Pi_i^{ab}(A) \rangle_t - \langle \Pi_i^{ab}(B) \rangle_t, \quad a \neq b. \quad (18)
\]

The next step in our analysis consists in imposing some constraints on the temporal evolution. In the present case it turns out that there are four distinct such possibilities:

\( e_1 \) Copy \( A \) evolves without any constraint, while copy \( B \) is restricted by the constraint that for an arbitrarily fixed site, say \( i = 0 \), \( \Pi_0^a(B) = 0 \), for \( a = 1, \ldots, N \).

\( e_2 \) Copy \( A \) evolves with \( \Pi_0^a(A) = 1 \) and copy \( B \) with \( \Pi_0^a(B) = 0 \), for \( a = 1, \ldots, N \).

\( e_3 \) Copy \( A \) evolves without any constraint, while copy \( B \) is restricted to having \( \Pi_0^{ab}(B) = 0 \), \( a \neq b \).

\( e_4 \) Copy \( A \) is subjected to \( \Pi_0^{ab}(A) = 1 \), while copy \( B \) is restricted to \( \Pi_0^{ab}(B) = 0 \), \( a \neq b \).

Ergodicity implies, for the evolution \( e_1 \), that

\[
\langle \Pi_i^a(A) \rangle_t = \langle \Pi_i^a \rangle \quad (19)
\]

and, with the help of conditional probability,

\[
\langle \Pi_i^a(B) \rangle_t = \frac{\langle \Pi_i^a(1 - \Pi_i^a) \rangle}{1 - \langle \Pi_i^a \rangle}. \quad (20)
\]

Equations (19), (20) relate, in a definitive way, the dynamical and thermal averages represented, respectively, by \( \langle \cdots \rangle_t \) and \( \langle \cdots \rangle \). Substitution of those equations into (17)

doi:10.1088/1742-5468/2009/08/P08002
Damage spreading and thermodynamic functions for the Ashkin–Teller model

gives us

$$F(e_1) = \frac{\langle \Pi_i \Pi_0 \rangle - \langle \Pi_i \rangle \langle \Pi_0 \rangle}{1 - \langle \Pi_0 \rangle}$$

(21)

which, with the help of (3), (5) and (7), can be expressed as

$$F(e_1) = \frac{\Gamma_{0i}}{2(1 - m^a)}.$$ 

(22)

For the evolution \((e_2)\) we have, in a similar way,

$$\langle \Pi_i^a(A) \rangle_t = \frac{\langle \Pi_0^a \Pi_i^a \rangle}{\langle \Pi_0^a \rangle},$$

(23)

and

$$\langle \Pi_i^a(B) \rangle_t = \frac{\langle \Pi_0^a(1 - \Pi_i^a) \rangle}{1 - \langle \Pi_0^a \rangle},$$

(24)

from which it follows that

$$F(e_2) = \frac{\Gamma_{0i}}{1 - (m^a)^2}.$$ 

(25)

In order to write the final equations (22) and (25) we have used the fact that \(m^a = m_0^a\) as a consequence of the lattice translational invariance. The results expressed by these equations mean that at first we compute numerically \(F(e_1)\) and \(F(e_2)\) (quantities related to DS). Then, we may determine the magnetization and the two-point correlation functions (thermal equilibrium quantities) as

$$m^a = 2 \frac{F(e_1)}{F(e_2)} - 1,$$

(26)

and

$$\Gamma_{0i}^a = 4 \frac{F(e_1)}{F(e_2)} (F(e_2) - F(e_1)),$$

(27)

for \(a = 1, 2, \ldots, N\).

For the evolution \((e_3)\) we find

$$\langle \Pi_i^{ab}(A) \rangle_t = \langle \Pi_i^{ab} \rangle$$

(28)

and

$$\langle \Pi_i^{ab}(B) \rangle_t = \frac{\langle \Pi_i^{ab}(1 - \Pi_0^{ab}) \rangle}{1 - \langle \Pi_0^{ab} \rangle},$$

(29)

for \(a \neq b\).

Thus, from (4), (6) and (8) we get

$$G(e_3) = \frac{\Gamma_{0i}^{ab}}{2(1 - M^{ab})}, \quad a \neq b.$$ 

(30)

doi:10.1088/1742-5468/2009/08/P08002
Finally, evolution \((e_4)\) implies that
\[
\langle \Pi^a_{i}(A) \rangle_t = \frac{\langle \Pi^a_{i} \Pi^b_{0} \rangle}{\langle \Pi^b_{0} \rangle},
\]
and
\[
\langle \Pi^a_{i}(B) \rangle_t = \frac{\langle \Pi^a_{i}(1 - \Pi^b_{0}) \rangle}{1 - \langle \Pi^b_{0} \rangle},
\]
for \(a \neq b\).

Therefore, in terms of \(M^{ab}\) and \(\Gamma^{ab}_{0i}\) we have
\[
G(e_4) = \frac{\Gamma^{ab}_{0i}}{1 - (M^{ab})^2}, \quad a \neq b.
\]
Thus, having determined \(G(e_3)\) and \(G(e_4)\) in a numerical simulation, we can use (30) and (33) to compute
\[
M^{ab} = 2 \frac{G(e_3)}{G(e_4)} - 1
\]
and
\[
\Gamma^{ab}_{0i} = 4 \frac{G(e_3)}{G(e_4)}(G(e_4) - G(e_3)).
\]

Since \(F(e_1), F(e_2), G(e_3)\) and \(G(e_4)\) are computed from selected combinations of damage types, the relations expressed by (22)–(25) and (30)–(33), which are exact for any translationally invariant lattice at all temperatures, allow us to determine numerically the thermal properties of the \(N\)-color Ashkin–Teller model.

As an example we considered the ferromagnetic three-color Ashkin–Teller model on a square lattice of linear size \(L = 60\) and with \(J_4 = 0.01J_2\). Periodic boundary conditions were applied and we computed the two-site correlation functions
\[
\Gamma^{(a)}(r) = \frac{1}{4} \sum_{i(r)} \Gamma^{(a)}_{0i} \quad (a = 1, 2, 3),
\]
measured with respect to the central site located at \((L/2, L/2)\). The two-site correlation functions \(\Gamma^{(a)}_{0i}\) are computed from (27). As the equilibria were approached we found that \(\Gamma^{(1)}(r) = \Gamma^{(2)}(r) = \Gamma^{(3)}(r)\) as expected from the permutation symmetry between the spin variables presented in the Hamiltonian. Initially a copy denoted by \(A\) with all spin variables \(\sigma^{(a)}_i(A) = 1\) is left to evolve according to a MC run during a time \(t_{eq} = 1 \times 10^4\) which is sufficient to allow the system to get close enough to thermal equilibrium. Then a second copy denoted by \(B\) is created by replicating copy \(A\) and introducing small modifications, the initial damage, on it. Both copies are left to evolve under the same ergodic dynamical rules during a time \(t_{av} = 1.8 \times 10^5\) and subjected to specific boundary conditions corresponding to the possibilities \((e_1)\) and \((e_2)\) mentioned above. In addition to that, each simulation was performed for \(M = 20\) different samples in order to reduce inherent statistical fluctuations for a given temperature. To locate the transition point we search for the temperature ratios \(T/T_C\) at which the functions \(\Gamma^{(a)}(r)\) show the slowest
Figure 1. The correlation function $\Gamma^{(1)}(r)$ versus $r$. The slowest decay was found for $T/T_C = 1.002$, in which case the plot of $\log_{10}[\Gamma^{(1)}(r)]$ versus $\log_{10} r$ is presented in the inset, leading to the estimate $\eta = 0.2521 \pm 0.0050$.

decay as a function of $r$. At criticality we expect that, for large $r$,

$$\Gamma^{(a)}(r) \sim r^{-\eta} \quad (a = 1, 2, 3). \quad (37)$$

In figure 1 we present the behavior of $\Gamma^{(1)}(r)$ for several values of $T/T_C$ (here $T_C$ is the usual Ising critical temperature at the decoupling point $J_4 = 0$). It is noted that the slowest decay occurs for $T/T_C = 1.002$. The inset in figure 1 shows a log–log plot of $\Gamma^{(1)}(r)$ versus $r$, at the observed critical point, from which we obtain $\eta = 0.2521 \pm 0.0050$. Therefore, for the three-color AT model we found evidence of a continuous transition of Ising type for $J_4/J_2 = 0.01$. The complete phase diagram for this particular case can be determined by the present method, as long as the transitions are continuous. We hope to address this problem in a future work.

Recently published results [9]–[11] for other nontrivial situations have established the accuracy of the present approach for obtaining critical properties of classical spin models in translationally invariant systems. We thus have presented new exact relations connecting some damage spreading functions to thermal equilibrium properties for the ferromagnetic $N$-color Ashkin–Teller model and we hope that such relations will become a useful guide to high precision numerical investigations.

References

[1] Stanley H E, Stauffer D, Kertész J and Hermann H J, 1987 Phys. Rev. Lett. 59 2326
[2] Derrida B and Weisbuch G, 1987 Europhys. Lett. 4 657
[3] Landau D P and Binder K, 2000 A Guide to Monte Carlo Simulations in Statistical Physics (Cambridge: Cambridge University Press)
[4] Puzzo M L R and Albano E, 2008 Commun. Comput. Phys. 4 207
[5] Coniglio A, de Arcangelis L, Hermann H J and Jan N, 1989 Europhys. Lett. 8 315
[6] Mariz A M, 1990 J. Phys. A: Math. Gen. 23 979
[7] Mariz A M, de Souza A M C and Tsallis C, 1993 J. Phys. A: Math. Gen. 26 L1007
doi:10.1088/1742-5468/2009/08/P08002
Damage spreading and thermodynamic functions for the Ashkin–Teller model

[8] Mariz A M, de Souza E S and Nobre F D, 1998 Physica A 257 429
[9] Anjos A S, Mariz A M, Nobre F D and Araujo I G, 2008 Phys. Rev. E 78 031105
[10] Anjos A S, Moreira D A, Mariz A M and Nobre F D, 2006 Phys. Rev. E 74 016703
[11] Anjos A S, Moreira D A, Mariz A M, Nobre F D and da Costa F A, 2007 Phys. Rev. E 76 041137
[12] Ashkin J and Teller E, 1943 Phys. Rev. 64 178
[13] Fan C, 1972 Phys. Lett. A 39 136
[14] Baxter R J, 1982 Exactly Solved Models in Statistical Mechanics (London: Academic)
[15] Wu F Y and Lin K Y, 1974 J. Phys. C: Solid State Phys. 7 L181
[16] Domany E and Riedel E K, 1979 Phys. Rev. B 19 5817
[17] Mariz A M, Tsallis C and Fulco P, 1985 Phys. Rev. B 32 6055
[18] Bezerra C G, Mariz A M, de Araujo J M and da Costa F A, 2001 Physica A 292 429
[19] Plascak J A and Sa Barreto F C, 1986 J. Phys. A: Math. Gen. 19 2195
[20] de Oliveira P M C and Sa Barreto F C, 1989 J. Stat. Phys. 57 53
[21] Plascak J A, Figueiredo W and Grandi B C S, 1999 Braz. J. Phys. 29 579
[22] Kamieniarz G, Kozlowski P and Dekeyser R, 1997 Phys. Rev. E 55 3724
[23] Pawlicki P, Kamieniarz G, Kozlowski P, Dekeyser R and Rogiers J, 1997 Acta Phys. Pol. A 92 453
[24] Badehdah M, Bekechi S, Benyoussef A and Touzani M, 2000 Physica B 291 394
[25] Ditzian R V, Banavar J R, Grest G S and Kadanoff L P, 1980 Phys. Rev. B 22 2542
[26] Chahine J, Drugowich de Felicio J R and Caticha N, 1989 J. Phys. A: Math. Gen. 22 1639
[27] Wiseman S and Domany E, 1993 Phys. Rev. E 48 4080
[28] Bekechi S, Benyoussef A, Elkenz A, Ettaki B and Loulidi M, 1999 Physica A 264 503
[29] Grest G S and Widom M, 1981 Phys. Rev. B 24 6508
[30] Fradkin E, 1984 Phys. Rev. Lett. 53 1967
[31] Bray A J, 1985 Phys. Rev. Lett. 54 1593
[32] Kardar M and Kaufman M, 1985 Phys. Rev. B 31 7282
[33] Shankar R, 1985 Phys. Rev. Lett. 55 453
[34] Goldschmidt Y Y, 1986 Phys. Rev. Lett. 56 1627
[35] Martins M J and de Felicio J R D, 1988 J. Phys. A: Math. Gen. 21 1117
[36] de Felicio J R D, Chahine J and Caticha N, 2003 Physica A 321 529
[37] Pielho F A P, da Costa F A, Bezerra C G and Mariz A M, 2008 Physica A 387 1538
[38] Calabrese P and Celi A, 2002 Phys. Rev. B 66 184410
[39] Calabrese P, Orlov E V, Pakhnin D V and Sokolov A I, 2004 Phys. Rev. B 70 094425
[40] Papanikolaou S, Luijten E and Fradkin E, 2007 Phys. Rev. B 76 134514
[41] Goswami P, Schwab D and Chakravarty S, 2008 Phys. Rev. Lett. 100 015703

doi:10.1088/1742-5468/2009/08/P08002