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Relaxation in the diluted XY model

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Abstract. The probabilistic cellular automata approach is used to estimate the relaxation of the magnetization in the quenched, site-diluted classical XY model. It is found that the relaxation can be described by an exponential law in two and three dimensions. For the initial time it has the Debye character. From the obtained curves an analytic expression is deduced which enables the phase diagram to be drawn in three dimensions. In two dimensions the final stage of the relaxation is always a non-magnetic one while in three dimensions it depends on the concentration of spins.

1. Introduction

Although the classical XY model with many modifications has been actively investigated in recent years (see e.g. Ariosa *et al* 1988, Berge *et al* 1986, Gerling and Landau 1983) the diluted version of the model is less popular. To the best of our knowledge the paper by Reeve and Betts (1975) is the only one. The authors, using high temperature series expansions, derived *inter alia* its phase diagram.

The aim of this paper is to estimate the relaxation of the magnetization in a site-diluted classical XY model in 2D and 3D. We shall use the probabilistic cellular automata approach. For technical reasons (lack of powerful computers) we do not aim at finding critical exponents nor at establishing precise values for the relaxation constants or critical concentrations. Rather, we want to show that having more computer power such things can, and probably should, be done.

2. The model

We consider a system of n classical XY spins located randomly on sites of a 2D or 3D cubic lattice. The concentration of spins is x. Once put in place the spins remain in their positions throughout the process. Hence we have the quenched site-diluted case. The spins may be rotated either by magnetic interactions, J, to nearest neighbours, or by random interactions with a continuous medium filling up the lattice. The latter interactions simulate thermal contact of the spins with a heat bath. The medium is characterized by two parameters—the friction constant, ρ, and the temperature, T. A similar approach using the Monte Carlo technique has been employed by Miyashita *et al* (1978). For time $t<0$ the system is in thermal equilibrium and an infinitely strong homogeneous external magnetic field is applied aligning all spins. At $t=0$ the field is switched off and the relaxation to a new equilibrium state begins.

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The spin at a site $i=(1,\ldots,N)$ is characterized by an angle $\alpha_i(t)$ it makes with a fixed arbitrary direction. The potential of magnetic interactions is

$$V(t)=-J\sum_{\langle i,j\rangle} s_i s_j \cos[\alpha_i(t)-\alpha_j(t)] \tag{1}$$

where $s_i(=0, 1)$ is the site occupation variable. The time evolution of the spin is given (we are looking for stationary solutions) by the Langevin equation

$$\rho d_t\alpha_i(t)=-J\sum_{\delta=1}^{q} s_{i+\delta}\sin[\alpha_i(t)-\alpha_{i+\delta}(t)]+\lambda_i(t) \tag{2}$$

where q is the number of nearest neighbours. The terms on the RHS represent the systematic (magnetic) and random (thermal) forces acting on the spin at site i. $\lambda(t)$ is the time derivative of the Wiener process, $W(T)$, with

$$\langle\lambda(t)\lambda(t')\rangle=2kT\rho\delta(t-t'). \tag{3}$$

For discrete time (2) can be written as

$$\alpha_i(t+\Delta t)=\alpha_i(t)-\rho^{-1}J\,\Delta t\sum s_{i+\delta}\sin[\alpha_i(t)-\alpha_{i+\delta}(t)]+\rho^{-1}\Delta W_i(t). \tag{4}$$

ΔW represents white noise and can be written as (Résibois and de Leener 1977)

$$\Delta W_i(t)=\sqrt{2kT\rho\,\Delta t}\;z_i(t) \tag{5}$$

where $z(t)$ are computer generated random variables with standard normal distribution. Scaling time to $t=t\rho J^{-1}$ (Gerling and Landau 1983) (4) becomes

$$\alpha_i(t+\Delta t)=\alpha_i(t)-\Delta t\sum s_{i+\delta}\sin[\alpha_i(t)-\alpha_{i+\delta}(t)]+\sqrt{2\tau\,\Delta t}\;z_i(t). \tag{6}$$

$\tau=kT/J$ is the reduced temperature and Δt is the time increment used in evaluation of (6). It should be small to ensure good accuracy, but not too small if, with restricted computer power, we want to reach larger times. In our case for $\Delta t=0.04\rho J^{-1}$, we iterated until $t=50\rho J^{-1}$, using an IBM AT microcomputer.

For a given concentration, x, of spins their positions on the lattice are randomly chosen, and their time evolution is calculated from (6). At each time step the magnetization, $m(t)$, is evaluated from

$$m(t)=N^{-1}\sum\cos\alpha_i(t). \tag{7}$$

This is then averaged over different initial localizations of spins

$$M(t)=\langle m(t)\rangle. \tag{8}$$

To speed up the computer calculations we have used discrete angles α_i, with a typical division of $2\pi/1000$. Therefore we were able to use mainly integer number arithmetics.

The equation of motion (6) depends, for a chosen time increment, on three parameters—dimensionality of the system, concentration of spins, $x=\Sigma s_i$, and reduced temperature τ. The relaxation curves following from (6) are shown, for some representative values of the parameters, in figure 1.

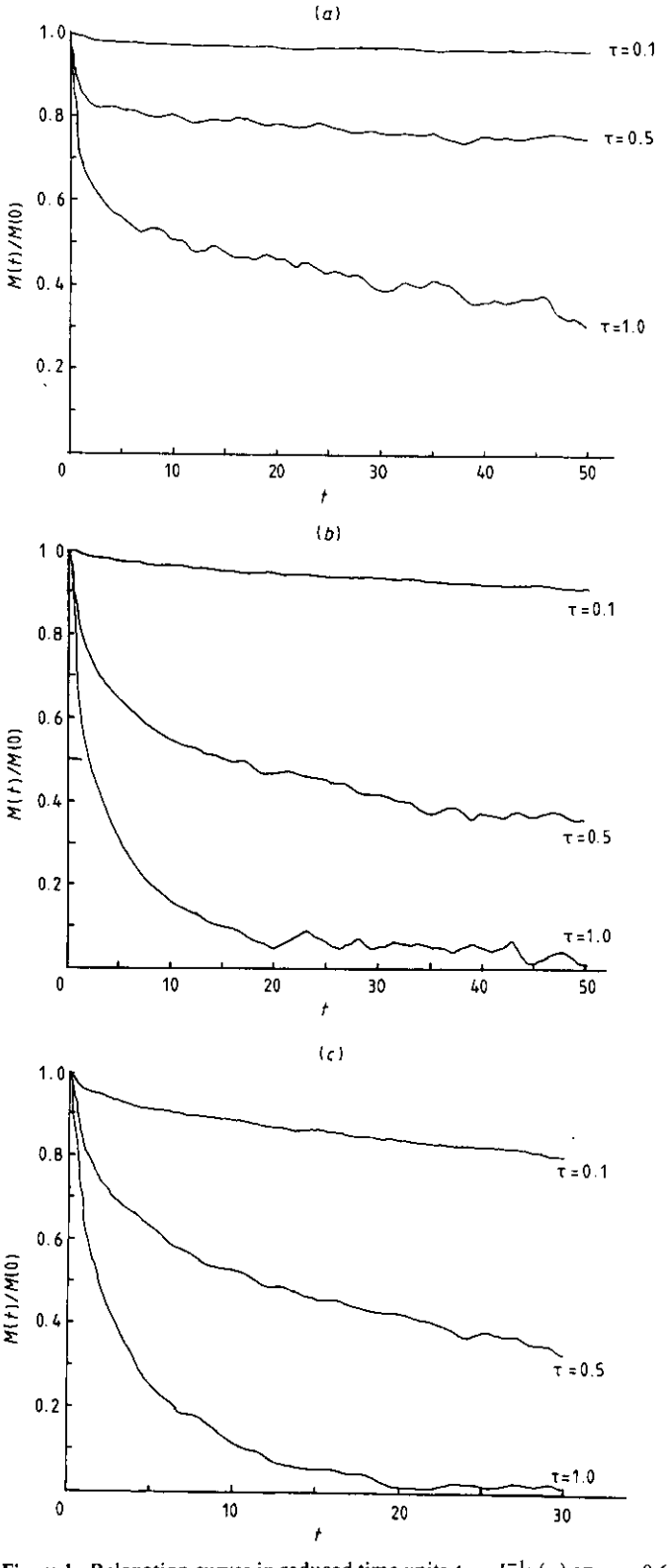

Figure 1. Relaxation curves in reduced time units $t = \rho J^{-1}$: (*a*) 3D, $x = 0.6$; (*b*) 3D, $x = 0.4$; (*c*) 2D, $x = 0.6$.

3. Results

It is possible, having several sets of curves as in figure 1, to find an analytic formula for relaxation of the magnetization which would fit the calculated curves (see figure 2). It seems that in 3D the initial relaxation behaves in a different way than that for larger times, although both seem to have an exponential character (see figure 3). We assume that

$$M(t) \propto \exp(-at^b) \tag{9}$$

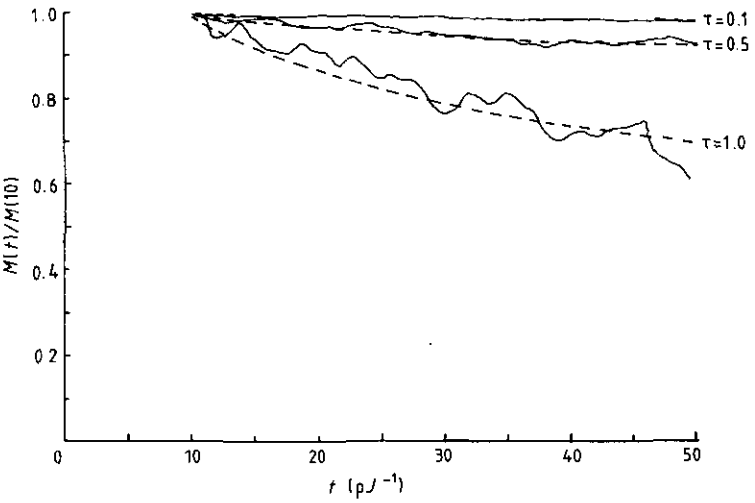

Figure 2. Relaxation of the magnetization in 3D calculated from the cellular automata (full line) and from equation (6) (broken line) for $x = 0.6$ and three values of the reduced temperature $\tau(=kT/J) = 0.1$, 0.5 and 1.0.

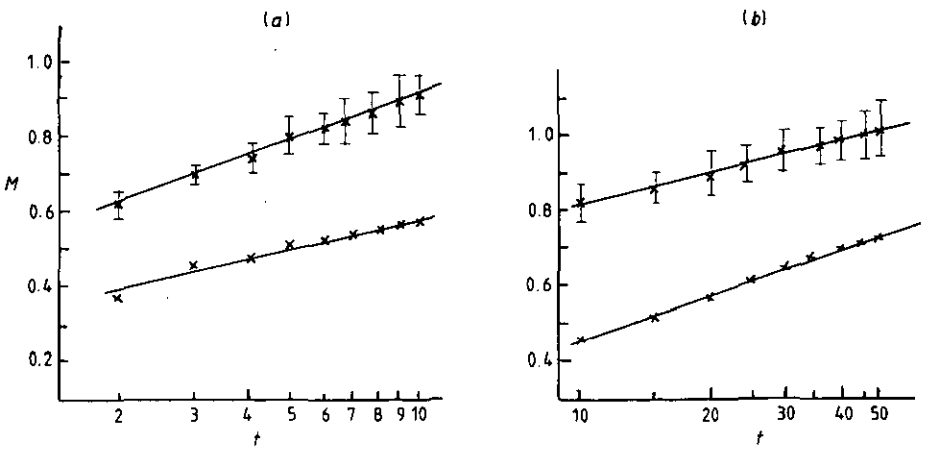

Figure 3. Plot of $M = \ln(-\ln(M(t)/M(0)))$, in arbitrary units, against $\ln t$ showing the exponential character of the CA curves. 3D, $x = 0.6$. Upper curves $\tau = 0.1$, lower curves $\tau = 0.5$. (*a*) Initial stage $2 \leq t \leq 10$; (*b*) longer times $10 \leq t \leq 50$. The error bars are confidence limits estimated from the observed scatter after 10 averaging.

where a and b are functions of x and τ. In 3D we get the short time estimate ($t < 10\rho J^{-1}$)

$$a = -0.16 + 0.42x - 0.29x^2 + (2.79 - 8.63x + 7.52x^2)\tau - (2.26 - 8.77x + 8.15x^2)\tau^2 \tag{10}$$

$$b = 1 - \frac{(1.2 - 7.25x + 14.3x^2)\tau}{\tau^2 + (1 - 5.75x + 11.56x^2)\tau + 0.23 - x + x^2} = 1 - \mathfrak{B}. \tag{11}$$

The initial relaxation may then be approximated by

$$M(t) \propto \exp(-at)(1 - at^{\mathfrak{B}} + \dots). \tag{12}$$

Hence at the early time steps the relaxation has a Debye-type character with the constant a given by (10). For $t > 10\rho J^{-1}$ we have

$$a = \frac{0.02}{x^{4.5}} + \frac{0.136}{x^{2.7}}\tau^2 \tag{13}$$

$$b = 1 - \frac{56x^3\tau}{\tau^2 + 64x^3\tau + 0.01(4.18 - 23x^2)}. \tag{14}$$

Since $a > 0$ the asymptotic behaviour of $M(t)$ changes when b changes sign: for $t \to \infty$ and $b > 0$ $\exp(-at^b) \to 0$ indicating relaxation to a non-magnetic state, while for $t \to \infty$ and $b < 0$ $\exp(-at^b) \to 1$ and the final state is magnetized. It is therefore possible to use the equation $b(x, \tau) = 0$ to estimate the critical temperature, τ_c, for the transition to a magnetic state as a function of x:

$$\tau_c = 0.5(8x^3 + \sqrt{64x^6 + 0.25(4.18 - 23x^2)}). \tag{15}$$

The threshold concentration, below which $\tau_c = 0$, is $x_c \simeq 0.321$ and agrees well with the estimation of Reeve and Betts (1975). The phase diagram is shown in figure 4.

In 2D, assuming the same exponential behaviour, equation (9), we get

$$a = 0.0275x^{-0.5} + (9.28x^2 + 0.558)^{-1}\tau^2 \tag{16}$$

$$b = 1 + \frac{(0.158 - 1.495x + 0.575x^2)\tau}{\tau^2 - (0.722 - 2.08x - 0.1x^2)\tau + 0.076 + 0.338x - 0.71x^2}. \tag{17}$$

Again the initial relaxation is given by (12) but with different values of $\mathfrak{B}$ and a. More specifically, $a_{2D} > a_{3D}$ while $\mathfrak{B}_{2D} < \mathfrak{B}_{3D}$, which indicates faster initial relaxation in 2D.

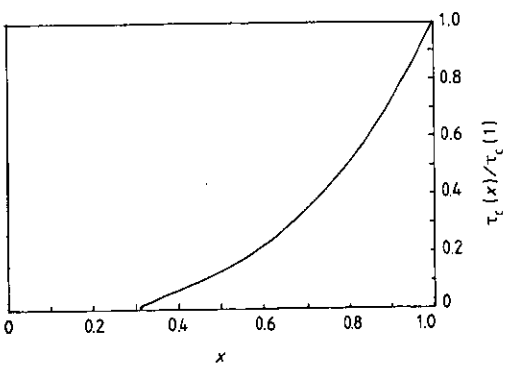

Figure 4. Phase diagram in 3D.

Here, as expected, $\tau_c = 0$ for all concentrations and the system relaxes always to a non-magnetic state.

The agreement between the cellular automata (z) and 'analytic' (y) curves were additionally checked by calculating their correlation coefficient

$$r = \sigma_{zy}(\sigma_{zz}\sigma_{yy})^{1/2} \tag{18}$$

where

$$\sigma_{zy} = \langle zy \rangle - \langle z \rangle \langle y \rangle. \tag{19}$$

The obtained values of r are higher for larger concentrations. At $x = 0.6$, $r = 0.896$ for $\tau = 0.1$ and $r = 0.892$ for $\tau = 0.5$ while at $x = 0.2$, $r = 0.875$ for $\tau = 0.1$ and $r = 0.617$ for $\tau = 0.5$.

4. Concluding remarks

We have presented relaxation curves of the initially magnetized state in 2D and 3D obtained via the cellular automata approach. From these curves we have 'guessed' the analytic formulae from which the phase diagram of figure 4 was constructed. It agrees with the one obtained earlier by Reeve and Betts (1975), giving a similar value for x_c and supporting the conjecture that $\tau_c(x)$ intersects the x axis with a finite slope. There is however a difference—our curve is concave while theirs was rather a straight line.

The very interesting question of finding the concentration threshold in 2D at which the Kosterlitz-Thouless transition appears, cannot be answered by the present approach since we have calculated only the magnetization.

For $x < x_c$ the relaxation is fast and therefore it is better described by (9) with a and b found from (10) and (11) rather than from (13) and (14).

Our system is macroscopically homogeneous since the dilution is random and there is no correlation among the vacancies. Initially all spins were aligned by the external field and then left to relax in the (macroscopically) same way. Therefore there are no propagating modes. A similar situation is encountered in the physics of phonons (see e.g. Petru 1987).

We had to consider small samples; 10^3 in 3D and 31^2 in 2D. Averaging was typically over 30 initial configurations—more for small x where the scatter was larger and less for larger x. The reason for such drastic limitations was the lack of fast computers. Increasing the computation time on our IBM AT computer by, say, ten hours, which we did in some cases for checking, did not improve drastically the quality of the results. More specifically, increasing the size of our system from 10^3 to 12^3 changed the value of $M(t = 10)$ by less than 0.5%. The change when the averaging was increased from 10 to 20 (for $x = 0.6$ and $\tau = 0.5$, which is a typical value with medium scatter) was less than 2%. The difference was even smaller when the time step, Δt, was decreased fourfold, to $\Delta t = 0.01 pJ^{-1}$. Finally, increasing twice the division of the angle α produced results identical to the previous ones up to four significant digits. Hence we decided to leave them at this level. It should however be stressed that our $M(t)$ curves are not smooth, the analytic equations are not unique and therefore (15) is only approximate. We hope this shows a way to calculate the relaxation properties of the diluted XY model.

Acknowledgments

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