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Diffusion in the one-dimensional Ising model

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Abstract. The critical dynamics of the one-dimensional Ising system with conserved magnetisation is studied by the real-space renormalisation group approach. The relaxation of odd and even spin-operator perturbations is calculated. The critical exponent obtained by an exact transformation is $z = 3$ in agreement with the conventional theory.

1. Introduction

Recent progress in the understanding of critical dynamics has been made by using the renormalisation group (RG) technique (Hohenberg and Halperin 1977). Most of the RG works are based on the Glauber model (Glauber 1963) and its generalisations. This model describes an Ising spins system, $\sigma_i = \pm 1$. The spins are assumed to flip independently in time with rates which are chosen to guarantee the ergodicity of the system. This model is purely relaxational and relaxes via an interaction with the heat bath. The continuum version of this model (Myerson 1976) was also generalised to describe conserved quantities and has been studied extensively since 1972 using the ϵ expansion around four and six dimensions (Halperin *et al* 1972, Hohenberg and Halperin 1977).

It is only in the last year that the real-space static RG technique (Niemeijer and van Leeuwen 1976) was generalised to the study of critical dynamics (Achiam and Kosterlitz 1978, Achiam 1978a, b, 1979a, b, c, d, Kinzel 1978, Mazenko *et al* 1978, Suzuki *et al* 1979, Chui *et al* 1979, Shiwa preprint). All of these works are based on the original Glauber model, and none of them include conserved quantities. Thus our knowledge of the critical dynamics of low-dimensional systems is restricted to only one universality class: the Ising system with non-conserved quantities.

In this work we are studying another dynamical universality class: the dynamics of an Ising system with a conserved magnetisation. The corresponding model with the continuum spin was studied by Halperin *et al* (1974) using the ϵ-expansion technique. They called this model 'model B' and found that the dynamic exponent, z, which characterises the dependence of the relaxation rate of the order parameter upon the correlation length is $z = 4 - \eta$ to all order of ϵ, where η, as well as other static exponents, have their standard definitions, e.g. Stanley (1971). This result is the one suggested by the conventional theory of van Hove (1954), and is expected to hold in all dimensions.

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However, the ϵ expansion itself is not valid for low dimensions, hence the generalisation of the above result to low-dimensional systems is not trivial at all.

In order to do it we started with a model in which the order parameter is conserved which was suggested by Kawasaki (1966). However, as we shall see in this paper, this model describes a mechanism of relaxation which is irrelevant in the RG sense. We studied a similar model which includes the model of Kawasaki as a special case. We applied the real-space time-dependent renormalisation group (TRG) approach to a one-dimensional Ising system which relaxes according to this model. We found that the conventional theory is correct for this universality class, a result which is not surprising.

The paper is organised as follows. In § 2, we represent the kinetic model and review the TRG technique. In § 3, we perform the transformation of the master equation using the decimation transformation. From the transformation we find the dynamic exponent z. In § 4, we discuss the results.

2. The model, the method and the notations

2.1. *The kinetic model*

This model describes the time-dependent behaviour of a large interacting spin system whose equilibrium is determined by an Ising Hamiltonian. The system is brought to a constrained equilibrium state. Then, at the time $t=0$ the constraint is removed, and the system relaxes towards the final equilibrium via an interaction with a heat bath which is not treated explicitly. The relaxation is not a total free relaxation as in the Glauber model (1963) but is restricted to conserve the total magnetisation. We assume the relaxation to be an instantaneous random spin-exchange transformation between two spins. This procedure can be described by an empirical master equation for the spin probability distribution, $P(\{\sigma\}, t)$, and a bare time scale, τ, of a spin system $\{\sigma = \pm 1\}$ as follows:

$$\begin{aligned}
&\tau \, \mathrm{d}P(\{\sigma\}, t)/\mathrm{d}t \\
&\quad = -\frac{1}{N}\Big[\sum_{ij} W_{ij}(\sigma_1, \ldots, \sigma_i, \ldots, \sigma_j, \ldots, \sigma_n) P(\sigma_1, \ldots, \sigma_i, \ldots, \sigma_j, \ldots, \sigma_n, t) \\
&\quad\quad - \sum_{ij} W_{ij}(\sigma_1, \ldots, \sigma_j, \ldots, \sigma_i, \ldots, \sigma_n) P(\sigma_1, \ldots, \sigma_j, \ldots, \sigma_i, \ldots, \sigma_n, t)\Big] \\
&\quad \equiv L(\sigma) P(\sigma, t) \equiv -\frac{1}{N} \sum_{ij} (1 - p_{ij}) W_{ij}(\sigma) P(\sigma, t)
\end{aligned} \tag{2.1}$$

where p_{ij} is a spin-exchange operator:

$$p_{ij} f(\sigma_1, \ldots, \sigma_i, \ldots, \sigma_j, \ldots, \sigma_n) = f(\sigma_1, \ldots, \sigma_j, \ldots, \sigma_i, \ldots, \sigma_n),$$

and the transition probability, W_{ij}, satisfies the detailed balance which ensures the ergodicity of the system:

$$(1 - p_{ij}) W_{ij}(\sigma) P_{\mathrm{e}}(\sigma) = 0, \tag{2.2}$$

and N is the number of lattice points.

The final equilibrium state, $P_{\mathrm{e}}(\sigma) \equiv P(\sigma, t=\infty)$ is given by a reduced Ising-like Hamiltonian, $\bar{H}$,

$$P_{\mathrm{e}}(\sigma) = \exp(-H/k_{\mathrm{B}}T) \equiv \exp(\bar{H})/Z \tag{2.3}$$

where the partition function Z normalises P_e,

$$\sum_{\{\sigma\}} P_e = 1. \tag{2.4}$$

The reduced Hamiltonian which is studied in this work is the usual nearest-neighbour (NN) Ising Hamiltonian,

$$\bar{H} = K \sum_i \sigma_i \sigma_{i+1}. \tag{2.5}$$

The master equation (2.1) can be written in a slightly different form:

$$\tau \, \mathrm{d}P(\sigma, t)/\mathrm{d}t = -\mathscr{L}\phi(\sigma, t) \tag{2.6}$$

where $\phi(\sigma, t)$ measures the deviation from equilibrium,

$$\phi(\sigma, t) \equiv P(\sigma, t)/P_e(\sigma). \tag{2.7}$$

From equation (2.2) we can see that $\mathscr{L}$ is given by

$$\mathscr{L} \equiv \sum_{ij} \mathscr{L}_{ij} \qquad \mathscr{L}_{ij} = -\frac{1}{N} P_e W_{ij}(\sigma)(1 - p_{ij}). \tag{2.8}$$

The relation (2.2) does not determine W_{ij} uniquely. We will use (Achiam and Kosterlitz 1978, Achiam 1978b, 1979a, b, c)

$$W_{ij}(\sigma_i\sigma_j) = [P_e(\sigma_1, \ldots, \sigma_j, \ldots, \sigma_i, \ldots, \sigma_n)/P_e(\sigma_1, \ldots, \sigma_i, \ldots, \sigma_j, \ldots, \sigma_n)]^{1/2}. \tag{2.9}$$

There is no *a priori* correlation between i and j. This is in contrast to the kinetic model of Kawasaki (1966) which assumes that i and j are nearest neighbours.

2.2. *The time-dependent* RG *transformation*

The time-dependent RG transformation is a transformation of the master equation (2.6) to a similar master equation which is defined on a scaled coordinate–time space. The transformation is performed in two steps:

2.2.1. The coordinate-space scaling. The kinetic equation (2.6) of the probability distribution of a set $\{\sigma\}$ is transformed to a new kinetic equation of a new probability distribution of a set of spin variables. The new spin variables, $\mu_\alpha = \pm 1$, are defined on a lattice with the same symmetry as the first one, but whose lattice constant is enlarged by a factor of b. The transformation is of the form

$$f'(\mu) = \sum_{\{\sigma\}} T(\mu, \sigma) f(\sigma) \tag{2.10}$$

and is applied to the two sides of equation (2.6). T is subject to the following conditions:

(i) $$\sum_{\{\mu\}} T(\mu, \sigma) = 1 \tag{2.11}$$

(ii) $$T(\mu, \sigma) \geq 0 \tag{2.12}$$

(iii) The transformation should not change the symmetry of the lattice.

T is time-independent. Hence the result of the transformation of the LHS of equation (2.6) is just the static RG transformation,

$$P'(\mu) = \sum_{\{\sigma\}} T(\mu, \sigma) P(\sigma). \tag{2.13}$$

The probability distribution can be represented in the parameter space $\boldsymbol{K} = \{K_a\}$ of the interactions appearing in $\bar{H}$ (see 2.3). Due to the conditions which T fulfil, the static RG transformation can be represented as a transformation of the parameter space

$$\boldsymbol{K}' = R\boldsymbol{K} \tag{2.14}$$

where $\boldsymbol{K}' = \{K'_a\}$ are the interactions of $P'(\mu)$. The fixed point of this transformation

$$\boldsymbol{K}^* = R\boldsymbol{K}^* \tag{2.15}$$

is associated with a critical point (or with zero correlation) (Wilson and Kogut 1974).

The transformation of the RHS of (2.6) is analysed in a similar way. The operator $\mathscr{L}$ depends on P via (2.8) and (2.9). Thus the transformation of P to P' determines the transformation of $\mathscr{L}(\sigma)$ into $\mathscr{L}'(\mu)$. The perturbation ϕ is represented in the parameter space by $\boldsymbol{h}$, the fields adjoint to the spin operators $\boldsymbol{O}(\mu)$,

$$\phi(\sigma) = 1 + (\boldsymbol{h} \cdot \boldsymbol{O}(\mu)). \tag{2.16}$$

Using this notation, the transformation of the RHS of (2.6) is

$$-\mathscr{L}'[(\boldsymbol{\Omega h}) \cdot \boldsymbol{O}(\mu)]. \tag{2.17}$$

Thus under the position transformation (2.6) becomes

$$\tau P'_e(\mu)\, \mathrm{d}/\mathrm{d}t\, [\boldsymbol{h} \cdot \boldsymbol{O}(\mu)] = -\mathscr{L}'[(\boldsymbol{\Omega h}) \cdot \boldsymbol{O}(\mu)] \tag{2.18}$$

where $\boldsymbol{h}' = \boldsymbol{\Lambda h}$ is the static RG transformation of the parameters $\boldsymbol{h}$.

2.2.2. The time scaling. Suppose that $\boldsymbol{\Lambda}$ and $\boldsymbol{\Omega}$ are scalars λ and ω. In such case the transformation

$$\tau' = b^z \tau \tag{2.19}$$

where

$$b^z = \lambda/\omega \tag{2.20}$$

will return the transformed kinetic equation to the form of (2.6). The standard RG suppositions identify z as the dynamic exponent. The RG suppositions, as well as their application to the case where $\boldsymbol{\Lambda}$ and $\boldsymbol{\Omega}$ are two non-commuting matrices, are discussed elsewhere (Achiam 1978b, 1979a, Achiam and Kosterlitz 1978 and unpublished report).

3. The time-dependent RG transformation

To perform the TRG of the model described by equations (2.3), (2.5), (2.6), (2.8) and (2.9) we have to know ϕ which is given by (2.7). However, this is equivalent to having the solution of (2.6), which we do not know. We can overcome this problem by using the ideas of the RG approach. It is sufficient to examine ϕ which spans only a subspace of the parameter space, as long as this subspace is invariant under the TRG transformation and gives the slowest relaxation. (Achiam 1979a, Achiam and Kosterlitz unpublished report). There are two families of such subspaces: perturbations which are even under spin reversal, and perturbations which are odd under spin reversal.

In this section we shall study the TRG of the even perturbations: the invariant subspace of the energy perturbation

$$\phi_1 = 1 + h_1 \sum_i (\sigma_i\sigma_{i+1} - \langle\sigma_i\sigma_{i+1}\rangle). \tag{3.1}$$

The odd subspace which gives a faster relaxation will be discussed in the appendix. According to the discussion in the previous section, we first have to perform the static RG of P_e and ϕ_1. The RG transformation we choose is the decimation transformation which scales the coordination space by a factor of $b = 3$ (Nelson and Fisher 1976). That is, T is given by

$$T = \prod_j \delta(\mu_j - \sigma_{3j}). \tag{3.2}$$

The calculation is easily done with the normalised probability distribution

$$P_e = \tfrac{1}{2}\prod_k P_e^k \qquad P_e^k \equiv \tfrac{1}{2}(1 + \zeta\sigma_k\sigma_{k+1}) \tag{3.3}$$

where

$$\zeta = \tanh K. \tag{3.4}$$

The RG transformation can be performed in each cell, j, which contains the σ_k, $k = 3j, 3j+1, 3j+2$, independently of the other cells. The result of the transformation is

$$P_e'^j(\mu_j, \mu_{j+1}) = \tfrac{1}{2}(1 + \zeta^3\mu_j\mu_{j+1}) \tag{3.5}$$

or, in the parameter space representation,

$$\zeta' = \zeta^3. \tag{3.6}$$

Equation (3.6) is not expressed in the usual form (2.14). However, this form can be achieved by expanding ζ in $\delta\zeta = \zeta - \zeta^*$ around the fixed-point solution $\zeta^* = 1$:

$$(\delta\zeta)' = 3\delta\zeta. \tag{3.7}$$

Going back to equation (3.1) and performing a few arithmetic steps, one can see that the perturbation field h_1 is also scaled according to (3.7). Thus we get $\lambda = 3$.

The calculation of the RG transformation of the RHS of (2.6) is more tedious. Before doing it, it is worth expressing the RHS explicitly. Evaluating the operator $1 - p_{ij}$ gives

$$(1 - p_{ij})\phi = h(\sigma_i - \sigma_j)(\sigma_{i-1} + \sigma_{i+1} - \sigma_{j-1} - \sigma_{j+1}). \tag{3.8}$$

The other factor which appears in $\mathscr{L}_{ij}$ is $W_{ij}P_e$. From (2.9), it follows that this quantity is invariant to permutations of σ_i and σ_j. Now, since equation (3.8) vanishes unless

$$\sigma_i = -\sigma_j \tag{3.9}$$

we can see that $\mathscr{L}_{ij}$ is independent of the spins σ_i and σ_j. We can now use (2.5), (2.9) and (3.9) to express W_{ij} as

$$W_{ij} = \exp\{-K[\sigma_i(\sigma_{i+1} + \sigma_{i-1}) + \sigma_j(\sigma_{j+1} + \sigma_{j-1})]\} \tag{3.10}$$

(if i and j are NN, the multiples terms have to be omitted). Multiplying P_e by W_{ij} results in the vanishing of the interactions around σ_i and σ_j. This is indicated in figure 1 by the

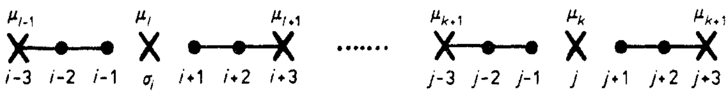

Figure 1. The configuration of spins that appear in $\mathscr{L}_{ij}$ whose RG transformation is studied in equations (3.11)–(3.17). The dots are the spins which are summed up while the X are the spins which become the new μ variables. The interactions which are cancelled in P_e by W_{ij} do not appear in the figure, while the other interactions are marked by a full line.

absence of the full line between the corresponding lattice points. For example, the configuration of i and j marked in figure 1 contributes to $P_e W_{ij}$

$$P_e W_{ij} \sim \frac{1}{Z} \exp[K(\sigma_{i-3}\sigma_{i-2} + \sigma_{i-2}\sigma_{i-1} + \sigma_{i+1}\sigma_{i+2} + \sigma_{i+2}\sigma_{i+3} + \sigma_{j-3}\sigma_{j-2}$$
$$+ \sigma_{j-2}\sigma_{j-1} + \sigma_{j+1}\sigma_{j+2} + \sigma_{j+2}\sigma_{j+3})]. \tag{3.11}$$

We shall now apply the RG transformation to the configuration illustrated in figure 1. The trace over a typical σ_n contributes two kinds of terms:

$$\operatorname*{Tr}_{\sigma_n} \exp(K\sigma_n\sigma_m) = 2\cosh K \xrightarrow[K\to\infty]{} e^K \tag{3.12a}$$

and

$$\operatorname*{Tr}_{\sigma_n} \sigma_n \exp(K\sigma_n\sigma_m) = 2\sigma_m \sinh K \xrightarrow[K\to\infty]{} \sigma_m e^K. \tag{3.12b}$$

In figure 1 we chose the σ_i and σ_j to be the new μ_l and μ_k variables where $i = 3l$ and $j = 3k$. Thus, the final contribution of (3.8) and (3.11) is

$$\exp(8K)(\mu_l - \mu_k)(\mu_{l-1} + \mu_{l+1} - \mu_{k-1} - \mu_{k+1}). \tag{3.13}$$

The other part of $P_e(\sigma)$ is of the spins before $i-3$, after $j+3$ and between $i+3$ and $j-3$. It gives the usual static RG transformation to the corresponding terms in $P'_e(\mu)$. Thus, using (3.10) this factor can be written as

$$P'_e(\mu) W_{lk}(\mu_l, \mu_k) \frac{1}{A^4} \tag{3.14}$$

where

$$A = [(e^{3K} + 3e^{-K})(e^{-3K} + 3e^K)]^{1/2} \xrightarrow[K\to\infty]{} 3^{1/2} e^{2K} \tag{3.15}$$

is the contribution to the partition function from the block $i \to i+3$ which is not included in (3.13). The RG transformation results through the combination of (3.14) with (3.13). Summing over all values of $i = 3l$ and $j = 3k$ gives

$$(1/9N) \sum_{lk} P'_e(\mu) W_{lk}(1 - p_{lk})\phi(\mu) = \tfrac{1}{27} \mathscr{L}'(\mu)\phi(\mu) \tag{3.16}$$

and thus

$$\omega_1 = 1/3^3. \tag{3.17}$$

There are three other kinds of contributions. If both σ_i and σ_j do not appear in T, (3.2), and are summed up in the trace, then

$$\sum_{\sigma_i\sigma_j} P_e W_{ij}(\sigma_i - \sigma_j) = 0 \tag{3.18}$$

because $P_e W_{ij}$ is independent of σ_i and σ_j. If only one of them, say i, becomes a μ variable under the RG transformation, then the two configurations of i and j drawn in figure 2 give

$$2\mu_l(\mu_{l+1}+\mu_{l-1}-\mu_k-\mu_{k-1})P'_e W_{lk}\exp(K\mu_k\mu_{k-1})\,e^{5K}/A^3. \tag{3.19}$$

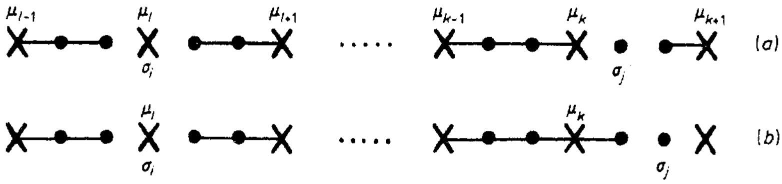

Figure 2. The configuration of the spins that appear in $\mathscr{L}_{ij}$ whose RG transformation is studied in equation (3.19). The notations are as in figure 1.

The extra exponent can be expanded, leading to three typical terms. One is a term similar to (3.14). Collecting this contribution and (3.16) gives $\omega = 1/3^2$. The other terms are proportional to $W_{lk}\mu_l\mu_k$, are invariant under the RG and are also scaled according to $\omega = 1/3^2$.

In all the terms which have been discussed above i and j were far enough apart. If we examine other configurations where i and j are less than six lattice constants apart, we see that the RG transformation contributes terms which vanish as $K\to\infty$. This case was studied by Kawasaki (1963). In his model he assumed i and j to be NN (see figure 3). The RG transformation of this term result with

$$P'_e(\mu)W_l(\mu)2\mu_l(\mu_{l-1}-\mu_{l+1})\,e^{3K}/A^2 \tag{3.20a}$$

$$P'_e(\mu)W_l(\mu)2\mu_l(\mu_{l+1}-\mu_{l-1})\,e^{3K}/A^2 \tag{3.20b}$$

where $W_l = \exp[-K\mu_l(\mu_{l+1}+\mu_{l-1})]$. These two contributions mutually cancel and thus do not contribute to the transformed kinetic equation.

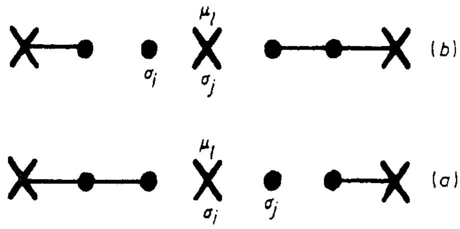

Figure 3. The configurations of the spins that appear in $\mathscr{L}_{ij}$ whose RG transformation is studied in equation (3.20a, b). The notations are as in figure 1.

4. Discussion

In the previous section we calculated the scale factors for the even perturbation, and found

$$\omega = \tfrac{1}{9} \qquad \lambda = 3. \tag{4.1}$$

Employing equation (2.20) we get the dynamic exponent

$$z = 3. \tag{4.2}$$

For the Ising model in one dimension $\eta = 1$, and hence (4.2) can be written as

$$z = 4 - \eta. \tag{4.3}$$

This is exactly as predicted by the conventional theory (van Hove 1954). This theory does not predict any anomaly in the transport coefficient. Thus the diffusion constant vanished as $\xi^{-2+\eta}$ where ξ is the correlation length which diverges at the critical point. From the conservation of the order parameter we can see that the relaxation rate varies as

$$\omega_m^r \sim \xi^z. \tag{4.4}$$

It is known (Kawasaki 1966) that the conventional theory value is an upper limit of z. Here we found that the z is actually at this upper limit. This result is expected from the study of a similar conserving model near four dimensions using the ϵ expansion (Halperin *et al* 1974). Due to the fact that in one dimension the RG transformation can be performed exactly, our result here is exact.

The RG calculation which was performed in this paper sheds light on the mechanism governing the slowing down of the order parameter relaxation. The model of Kawasaki suggests that the conservation mechanism is of a short-range nature, i.e. the spins which exchange their values are nearest neighbours. We found that this mechanism is irrelevant in the RG sense, and that the leading mechanism is of long range.

In this paper we also examine the result of the effective antiferromagnetic perturbation as represented by the odd subspace of spin perturbations. The result presented in the appendix shows that the antiferromagnetic perturbation relaxes faster than the energy perturbation.

Appendix

The antiferromagnetic-like perturbation

$$\phi_2 = 1 + h_2 \sum_j (-1)^j \sigma_j \tag{A1}$$

is a perturbation which conserves magnetisation. Thus we must check whether it yields a slower relaxation than that of the energy like perturbation ϕ_1 (3.1). Each of the two perturbations, ϕ_1 and ϕ_2, form an invariant parameter subspace of the kinetic equation (2.1). Thus we can study each of them separately. In this appendix we shall calculate the z_a corresponding to ϕ_2 and find it to be smaller than (4.2).

Using the decimation in $b = 3$ blocks (3.2), we find the recursion relation

$$h_2' = h_2\{1 + 2[\exp(-4K) - 1][\exp(-4K) + 3]^{-1}\}. \tag{A2}$$

At the fixed point $K = \infty$

$$\lambda = \tfrac{1}{3}. \tag{A3}$$

The rules for calculating the contributions of different configurations of i and j to the renormalisation of the RHS of (2.6) are the same as for the energy perturbation. Thus, the configuration of figure 1 in which $i = 3l$ and $j = 3K$, and are far enough apart, contribute a functional form which is similar to (3.16), with the factor

$$\exp(8K)/A^4 \xrightarrow[K \to \infty]{} \tfrac{1}{9}. \tag{A4}$$

Thus we obtain $\omega=\frac{1}{9}$ and $\omega/\lambda=\frac{1}{3}$, which results in

$$Z_a=1. \tag{A5}$$

As in the energy perturbation case, the other configurations contribute to the RG transformation terms which vanish close to the fixed point. We thus obtain the same phenomenon we found for the energy-like perturbation. The relevant conservation mechanism is of long range. However, the antiferromagnetic-like perturbation relaxes faster than the energy-like perturbation. The slowest time scale is that of the energy-like perturbation, $Z=3$.

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