# CRITICAL SLOWING DOWN AND NONLINEAR RESPONSE IN AN EXACTLY SOLVABLE STOCHASTIC MODEL

# TH.W. RUIJGROK and J.A. TJON

Instituut voor Theoretische Fysica, Rijksuniversiteit te Utrecht, Utrecht, Nederland

### Received 2 November 1972

## **Synopsis**

The master equation for a stochastic Ising model with long-range interaction is studied and the spectrum of the transition matrix is solved exactly in the limit of an infinite system. The model is then used to illustrate critical slowing down, nonlinear response, macroscopic equations and fluctuations outside equilibrium.

1. Introduction. The main purpose of the present paper is to study fluctuations and response in a nonlinear system, especially near the critical temperature. In order to do so we choose a spin system similar to that of Griffiths, Weng and Langer<sup>1</sup>), for which the molecular-field approximation is exact. Although this approximation has been used<sup>2</sup>) to describe the slowing down of relaxation near the critical temperature, no attempt has been made to solve the master equation, other than for a one-dimensional system<sup>3</sup>) or in a high-temperature expansion<sup>4</sup>).

For the present model<sup>1</sup>), in which each spin has an equally strong Ising interaction with any other spin, it is possible to give an exact solution of the master equation in the limit of an infinite number of spins (section 4). This solution is then used to find the critical exponents arising in the calculation of autocorrelation functions of magnetization and energy. The results are described in section 5. In addition, however, the model provides another example<sup>5</sup>) where a systematic method due to Van Kampen<sup>5</sup>) leads to the proper macroscopic equation and the correct (i.e. linear Fokker-Planck) equation, describing fluctuations in a non-linear system, also outside equilibrium. These equations are derived and discussed in section 6 and compared with Kubo's theory<sup>6</sup>) of linear response. The effect of nonlinearity on the critical slowing down is calculated.

Preliminaries are given in section 2, where the equilibrium properties are derived and in section 3, where the master equation as given by Glauber<sup>7</sup>), is written in a simplified form.

2. Equilibrium. Consider a system of N particles with spin one half in an external magnetic field B and with a ferromagnetic Ising pair interaction, which is the same for each pair and has a strength inversely proportional to N. The hamiltonian for this system is

$$H = -(J/2N) M^2 - \mu BM, \tag{2.1}$$

where  $M = \sum_{j=1}^{N} \sigma_j^z$  is twice the z component of the total spin and  $\mu$  is the magnetic moment of each particle. The partition function can be written in the form  $Z = \sum_{M=-N}^{N} Z(M)$  with  $\Delta M = 2$  and

$$Z(M) = F(M) e^{(K/2N) M^2 + HM}, (2.2)$$

where

$$F(M) = \frac{N!}{\left[\frac{1}{2}(N+M)\right]! \left[\frac{1}{2}(N-M)\right]!},$$
(2.3)

is the number of states with a given M,  $K = \beta J$  and  $H = \beta \mu B$ . A dimensionless temperature is defined by T = 1/K.

The value of  $M = Nm_{eq}$  for which Z(M) attains an extremum can be easily derived. We obtain the following equation for  $m_{eq}$ 

$$m_{\rm eq} = \tanh X(m_{\rm eq}), \tag{2.4}$$

with

$$X(m) = Km + H. (2.5)$$

It can be shown in the usual way that for zero field there is a critical temperature at  $K = T_c = 1$ . Above this temperature eq. (2.4) has only one solution  $m_+$ , corresponding to the stable equilibrium state. For  $T < T_c$  there is a critical field

$$H_{c} = [K(K-1)]^{\frac{1}{2}} - \ln [K^{\frac{1}{2}} + (K-1)^{\frac{1}{2}}], \qquad (2.6)$$

such that for  $0 < H < H_c$  eq. (2.4) has two additional solutions,  $m_-$  corresponding to the metastable state and  $m_0$ , giving an unstable equilibrium. The static susceptibility per spin can be calculated from  $m_+$  and we obtain

$$\frac{\chi}{\mu^2 \beta} = \frac{\mathrm{d}m_+}{\mathrm{d}H} = \frac{1 - m_+^2}{1 - K(1 - m_+^2)}.$$
 (2.7)

In the neighbourhood of the critical temperature we have for H = 0

$$\chi(T)/\mu^2\beta \approx 1/2 \, (T_c - T)$$
 for  $T \leqslant T_c$   
and  $\chi(T)/\mu^2\beta \approx 1/(T - T_c)$  for  $T \geqslant T_c$ . (2.8)

Fluctuations in the magnetic moment are related to the static susceptibility by

$$\overline{M^2} - \overline{M}^2 = N \frac{\mathrm{d}m_+}{\mathrm{d}H} = \frac{N\chi}{\mu^2 \beta}.$$
 (2.9)

In the same way the fluctuations in the total energy are given by

$$\overline{E^2} - \bar{E}^2 = \frac{NC_H}{k\beta^2} = \frac{N}{\beta^2} (Km_+ + H)^2 \frac{\mathrm{d}m_+}{\mathrm{d}H}, \qquad (2.10)$$

where  $C_H$  is the specific heat at constant magnetic field. In figs. 1, 2 and 3 we have plotted the magnetization  $m_+$ , the inverse  $(\chi/\mu^2\beta)^{-1}$  of the static susceptibility and the specific heat  $C_H/k$ , all for  $h = \mu B/J = 10^{-3}$ , as a function of the temperature. Observe that the limits  $T \to T_c$  and  $h \to 0$  may not be interchanged, since

$$\lim_{h \to 0} \lim_{T \to T_c} (C_H/k) = 1 \quad \text{and} \quad \lim_{T \to T_c} \lim_{h \to 0} (C_H/k) = 1.5. \tag{2.11}$$

In closing this section on equilibrium properties we want to remark that, in order to see the phase transition occur in a very small temperature interval, an unexpectedly large number of spins must be present. This was already shown for another spin system with long-range interaction by Kittel and Shore<sup>8</sup>). In our case this can be seen in figs. 1-3, where the corresponding quantities have also been plotted for N = 10000 and N = 20000. From these figures it should be clear that,

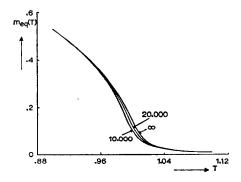
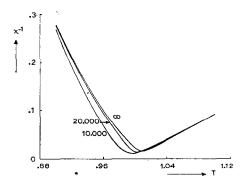


Fig. 1. Magnetization for  $h = 10^{-3}$ , N = 10000, 20000 and  $\infty$  in the interval  $0.9 \le T \le 1.1$ .

in order to perform a numerical calculation of a phase transition, which is to be correct to within a few millidegrees of the transition temperature, one should take more than 100000 spins. Since this is a prohibitively large number for the numerical solution of the equations, which describe the nonequilibrium behaviour of a large spin system, asymptotic methods must be used for this case. These will be explained in sections 3 and 4.



2.4 C<sub>H</sub>
1.6
1.000
0.88
1.96
1.04
1.12

Fig. 2. Inverse susceptibility for  $h = 10^{-3}$ , N = 10000, 20000 and  $\infty$  in the interval  $0.9 \le T \le 1.1$ .

Fig. 3. Specific heat for  $h = 10^{-3}$ , N = 10000, 20000 and  $\infty$  in the interval  $0.9 \le T \le 1.1$ .

3. The stochastic equations. We consider a spin system in interaction with a heat bath at temperature T. A complete dynamical treatment including all degrees of freedom of this heat bath (e.g. a harmonic lattice) is out of the question and also not desired for a macroscopic description of the spin system alone. For these reasons the time dependence of the spin system is described by a stochastic process. In order to keep this process as simple as possible we choose the transitions such that in each step only one spin flips from up  $(\sigma = +1)$  to down  $(\sigma = -1)$  or vice versa. The transition probability per unit time  $w_M(\sigma_j)$  for the change  $\sigma_j \to -\sigma_j$ , when the total spin is  $M = \sum_j \sigma_j$ , will be chosen such that detailed balance is satisfied. This means that

$$w_{M}(\sigma_{j}) P_{eq}(\{\sigma_{l}\}) = w_{M'}(-\sigma_{j}) P_{eq}(\{\sigma_{l}\}),$$
(3.1)

where  $M' = M - 2\sigma_j$  and  $\{\sigma'_i\}$  differs from  $\{\sigma_i\}$  only in that the jth spin is flipped. The equilibrium spin distribution is

$$P_{\rm eq}(\{\sigma_l\}) = Z^{-1} \exp\left[ (K/2N) M^2 + HM \right]. \tag{3.2}$$

One choice for the transition probability which satisfies eq. (3.1) is

$$w_{M}(\sigma_{i}) = \exp\left[-\sigma_{i}X(M/N)\right],\tag{3.3}$$

where X(m) is given by eq. (2.5). This choice is not unique and it differs for example from the function taken in ref. 1 and by Suzuki and Kubo<sup>2</sup>). As a consequence we shall find that in the macroscopic equation the nonlinear effects are different for the two cases. As long, however, as the transition probability only depends on the total spin and on the spin under consideration, the particular form of  $w_M(\sigma_i)$  will not influence our discussion.

In terms of the transition probabilities the master equation can be written in the form

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\{\sigma_i\}, t) = \sum_{l=1}^{N} w_{M'}(-\sigma_j) P(\{\sigma_l\}, t) - P(\{\sigma_l\}, t) \sum_{l=1}^{N} w_{M}(\sigma_j). \tag{3.4}$$

The probability  $P(\sigma_1, ..., \sigma_N, t)$  to find the spin system at time t in the state  $|\sigma_1 \cdots \sigma_N\rangle$  has the property that it approaches  $P_{eq}(\sigma_1, ..., \sigma_N)$  for  $t \to +\infty$ . Eq. (3.4) can be written in a simplified form when we introduce the state

$$|P(t)\rangle = \sum_{\{\sigma_j\}} P(\sigma_1, \dots, \sigma_N, t) |\sigma_1 \cdots \sigma_N\rangle.$$
 (3.5)

Then (3.4) becomes

$$\frac{\mathrm{d}|P(t)\rangle}{\mathrm{d}t} = \tilde{W}|P(t)\rangle,\tag{3.6}$$

with

$$\tilde{W} = \sum_{j=1}^{N} (\sigma_j^x - 1) e^{-X(M_j N) \sigma_j^z}, \tag{3.7}$$

where now  $M = \sum_{i=1}^{N} \sigma_i^z$  and  $\sigma_j^x$  and  $\sigma_j^z$  are Pauli spin operators. Introducing the density operator

$$\varrho_{\rm eq} = Z^{-1} \exp \left[ (K/2N) M^2 + HM \right],$$
 (3.8)

and the state  $|1\rangle = \sum_{\{\sigma_i\}} |\sigma_1 \cdots \sigma_N\rangle$ , the equilibrium state can be written as

$$|P_{\rm eq}\rangle = \varrho_{\rm eq} |1\rangle. \tag{3.9}$$

Normalization of the probability  $P(\sigma_1, ..., \sigma_N, t)$  means that for all times one should have

$$\langle 1 \mid P(t) \rangle = 1. \tag{3.10}$$

The constancy of  $\langle 1 | P(t) \rangle$  is indeed easily proved, using eq. (3.6) and the fact that  $(\sigma_j^x - 1) | 1 \rangle = 0$ . Furthermore, it is easily seen that the equilibrium state,

for which

$$\langle 1 \mid P_{eq} \rangle = 1, \tag{3.11}$$

satisfies

$$\tilde{W}|P_{\rm eg}\rangle = 0, \tag{3.12}$$

which means that it is an eigenstate of  $\tilde{W}$  with eigenvalue zero.

The whole treatment becomes more nearly symmetric if the following transformations are performed:

$$|\psi(t)\rangle = \varrho_{\rm eq}^{-\frac{1}{2}}|P(t)\rangle,\tag{3.13}$$

$$|0\rangle = \varrho_{\text{eq}}^{-\frac{1}{2}} |P_{\text{eq}}\rangle = \varrho_{\text{eq}}^{\frac{1}{2}} |1\rangle, \tag{3.14}$$

$$W = \varrho_{eq}^{-\frac{1}{2}} \tilde{W} \varrho_{eq}^{\frac{1}{2}}. \tag{3.15}$$

From these definitions we obtain

$$\frac{\mathrm{d}|\psi(t)\rangle}{\mathrm{d}t} = W|\psi(t)\rangle,\tag{3.16}$$

$$\langle 0 \mid \psi(t) \rangle = 1, \tag{3.17}$$

and

$$W|0\rangle = 0. (3.18)$$

A simple calculation leads to the following form for W

$$W = \sum_{j=1}^{N} e^{-\frac{1}{2}X(M/N)\sigma_{j}^{z}} (\sigma_{j}^{x} - 1) e^{-\frac{1}{2}X(M/N)\sigma_{j}^{z}},$$
(3.19)

which is clearly a hermitean operator with therefore only real eigenvalues. Since this operator can also be written as

$$W = -\frac{1}{2} \sum_{j=1}^{N} B_j^* B_j, \tag{3.20}$$

with

$$B_i = (1 - \sigma_I^x) \exp \left[-\frac{1}{2}X(M/N) \sigma_I^z\right],$$

it is clear that W has no positive eigenvalues. It can even be proved<sup>9</sup>) that for finite N all eigenvalues are nondegenerate. The different terms in (3.20) do not

commute and for an evaluation of the eigenvalue spectrum the complete operator W must therefore be considered. This is most easily done by starting from the following expression, obtained from eq. (3.19) by permuting  $\sigma_J^x - 1$  to one side

$$W = -N \cosh X + 2J_z \sinh X + 2 e^{-K/N} J_x.$$
 (3.21)

Here  $J_{\alpha}$  is the operator for the total spin defined as  $J_{\alpha} = \frac{1}{2} \sum_{i=1}^{N} \sigma_{i}^{\alpha}$  and with  $X = (2K/N) J_{z} + H$ . We now note from eq. (3.21), that this operator W, which acts in the  $2^{N}$ -dimensional space of the states  $|\sigma_{1} \cdots \sigma_{N}\rangle$ , commutes with  $J^{2}$  [eigenvalues j(j+1)]. The eigenvalue problem is therefore reduced to a number of independent eigenvalue problems in (2j+1)-dimensional spaces. The largest possible value of j is  $\frac{1}{2}N$ , corresponding to the (N+1)-dimensional subspace, which is spanned by the totally symmetric states with a definite value of the z component of the total spin, *i.e.*, by

$$|M\rangle = \sum_{\{\sigma_i\}_M} |\sigma_1 \cdots \sigma_N\rangle \qquad (M = -N, -N + 2, \dots, +N).$$
 (3.22)

Because  $|M\rangle = J_{-}^{N-M}|N\rangle$  and  $J_{-}$  commutes with  $J^2$ , these states indeed have the same total spin as  $|N\rangle = |1, 1, ..., 1\rangle$ , i.e.,  $j = \frac{1}{2}N$ . Since  $|0\rangle = \varrho_{eq}^{\frac{1}{2}}|1\rangle$  and

$$|1\rangle = \sum_{M} |M\rangle,\tag{3.23}$$

also the equilibrium state  $|0\rangle$  is contained in this (N+1)-dimensional space with  $j=\frac{1}{2}N$ . Eigenstates belonging to a subspace with  $j<\frac{1}{2}N$  necessarily have strictly negative eigenvalues, because of the nondegeneracy of the spectrum. Any initial state orthogonal to the space with  $j=\frac{1}{2}N$  therefore disappears completely as  $t\to +\infty$ . Moreover, as long as we are not interested in correlation functions between many individual spins we only have to know the spectrum W for values of j which are of order  $\frac{1}{2}N$ . In particular, we have studied in detail the case of  $j=\frac{1}{2}N$ , although the method also applies for the cases that  $j=\frac{1}{2}N-j'$  with j' finite. The relevance of only this (N+1)-dimensional subspace corresponds to the fact that a configuration  $(\sigma_1,\ldots,\sigma_N)$  is completely specified by the value of  $M=\sum_{j}\sigma_{j}$ . This means that the distribution  $P(\{\sigma_i\},t)$  actually depends only on M and t and can therefore be written as P(M,t). It can be calculated as

$$P(M,t) = \langle M | P(t) \rangle = \langle M | \varrho_{eq}^{\frac{1}{2}} | \psi(t) \rangle. \tag{3.24}$$

From eqs. (3.10), (3.22) and (3.23) it follows that this P(M, t) is properly normalized, so that

$$\sum_{M} P(M, t) = 1. {(3.25)}$$

With the standard expressions for the matrix elements of  $J_z$  and  $J_x$  the master equation (3.6) can now be cast in the form

$$\frac{\partial P(M,t)}{\partial t} = \sum_{M'} \tilde{W}(M \mid M') P(M',t), \qquad (3.26)$$

where the matrix elements  $\tilde{W}(M \mid M')$  are derived from the expression (3.21) and are found to be

$$\tilde{W}(M \mid M) = -N \cosh X + M \sinh X, 
\tilde{W}(M \mid M+2) = \frac{1}{2} (N+M+2) e^{-2K/N} e^{-X}, 
\tilde{W}(M \mid M-2) = \frac{1}{2} (N-M+2) e^{-2K/N} e^{X},$$
(3.27)

all other  $\tilde{W}(M \mid M')$  equal to zero and X = K(M/N) + H.

The derivation of the macroscopic and Fokker-Planck equations in section 6 will be based on this form of the master equation.

In the next section eq. (3.21) will be used to calculate the spectrum of W. This is of importance for the determination of correlation functions in section 5 and also for a discussion of the macroscopic equation in the last section.

4. The spectrum of the transition matrix. Holstein and Primakoff have given a representation of angular-momentum operators in terms of Bose operators a and  $a^*$ . For a total angular momentum  $j = \frac{1}{2}N$  one has

$$L_{x} = \frac{1}{2}N^{\frac{1}{2}} \left[ a^{*} \left( 1 - \frac{a^{*}a}{N} \right)^{\frac{1}{2}} + \left( 1 - \frac{a^{*}a}{N} \right)^{\frac{1}{2}} a \right],$$

$$L_{y} = \frac{1}{2i} N^{\frac{1}{2}} \left[ a^{*} \left( 1 - \frac{a^{*}a}{N} \right)^{\frac{1}{2}} - \left( 1 - \frac{a^{*}a}{N} \right)^{\frac{1}{2}} a \right],$$

$$L_{z} = a^{*}a - \frac{1}{2}N.$$
(4.1)

This is indeed a representation of the usual commutation relations, provided the number l of quanta is restricted by  $0 \le l \le N$ . Calculation of the total angular momentum gives  $L^2 = \frac{1}{2}N(\frac{1}{2}N+1)$ . In order to apply this method to our problem of finding the eigenvalues of W [eq. (3.21)] we perform a rotation around the y axis and define

$$J_{y} = L_{y}, \qquad J_{x} = -pL_{z} - mL_{x}, \qquad J_{z} = -mL_{z} + pL_{x},$$
 (4.2)

where m and p are as yet undefined parameters, such that  $p^2 + m^2 = 1$ . Since we shall be interested in the case with a number of quanta which is small compared

to  $N^{\frac{1}{2}}$ , the square roots occurring in (4.1) can be expanded, and we obtain

$$J_{x} = \frac{1}{2}Np - \frac{1}{2}mN^{\frac{1}{2}}(a + a^{*}) - pa^{*}a$$

$$+ (m/4N^{\frac{1}{2}})(a^{*}a^{*}a + a^{*}aa) + \mathcal{O}(N^{-3/2}),$$

$$J_{y} = \frac{1}{2}N^{\frac{1}{2}}(a - a^{*}) + (i/4N^{\frac{1}{2}})(a^{*}a^{*}a - a^{*}aa) + \mathcal{O}(N^{-3/2}),$$

$$J_{z} = \frac{1}{2}Nm + \frac{1}{2}pN^{\frac{1}{2}}(a + a^{*}) - ma^{*}a$$

$$- (p/4N^{\frac{1}{2}})(a^{*}a^{*}a + a^{*}aa) + \mathcal{O}(N^{-3/2}).$$

$$(4.3)$$

Substitution of these expressions into eq. (3.21) yields a series in descending powers of  $N^{\frac{1}{2}}$ . Because we are first of all interested in the smallest eigenvalues of W we want to choose the parameters p and m in such a way that the terms  $\mathcal{O}(N)$  and  $\mathcal{O}(N^{\frac{1}{2}})$  disappear. The former is achieved by taking for m a solution of

$$m = \tanh X(m), \tag{4.4}$$

which is the same as eq. (2.4) for the equilibrium magnetization. It has one solution  $m_+$  if  $T > T_c = 1$  and three solutions  $m_+$ ,  $m_-$  and  $m_0$  if  $T < T_c$  and  $H < H_c$ . The terms of order  $N^{\frac{1}{2}}$  cancel if p is taken as the positive square root  $p = +(1 - m^2)^{\frac{1}{2}}$ . The remaining finite terms give

$$-W = A_i a^* a + \frac{1}{2} B_i (a^* a^* + aa) + D_i + \mathcal{O}(N^{-\frac{1}{2}}), \tag{4.5}$$

with

$$A_{i} = 2K(1 - m_{i}^{2})^{\frac{1}{2}} \left[ \frac{1}{2}K(1 - m_{i}^{2}) - 1 \right] + 2/(1 - m^{2})^{\frac{1}{2}},$$

$$B_{i} = 2K(1 - m_{i}^{2})^{\frac{1}{2}} \left[ \frac{1}{2}K(1 - m_{i}^{2}) - 1 \right],$$

$$D_{i} = \frac{1}{2}K(1 - m_{i}^{2})^{3/2},$$

$$(4.6)$$

where  $m_i$  is one of the solutions of eq. (4.4). Also the operators a and  $a^*$  depend on which  $m_i$  is taken (since in (4.3)  $J_x$ ,  $J_y$  and  $J_z$  do not depend on i, but m and p do) but this is not indicated explicitly. In the limit of an infinite number of spins the right-hand side of eq. (4.5) can be diagonalized by a Bogoliubov transformation. This is always possible, provided  $A_i - B_i$  and  $A_i + B_i$  are both positive. We find  $A_i - B_i = 2/(1 - m_i^2)^{\frac{1}{2}}$  and  $A_i + B_i = 2(1 - m_i^2)^{3/2} [1/(1 - m_i^2) - K]^2$ . From this it is clear that only for the following two cases is diagonalization impossible: a)  $T = T_c = 1$  and H = 0; b)  $T < T_c$  and  $H = H_c$  for i = - and i = 0, because in this case  $m_- = m_0 = -(T_c - T)^{\frac{1}{2}}$ . These are exactly the cases for which large

fluctuations occur and the number of quanta involved is not finite. For all other cases the canonical transformation

$$c = \frac{1}{2} (\varphi_i - \varphi_i^{-1}) a^* + \frac{1}{2} (\varphi_i + \varphi_i^{-1}) a, \tag{4.7}$$

with

$$\varphi_t = +[|1 - K(1 - m_t^2)|]^{\frac{1}{2}},\tag{4.8}$$

brings W into the form

$$-W = \lambda_i c^* c + \Delta_i. \tag{4.9}$$

The eigenvalues of -W are given by

$$\mu_i(l) = l\lambda_i + \Delta_i \qquad (l = 0, 1, 2, ...),$$
 (4.10)

with

$$\lambda_i = 2 \left| \left[ 1/(1 - m^2)^{\frac{1}{2}} \right] - K(1 - m_i^2)^{\frac{1}{2}} \right| \quad (i = \pm, 0). \tag{4.11}$$

If eq. (4.4) has only one solution, then  $\Delta_+=0$ . If it has three solutions, then  $\Delta_+=\Delta_-=0$  and  $\Delta_0=\lambda_0$ . Since  $\Delta_0$  is positive the i=0 solutions are indeed unstable and will decay completely.

In this way we have shown that every small eigenvalue of -W belongs to one of at most three classes. In each class the eigenvalues are equidistant and their number is small compared to  $N^{\frac{1}{2}}$ . This structure has been confirmed by a numerical diagonalization of W for N=100.

In the exceptional cases a) and b) eq. (4.5) takes the form

$$-W = -\frac{1}{2}K^{\frac{1}{2}}(a-a^*)^2. \tag{4.12}$$

Introducing the canonical coordinate and momentum  $q = (a + a^*)/\sqrt{2}$  and  $p = (a - a^*)/i \sqrt{2}$ , eq. (4.12) becomes  $-W = K^{\frac{1}{2}}p^2$ , which shows that W now has a continuous spectrum. This is in agreement with the fact that in these exceptional cases the level spacings  $\lambda_l$ , as given by eq. (4.11), are equal to zero.

It should be stressed that in eq. (4.9) the transition matrix is written either with i=+, or with i=-, or with i=0 and not as a sum of the three expressions. This implies that  $\mu_+(l_1) + \mu_-(l_2) + \mu_0(l_3)$  is not an eigenvalue of -W. If the eigenstate of -W, belonging to the eigenvalue  $\mu_i(l)$ , is indicated by  $|l,i\rangle$ , then the Hilbert space is spanned by the union of the three sets  $|l,i\rangle$  and product states do not occur. Any state can therefore be written as  $|\psi(t)\rangle = |\psi_+(t)\rangle + |\psi_-(t)\rangle + |\psi_0(t)\rangle$  and the distribution of the total spin accordingly becomes  $P(M, t) = P_+(M, t) + P_-(M, t) + P_0(M, t)$ , where the relaxation times occurring in  $P_1(M, t)$  are  $\mu_1^{-1}(l)$ .

In appendix I we have calculated the distributions  $P_{i,i}(M)$  for the eigenstates  $|l,i\rangle$ . It is found that  $P_{i,i}(M)$  is different from zero only for values of M around  $Nm_i$ . The width of the distribution is proportional to  $[(l+\frac{1}{2})N]^{\frac{1}{2}}$ . Introducing the variable y by  $M=Nm_i+\varphi_i^{-1}(1-m_i^2)^{\frac{1}{2}}y(2N)^{\frac{1}{2}}$  and denoting the equilibrium distribution  $P_{0,i}(M)$  by  $P_i^{eq}(y)$ , we obtain the expression

$$P_{i,i}(M) = [H_i(y)/(2^i l!)^{\frac{1}{2}}] P_i^{eq}(y). \tag{4.13}$$

 $H_1(y)$  is a Hermite polynomial.  $P_+^{eq}(y)$  and  $P_-^{eq}(y)$  are the distributions of magnetization for the stable and metastable equilibrium states, which are both eigenstates of W with eigenvalue zero. The distribution  $P_0^{eq}(y)$  decays completely (with relaxation time  $\Delta_0^{-1}$ ) and therefore does not correspond to a physically realizable state, *i.e.*,  $P_0^{eq}(y)$  cannot be positive for all y.

The distributions  $P_{l,\pm}(M)$  are centred around the equilibrium values  $Nm_{\pm}$  with a width which is small compared to their separation. This implies that, as long as the difference in magnetization of an initial state and the final equilibrium state is of the order of  $\sqrt{N}$ , i.e., close to equilibrium, the initial state can be expanded in the states of one of the sets  $|l,\pm\rangle$ , with expansion coefficients which are independent of N. The time evolution is then simply obtained by multiplying each term with the factor  $e^{-l\lambda_{\pm}t}$ . If the difference in magnetization between the initial and the equilibrium state is of the order N a knowledge of the complete spectrum is required and the expansion method is no longer very appropriate. It is known<sup>5</sup>) that in this case a simpler description can be given using a macroscopic equation and a Fokker-Planck equation. For the present model this will be discussed in section 6.

We now turn to the part of the spectrum where the eigenvalues are of order N. In particular we want to calculate the number of eigenvalues of -W between  $N\varepsilon$  and  $N(\varepsilon + d\varepsilon)$ . We call this number  $N\varrho(\varepsilon) d\varepsilon$ , anticipating that the density is independent of N. Introducing the operators w = -W/N,  $x = 2J_x/N$ ,  $y = 2J_y/N$  and  $z = 2J_z/N$ , we can write eq. (3.21) as

$$w = \cosh X(z) - z \sinh X(z) - x e^{-K/N},$$
 (4.14)

with

$$X(z) = Kz + H. (4.15)$$

The commutation relations between x, y and z are

$$[x, y] = (2i/N) z,$$
  $[y, z] = (2i/N) x,$   $[z, x] = (2i/N) y.$  (4.16)

Since the total spin is  $j = \frac{1}{2}N$ , we also have

$$r^2 \equiv x^2 + y^2 + z^2 = 1 + 2/N. \tag{4.17}$$

In the limit  $N \to \infty$  the operators x, y and z are mutually commuting and r = (x, y, z) becomes a unit vector. The operator w indeed becomes independent of N. From this we derive

$$\varrho(\varepsilon) = (1/4\pi) \int \delta \left[ w(\mathbf{r}) - \varepsilon \right] \delta (r - 1) \, \mathrm{d}\mathbf{r}. \tag{4.18}$$

Performing first the y and then the x integration leads to the expression

$$\varrho(\varepsilon) = (1/2\pi) \int dz \left\{ \left[ (1-z^2)^{\frac{1}{2}} + g(z) - \varepsilon \right] \left[ (1-z^2)^{\frac{1}{2}} - g(z) + \varepsilon \right] \right\}^{-\frac{1}{2}}, \quad (4.19)$$

with

$$g(z) = \cosh X(z) - z \sinh X(z). \tag{4.20}$$

The integration in (4.19) extends over that region of the interval (-1, +1) for which

$$g(z) - (1 - z^2)^{\frac{1}{2}} < \varepsilon < g(z) + (1 - z^2)^{\frac{1}{2}}.$$
 (4.21)

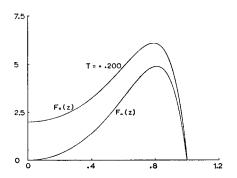


Fig. 4.  $F_{+}(z)$  and  $F_{-}(z)$  for T = 0.2 and B = 0.

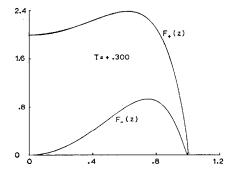


Fig. 5.  $F_{+}(z)$  and  $F_{-}(z)$  for T = 0.3 and B = 0.

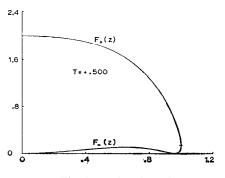


Fig. 6.  $F_{+}(z)$  and  $F_{-}(z)$  for T = 0.5 and B = 0.

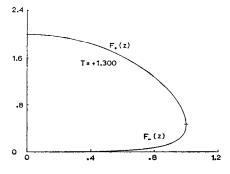


Fig. 7.  $F_{+}(z)$  and  $F_{-}(z)$  for T = 1.3 and B = 0.

In order to illustrate these regions we have plotted the functions  $F_{\pm}(z) = g(z) \pm (1-z^2)^{\frac{1}{2}}$  for different temperatures and for H=0. The results are shown in figs. 4-7. Each value of  $F_+$  and  $F_-$  for which  $F_+(z)$  or  $F_-(z)$  has a vanishing derivative corresponds to an extremum or even a singularity in  $\varrho(\varepsilon)$ . By expanding  $F_{\pm}(z)$  around these points and neglecting all but the first term in the Taylor series, we can easily determine the behaviour of  $\varrho(\varepsilon)$  in the corresponding neighbourhood. In this way we find:

for  $\varepsilon \downarrow 0$ 

$$\varrho(\varepsilon) \to \text{constant} \neq 0 \quad \text{for all} \quad T \neq T_c,$$
 (4.22)

$$\varrho(\varepsilon) \approx \varepsilon^{-1/3}$$
 if  $T = T_c = 1$ ; (4.23)

for  $\varepsilon \uparrow 2$ 

$$\varrho(\varepsilon) \to \text{constant} \neq 0 \quad \text{if} \quad T > 2^{\frac{1}{2}} - 1 = 0.414 \dots,$$
 (4.24)

$$\varrho(\varepsilon) \approx -\log(2-\varepsilon) \quad \text{if} \quad T < 2^{\frac{1}{2}} - 1,$$
 (4.25)

$$\varrho(\varepsilon) \approx (2 - \varepsilon)^{-1/4}$$
 if  $T = 2^{\frac{1}{2}} - 1$ ; (4.26)

for  $\varepsilon \downarrow 2$ 

$$\varrho(\varepsilon) \to 0 \quad \text{if} \quad T \geqslant 2^{\frac{1}{2}} - 1,$$
 (4.27)

$$\varrho(\varepsilon) \approx -\log(\varepsilon - 2) \quad \text{if} \quad T < 2^{\frac{1}{2}} - 1.$$
(4.28)

For  $T < T_c$  the function  $F_-(z)$  develops a minimum and a maximum in the interior of the interval (0, 1). The minimum occurs for  $\tanh Kz = z$ , *i.e.*, when z is equal to the equilibrium magnetization.  $F_-(z)$  vanishes at this point and there is a finite contribution to  $\varrho$  ( $\varepsilon = 0$ ).

Writing  $\varepsilon_0$  for the maximum value of  $F_-(z)$ , it can be shown that this gives rise to a singularity in  $\rho(\varepsilon)$  of the form

$$\rho(\varepsilon) \approx -\log |\varepsilon - \varepsilon_0|$$
 if  $T < T_c$ .

With decreasing temperature the position  $\varepsilon_0$  of this singularity moves to the right and eventually becomes even larger than 2, which is the fixed position where for  $T < 2^{\frac{1}{2}} - 1$  the other singularity occurs. A numerical calculation of  $\varrho(\varepsilon)$ , using eq. (4.19) has been performed for the same temperatures for which  $F_+(z)$  and  $F_-(z)$  were determined. The peculiarities of this function, shown in figs. 8-11, can all be understood on the basis of the previous remarks and the forms of  $F_+(z)$  and  $F_-(z)$ .

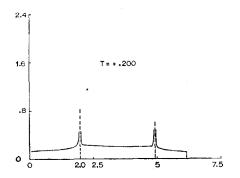


Fig. 8.  $\varrho(\varepsilon)$  for T=0.2 and B=0.

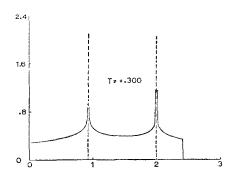


Fig. 9.  $\varrho(\varepsilon)$  for T = 0.3 and B = 0.

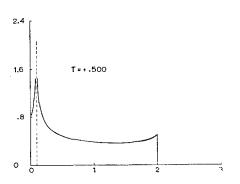


Fig. 10.  $\varrho(\varepsilon)$  for T=0.5 and B=0.

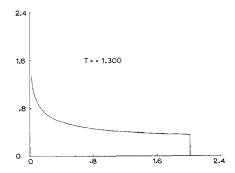


Fig. 11.  $\varrho(\varepsilon)$  for T=1.3 and B=0.

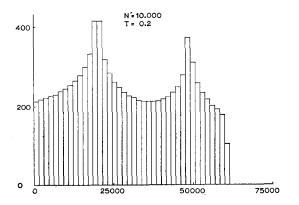


Fig. 12. The exact density of eigenvalues for N = 10000, T = 0.2 and B = 0.

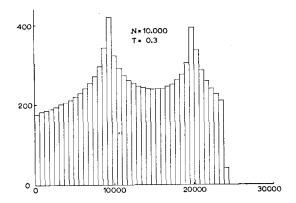


Fig. 13. The exact density of eigenvalues for N = 10000, T = 0.3 and B = 0.

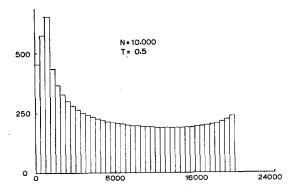


Fig. 14. The exact density of eigenvalues for N = 10000, T = 0.5 and B = 0.

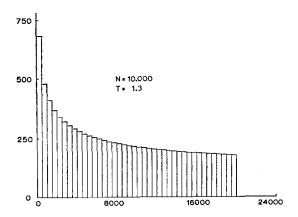


Fig. 15. The exact density of eigenvalues for N = 10000, T = 1.3 and B = 0.

For large but finite values of N we have used a numerical method, explained by Wilkinson<sup>11</sup>), to calculate the density of eigenvalues. For some temperatures and zero field, the results are given in figs. 12–15. In all cases the structure of the function  $\varrho(\varepsilon)$  is completely recovered. In particular we find for some temperatures the occurrence of an accumulation point of eigenvalues. This should be compared with the accumulation point in the spectrum of the diode model, found by Van Kampen<sup>12</sup>). His suggestion that this is a general feature of nonlinear systems has thus been confirmed for these cases. The physical meaning of the states below and above the accumulation point is, however, quite different in the two models. For the diode the small eigenvalues are said to be determined by the RC time of the circuit, so that they describe macroscopic deviations from equilibrium. In the present case the small eigenvalues, given by eq. (4.10) and concentrated at the point  $\varepsilon = 0$ , will suffice to describe the macroscopic behaviour (see section 6). The finite part of  $\varrho(\varepsilon)$  describes processes with a characteristic decay time of 1/N times the average time between two flips of a single spin.

5. Correlations and dynamical susceptibility. In this section we first calculate the equilibrium autocorrelation functions  $\overline{M(t)} \, M(0)^{\text{eq}}$  and  $\overline{E(t)} \, E(0)^{\text{eq}}$  of the total magnetization and energy. These are defined as follows. Let  $P_{M_0}(M, t)$  be the distribution of magnetization which for t = 0 is given by  $P_{M_0}(M, 0) = \delta_{MM_0}$ . With this distribution the average magnetization at a later time is  $M_{M_0}(t) = \sum_{M} MP_{M_0}(M, t)$ . The average of the product  $M_{M_0}(t) M_0$  over the equilibrium distribution  $P_{+}^{\text{eq}}(M_0)$  (with only one maximum near  $Nm_+$ ) can be written as

$$\overline{M(t) \ M(0)}^{\text{eq}} = \langle 0, + | \ M e^{Wt} \ M | 0, + \rangle = \sum_{l=0}^{\infty} e^{-\mu_{+}(l) t} |U(l)|^{2}, \tag{5.1}$$

where  $\mu_+(l)$  is given by (4.10) and  $U(l) = \langle l, + | M | 0, + \rangle$ . Similarly the equilibrium value of M itself can be written as  $\overline{M}^{\text{eq}} = \sum_M M P_+^{\text{eq}}(M) = \langle 0, + | M | 0, + \rangle = U(0)$ , so that

$$\overline{M(t)} \ \overline{M(0)}^{\text{eq}} - (\overline{M}^{\text{eq}})^2 = \sum_{l=1}^{\infty} e^{-\mu_{+}(l)t} |U(l)|^2.$$
 (5.2)

The matrix elements U(l) can be calculated, using  $M = 2J_z$  and substituting the expression (4.3) for  $J_z$ , but now via (4.7) in terms of c and  $c^*$ . We find

$$\varphi_{M}^{\text{eq}}(t) = \overline{M(t) M(0)}^{\text{eq}} - (\overline{M}^{\text{eq}})^{2} = (N\chi/\mu^{2}\beta) e^{-\lambda_{+}t},$$
 (5.3)

where  $\lambda_+$  is given by (4.11) and  $\chi$  is the static susceptibility, as calculated in (2.7). In the same way we find for the energy autocorrelation function

$$\varphi_E^{\text{eq}}(t) = \overline{E(t) E(0)}^{\text{eq}} - (\bar{E}^{\text{eq}})^2 = (NC_H/k\beta^2) e^{-\lambda_1 t},$$
 (5.4)

where  $c_H$  is the specific heat at constant field of eq. (2.10). Since the energy  $E(M) = -(J/2N) M^2 - \mu BM$  contains a quadratic term in the magnetization one would expect that the autocorrelation function should also contain the second relaxation time  $e^{-2\lambda + t}$ . It turns out, however, that the corresponding term is of lower order in N. These terms have been deleted in eqs. (5.3) and (5.4). For t = 0 the correlation functions indeed reduce to the static values of eq. (2.9) and (2.10).

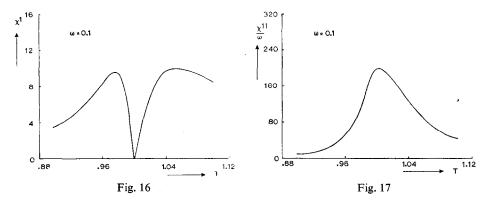


Fig. 16. Temperature dependence of  $\chi'_{eq}(\omega)$  for  $\omega = 0.1$  in the interval  $0.9 \le T \le 1.1$ . The unit along the ordinate is  $\mu^2 \beta$ .

Fig. 17. Temperature dependence of  $\omega^{-1}\chi_{eq}^{"}(\omega)$  for  $\omega=0.1$  in the interval  $0.9 \le T \le 1.1$ . The unit along the ordinate is  $\mu^2\beta$ .

The spectral densities of fluctuations  $S(\omega) = (2/\pi) \int_0^\infty \cos \omega t \varphi^{eq}(t) dt$  follow from eqs. (5.3) and (5.4):

$$S_{M}(\omega) = \frac{2}{\pi} \frac{N\chi}{\mu^{2}\beta} \frac{\lambda_{+}}{\omega^{2} + \lambda_{+}^{2}}$$
 (5.5)

and

$$S_E(\omega) = \frac{2}{\pi} \frac{Nc_H}{k\beta^2} \frac{\lambda_+}{\omega^2 + \lambda_+^2}.$$
 (5.6)

Using the autocorrelation function  $\varphi_M^{eq}(t)$  one can define the dynamical susceptibility  $\chi_{eq}(\omega) = \chi'_{eq}(\omega) - i\chi''_{eq}(\omega)$  by

$$\chi_{eq}(\omega) = -\frac{\beta \mu^2}{N} \int_0^{\infty} \frac{d\varphi_M^{eq}(t)}{dt} e^{-i\omega t} dt.$$
 (5.7)

Since  $\varphi_{M}^{eq}(t)$  [eq. (5.3)] is monodispersive we obtain for  $\chi_{eq}(\omega)$  a simple Debye form

$$\chi_{eq}(\omega) = \frac{\lambda_{+}}{\lambda_{+} + i\omega} \chi, \tag{5.8}$$

from which

$$\chi'_{eq}(\omega) = \frac{\lambda_+^2}{\lambda_+^2 + \omega^2} \chi \quad \text{and} \quad \frac{\chi'''_{eq}(\omega)}{\omega} = \frac{\lambda_+}{\lambda_+^2 + \omega^2} \chi.$$
(5.9)

For fixed  $\omega$  the temperature dependence of these two functions is shown in figs. 16 and 17. Since  $\lambda_+$  approaches zero when  $T \to T_c$  it is clear that for nonzero frequency the critical index of slowing down of  $\chi'_{eq}(\omega)$  is different from that of the static susceptibility. For  $\omega = 0$  it is the same. For a model with nearest-neighbour interaction the same effect has been found by Yahata<sup>4</sup>).

6. Macroscopic law and Fokker-Planck equation. In this section we want to study the relaxation of a state which has a macroscopic deviation from equilibrium. It has been remarked by Nishikawa<sup>13</sup>) and Matsudaira<sup>2</sup>) that when nonlinear effects are present the monodispersive relaxation is changed to a polydispersive one. For the model under consideration we shall find the same phenomenon. In addition to this we want to discuss relaxation near the critical point, non-equilibrium fluctuations and the question when linear-response theory breaks down.

In order to study these problems we start from the master equation in the form of eq. (3.26), i.e.,

$$\frac{\mathrm{d}P(M,t)}{\mathrm{d}t} = \sum_{M'} \tilde{W}(M \mid M') P(M',t), \tag{6.1}$$

where  $\tilde{W}(M \mid M')$  is given by eq. (3.27). Following Van Kampen<sup>5</sup>) we can derive from this a macroscopic equation for the average magnetization (per particle) m(t) and a linear Fokker-Planck equation, which gives a detailed description of the fluctuations of the magnetization. This is done by introducing a new variable x instead of M through  $M = Nm(t) + xN^{\frac{1}{2}}$ . The function m(t) will be chosen later. From the appearance of  $N^{\frac{1}{2}}$  it is clear that it is assumed that for all times the width of the distribution P(M, t) around the average value Nm(t) is of the order  $N^{\frac{1}{2}}$ . It can be shown that if this holds at the initial time it will hold forever. From now on we restrict ourselves to distributions of this kind. The new distribution function will be indicated by P(x, t). Expanding P(M', t) = P(x', t) in the right-hand side of eq. (6.1) around x and expanding the M' dependence of  $\tilde{W}(M \mid M')$  around Nm(t), we collect powers of  $N^{\frac{1}{2}}$  in eq. (6.1). The term of O(N) vanishes. In order to let the term  $O(N^{\frac{1}{2}})$  also be zero we must choose m(t) such that it satisfies

$$\frac{\mathrm{d}m(t)}{\mathrm{d}t} = -\beta_1(m),\tag{6.2}$$

with

$$\beta_1(m) = 2 [m \cosh X(m) - \sinh X(m)].$$
 (6.3)

From

$$\overline{M(t)} = \sum_{M} MP(M, t) = \sum_{x} [Nm(t) + N^{\frac{1}{2}}x] P(x, t) = Nm(t) + O(N^{\frac{1}{2}}),$$
(6.4)

it follows indeed that

$$m(t) = [M(t)/N] + \mathcal{O}(1/N^{\frac{1}{2}}),$$
 (6.5)

so that the initial value of m(t) in eq. (6.2) is well defined by the macroscopic magnetization at t = 0.

The remaining terms, a constant and terms of higher order in  $N^{-\frac{1}{2}}$ , determine the fluctuations. Deviations from the linear Fokker-Planck equation occur for finite N. For N tending to infinity only the constant remains and gives the following Fokker-Planck equation, which is now linear in x

$$\frac{\partial P(x,t)}{\partial t} = \frac{\mathrm{d}\beta_1}{\mathrm{d}m} \frac{\partial}{\partial x} \left[ x P(x,t) \right] + \frac{1}{2}\beta_2(m) \frac{\partial^2 P}{\partial x^2}, \tag{6.6}$$

where

$$\beta_2(m) = 4 \left[ \cosh X(m) - m \sinh X(m) \right]$$
 (6.7)

and m = m(t) is the solution of eq. (6.2). The normalization of P(x, t) is such that  $\sum_{x} P(x, t) = 1$  with  $\Delta x = 2/N^{\frac{1}{2}}$ . This can be changed into  $\int P(x, t) dx = 1$ , provided the new P(x, t) is  $\frac{1}{2}N^{\frac{1}{2}}$  times as large as the old one. It of course still satisfies eq. (6.6).

Let us now consider eq. (6.2) in some more detail. The stationary points, given by the zeros of  $\beta_1(m)$ , are the equilibrium values of the average magnetization [see eq. (2.4)]. From the form of  $\beta_1(m)$ , an example of which is shown in fig. 18,

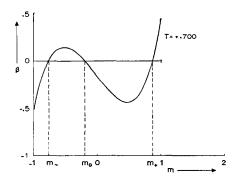


Fig. 18.  $\beta_1(m)$  as function of m for T = 0.7 and  $H = \frac{1}{2}H_c(T)$  [eq. (2.6)].

it is easily seen that the so-called stable  $(m_+)$  and metastable  $(m_-)$  solutions indeed are stable and the third solution  $(m_0)$ , if it exists, is unstable. We have not succeeded in finding the general solution of eq. (6.2). Numerical solutions are, however, easily obtained. In figs. 19 and 20 we show the function  $\ln |m(t) - m(\infty)|$  for two temperatures and for zero field. Away from the critical temperature only one relaxation time plays a role. It is equal to the inverse of  $\lambda_+$  or  $\lambda_-$  [given by eq. (4.11)] depending on whether m(t) tends to  $m_+$  or to  $m_-$  and provided m(t=0) is not too close to  $m_0$ . For temperatures close to  $T_c$  the higher eigenvalues [eq. (4.10)] become important.

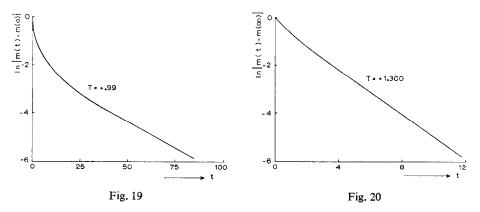


Fig. 19. Logarithmic plot of  $m(t) - m(\infty)$  for T = 0.99. The relaxation time  $\tau = \lambda_+^{-1}$  is  $\tau = 24.67$ . Fig. 20. Same as fig. 19 for T = 1.3. The relaxation time is  $\tau = 2.167$ .

In appendix II it is shown (for  $T > T_c$  and zero field) that the general solution of eq. (6.2) can always be written in the form

$$m(t) = \sum_{n=0}^{\infty} c_n e^{-(2n+1)(\lambda t + B)}, \qquad (6.9)$$

where B is determined by the initial value m (t = 0) and  $\lambda$  is given by eq. (4.11). The coefficients  $c_n$  are positive, they do not depend on the initial condition and are therefore completely determined by the function  $\beta_1(m)$  in the differential equation (6.2). Only the odd eigenvalues among the ones given by eq. (4.10) occur in eq. (6.9). This is caused by the fact that  $\beta_1(m)$  is an odd function of m. When a magnetic field is applied this property will be destroyed and also the even eigenvalues will come into play. Obviously the higher eigenvalues of the transition matrix, i.e., those proportional to N, do not enter the expansion (6.9) at all. These are only important for the very short time behaviour of a finite system.

For small, but macroscopic deviations from equilibrium eq. (6.2) can be solved analytically. Let us take as initial state the equilibrium at a field  $B + \Delta B$ . Then switching off  $\Delta B$  at t = 0, gives, as solution of eq. (6.2) and neglecting terms of

order  $(\Delta B)^2$ ,

$$m(t) = m_{eq}(B) + [m_{eq}(B + \Delta B) - m_{eq}(B)] e^{-\lambda_{\pm} t},$$
 (6.10)

where  $\lambda_{\pm}$  is given by eq. (4.11) and the plus (minus) sign must be chosen when m(t=0) is greater (less) than  $m_0$ . Expanding  $m_{\rm eq}(B+\Delta B)$  and combining eqs. (2.7) and (5.3), eq. (6.10) can be written as

$$m(t) = m_{\text{eq}}(B) + \Delta B \left(\beta \mu / N\right) \left[ \overline{M(t) M(0)}^{\text{eq}} - (\overline{M}^{\text{eq}})^2 \right] + \mathcal{O}(\Delta B^2). \tag{6.11}$$

If, following Kubo and Tomita<sup>14</sup>), we define the linear-response function  $\varphi_M(t)$  by

$$m(t) - m_{eq}(B) = \Delta B (\beta \mu | N) \varphi_{M}(t) + \mathcal{O}(\Delta B^{2}), \tag{6.12}$$

we see by comparison with eq. (6.11) that

$$\varphi_{M}(t) = \varphi_{M}^{eq}(t). \tag{6.13}$$

This well-known, but still amazing equality, states that an equilibrium fluctuation decays with the same rate as a nonequilibrium state, provided the initial disturbance is small on a macroscopic scale. The reason is, of course, that a nonequilibrium state decays just because of the fluctuations and that these fluctuations are almost the same as in equilibrium. At the end of this section this will be verified explicitly by calculating the nonequilibrium fluctuations from the Fokker-Planck equation.

Before doing this we first discuss for which values of  $K = \beta J$ ,  $h = \mu B/J$  and  $\Delta h = \mu \Delta B/J$  the solution (6.10) of the linearized equation is a good approximation. By expanding  $\beta_1(m)$  in powers of K it can easily be seen that in the high-temperature limit the linear approximation (6.10) becomes exact. For a dynamical system this is known<sup>15,16</sup>) to hold quite generally. In order to make a comparison for finite temperatures we define<sup>16</sup>)  $R_{\rm ex}(t) = m(t) - m_{\rm eq}(B)$  and, using eqs. (2.7) and (5.3),

$$R_{K-T}(t) = \Delta B \left( \beta \mu / N \right) \left[ \overline{M(t) M(0)}^{eq} - (\overline{M}^{eq})^2 \right],$$

or

$$R_{K-T}(t) = \frac{K(1-m_+^2)}{1-K(1-m_+^2)} e^{-\lambda_+ t} \Delta h.$$
 (6.14)

In fig. 21  $R_{\text{ex}}$  and  $R_{K-T}$  are shown as functions of K for h=0,  $\Delta h=0.1$  and t=1. It is indeed confirmed that for high temperatures  $R_{\text{ex}}$  and  $R_{K-T}$  become equal. The discrepancy is largest near the critical point K=1.

For the X-Y model it was shown<sup>16</sup>) that linear-response theory is a very bad approximation near a critical point. The same conclusion can now be drawn for

the present stochastic model. To be more precise we can ask the following question. When T is just below the critical temperature, say  $T_c - T = 10^{-2}$ , and the initial field h is switched off completely, how small should this field be in order for the linear approximation still to be correct? We can show that in the expansion of  $\beta_1(m)$  around the equilibrium value  $m_{eq}$  at zero field the first two non-vanishing terms are of the same size when h is greater than or of the order of magnitude of the critical field as given by eq. (2.6). From this follows that the linear theory fails if

$$h \geqslant (T_c - T)^{3/2}$$
, or  $h \geqslant 10^{-3}$  if  $T_c - T = 10^{-2}$ . (6.15)

This can be seen very clearly in fig. 22, where we show  $|R_{ex}(t) - R_{K-T}(t)|/R_{ex}(t)$  as a function of the switch-off field h for  $h \gg h_c = 0.008$ . The temperature is T = 0.95 and the time is half the relaxation time for this temperature, i.e., t = 2.337. Since  $R_{K-T}(t)$  is proportional to h the linearity of the curve in fig. 22 indicates that  $R_{ex}(t)$  has become independent of h, as it should, because of the almost complete saturation of the initial magnetization.

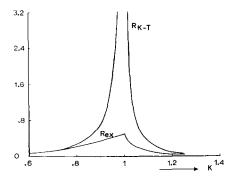


Fig. 21.  $R_{\text{ex}}$  and  $R_{K-T}$  as functions of K for h = 0,  $\Delta h = 0.1$  and t = 1.

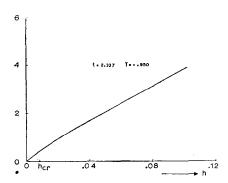


Fig. 22.  $|(R_{ex} - R_{K-T})/R_{ex}|$  as function of h for T = 0.95 and  $t = \frac{1}{2}\tau$ .

As final part of this section we now want to discuss the solution of the Fokker–Planck equation (6.6). If it is allowed to neglect the time dependence of  $\beta'_0 = \mathrm{d}\beta_1/\mathrm{d}m$  and of  $\beta_2(m)$  we can find solutions of eq. (6.6) with a single relaxation time. These solutions are given by

$$P_{l}(x,t) = e^{-\gamma_{l}t} \varphi_{l} \left[ (\beta'_{1}/\beta_{2})^{\frac{1}{2}} x \right] \qquad (l = 0, 1, 2, ...), \tag{6.16}$$

with

$$\gamma_l = l\beta_1' \tag{6.17}$$

and  $\varphi_l$  the *l*th Hermite function. Since  $\beta_2 > 0$  for all |m| < 1, this solution can only hold when  $\beta'_1 > 0$ , which is satisfied as long as the instantaneous value of

m(t) is not too close to the unstable equilibrium state  $m_0$ . In the linear approximation of eq. (6.2)  $\gamma_1 = \beta_1'$  is equal to the relaxation rate of m(t). From this it is clear that the assumption of negligible time dependence of  $\beta_1'$  and  $\beta_2$  is satisfied for large l values. With eq. (6.16) we can therefore give a correct description of rapid fluctuations outside equilibrium. The slow fluctuations, which determine the width of the distribution P(x, t), should be calculated differently. This width  $\sigma(t)$  can be determined for the special initial state  $P(x, 0) = \delta(x - x_0)$ . The general solution is (see e.g. ref. 5)

$$P(x,t) = \frac{1}{\sigma(t) (2\pi)^{\frac{1}{2}}} \exp\left(-\frac{(x-x_0 e^{-s(t)})^2}{2\sigma^2(t)}\right), \tag{6.18}$$

with

$$s(t) = \log \{ \beta_1 [m(0)] / \beta_1 [m(t)] \}$$
(6.19)

and

$$\sigma^{2}(t) = e^{-2s(t)} \int_{0}^{t} \beta_{2} [m(t')] e^{2s(t')} dt'.$$
 (6.20)

During the motion m(t) the function  $\beta_1$  [m(t)] does not change sign, so that s(t) is well defined by eq. (6.19). Again in the linear approximation of eq. (6.2) the functions s(t) and  $\sigma^2(t)$  can be calculated exactly. We find

$$s(t) = \lambda_{+}t \tag{6.21}$$

and

$$\sigma^{2}(t) = (\chi/\mu^{2}\beta) (1 - e^{-2\lambda_{+}t}), \tag{6.22}$$

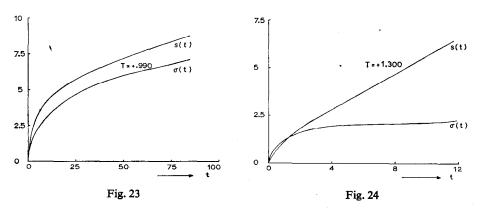


Fig. 23. s(t) and  $\sigma(t)$  for T=0.99. The relaxation time  $\tau=\lambda_+^{-1}$  is  $\tau=24.67$ . Fig. 24. Same as fig. 23 for T=1.3. The relaxation time is  $\tau=2.167$ .

where  $\lambda_+$  and  $\chi$  are given by eqs. (4.11) and (2.7), respectively. It is again the smallest non-vanishing eigenvalue of the transition matrix which determines the nonequilibrium fluctuations. Higher eigenvalues play a role only under conditions when the nonlinear part of  $\beta_1(m)$  is important. For such a case we have used eqs. (6.19) and (6.20) to calculate s(t) and  $\sigma(t)$ . The results are shown in figs. 23 and 24.

### APPENDIX I

For the eigenstates  $|l, i\rangle$  found in section 4, we now want to calculate the distribution of the magnetization. According to eq. (3.24) and omitting the index i, this distribution is given by

$$P_{l}(M) = \langle M | \varrho_{eq}^{\frac{1}{2}} | l \rangle, \tag{I.1}$$

where the state  $|M\rangle$ , defined by eq. (3.22), satisfies

$$J_z |M\rangle = \frac{1}{2}M |M\rangle. \tag{I.2}$$

Using the transformation (4.7) from the a and  $a^*$  operators to the c and  $c^*$  operators, we can write the expression (4.3) for  $J_z$  as

$$J_z = \frac{1}{2}Nm + (N^{\frac{1}{2}}/2\varphi)(1 - m^2)^{\frac{1}{2}}(c + c^*) + \mathcal{O}(1). \tag{I.3}$$

With these three formulae  $P_i(M)$  now becomes

$$P_{i}(M) = \varrho_{eq}^{\frac{1}{2}}(M) (2/M) \langle M | J_{z} | l \rangle = (2/M) \left\{ \frac{1}{2} Nm \langle M | \varrho_{eq}^{\frac{1}{2}} | l \rangle + (N^{\frac{1}{2}}/2\varphi) (1 - m^{2})^{\frac{1}{2}} [l^{\frac{1}{2}} \langle M | \varrho_{eq}^{\frac{1}{2}} | l - 1 \rangle + (l + 1)^{\frac{1}{2}} \langle M | \varrho_{eq}^{\frac{1}{2}} | l + 1 \rangle ] \right\}.$$
(I.4)

Introducing instead of M the new variable y, defined by

$$M = Nm + [(2N)^{\frac{1}{2}}/\varphi] (1 - m^2)^{\frac{1}{2}} y, \qquad (I.5)$$

eq. (I.4) takes the form

$$2^{\frac{1}{2}}yP_{l}(y) = l^{\frac{1}{2}}P_{l-1}(y) + (l+1)^{\frac{1}{2}}P_{l+1}(y).$$
(I.6)

With

$$P_l(y) = [H_l(y)/(2^l l!)^{\frac{1}{2}}] P^{eq}(y)$$
 and  $H_0(y) \equiv 1$ , (I.7)

this recurrence relation becomes

$$yH_{l}(y) = lH_{l-1}(y) + \frac{1}{2}H_{l+1}(y), \tag{I.8}$$

which is the defining equation for Hermite polynomials. The normalization of  $P^{eq}(y)$  is arbitrary. Eq. (I.7) is identical with eq. (4.13) of the main text.

### APPENDIX II

For temperatures above  $T_c$  and for zero field we shall prove that the general solution of eq. (6.2) can be written in the form

$$m(t) = \sum_{n=0}^{\infty} c_n e^{-(2n+1)(\lambda t + B)}, \qquad (II.1)$$

where B is determined by the initial value m(0) and the  $c_n$  are positive constants, independent of m(0).

Defining Y(t) = Km(t) and

$$G(Y) = 2(Y \cosh Y - K \sinh Y), \tag{II.2}$$

eq. (6.2) becomes

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = -G(Y). \tag{II.3}$$

From G(Y) > 0 and G(0) = 0 follows that Y(t) decreases monotonically to zero. Moreover, Y(t) is completely monotonic, *i.e.*,

$$(-1)^n \frac{\mathrm{d}^n Y}{\mathrm{d}t^n} \geqslant 0 \quad \text{in} \quad 0 \leqslant t < \infty.$$
 (II.4)

This follows from the equation

$$(-1)^n \frac{\mathrm{d}^n Y}{\mathrm{d}t^n} = \left(G(Y) \frac{\mathrm{d}}{\mathrm{d}Y}\right)^n Y \tag{II.5}$$

and from the fact that all derivatives of G(Y) are positive. These conditions are sufficient<sup>17</sup>) for the existence of a bounded, non-decreasing function  $\alpha(\omega)$ , such that

$$Y(t) = \int_{0}^{\infty} e^{-\omega t} d\alpha (\omega).$$
 (II.6)

If we put  $\alpha(0) = 0$  this representation is unique and it defines a function which is analytic in the right half-plane  $t = \sigma + i\tau$  with  $\sigma > \sigma_c$ . The point at infinity is a possible exception. The point  $t = \sigma_c$  is a singular point of Y(t) (ref. 17, p. 48,

theorem 5b). In our case it is given by

$$\sigma_{\rm c} = -\int_{Y(0)}^{\infty} {\rm d}Y/G(Y), \tag{II.7}$$

which is finite and negative.

If we now change to the variable

$$x = e^{-\lambda t}, (II.8)$$

with

$$\lambda = 2(1 - K),\tag{II.9}$$

eq. (II.3) becomes

$$\frac{\mathrm{d}Y}{\mathrm{d}x} = \frac{1}{\lambda x} G(Y). \tag{II.10}$$

The solution depends on how Y approaches zero when  $t \to \infty$  or  $x \to 0$ . This condition can be removed by introducing  $z = (dY/dx)_{x=0} x$ . The differential equation then becomes

$$\frac{\mathrm{d}Y}{\mathrm{d}z} = \frac{1}{\lambda z} G(Y),\tag{II.11}$$

to be solved under the condition  $(dY/dz)_{z=0} = 1$ . Since  $(dY/dx)_{x=0} > 0$  it can be written as  $(dY/dx)_{x=0} = e^{-B}$  with B real. In order to prove eq. (II.1) it remains therefore to show that the solution Y(z) of eq. (II.1) with  $(dY/dz)_{z=0} = 1$  can be expanded in a power series in z. For that it is sufficient that Y(z) be analytic in a finite region around the origin. Since the strip  $t = \sigma + i\tau$  with  $\sigma > \sigma_c$  and  $-(\pi/\lambda) \le \tau < \pi/\lambda$ , is mapped into the interior of the circle  $|z| < e^{-\lambda \sigma_c - B}$  and since Y(t) is analytic in this strip, we conclude that Y(z) is analytic inside this circle, with the possible exception of the point z = 0, i.e., the image of  $t = \infty$ . For  $z \to 0$  we have, however,  $Y \to 0$  and for small Y the function G(Y), as given by eq. (II.2), behaves as  $\lambda Y$ , so that for small z the differential equation (II.11) becomes

$$\frac{\mathrm{d}Y}{\mathrm{d}z} \approx \frac{Y}{z},$$
 (II.12)

with the solution  $Y(z) \approx z$ . So far this holds only for real and positive values of z, which are sufficiently small. The analytic continuation of Y(z) must, however, also satisfy eq. (II.11). From this follows that  $Y(z) \approx z$  also for complex z and

this implies that the complex derivative  $(dY/dz)_{z=0} = 1$  exists, so that Y(z) is indeed analytic inside a finite region around z = 0.

Notice that it is essential in the proof, that for small Y the function G(Y) behaves like  $\lambda Y$ . A dependence like  $Y^3$  would make the function Y(z) nonanalytic in z = 0. As was remarked already in the main text, the occurrence of only odd powers in

$$Y(z) = K \sum_{n=0}^{\infty} c_n z^{2n+1}, \tag{II.13}$$

is obviously caused by G(Y) being odd in Y. Eq. (II.13) shows that the function  $\alpha(\omega)$  of eq. (II.6) is a step function. Since  $\alpha(\omega)$  is non-decreasing all coefficients  $c_n$  are positive and independent of the initial condition, because this was already removed in going from eq. (II.10) to eq. (II.11).

# REFERENCES

- 1) Griffiths, R.B., Weng, C.Y. and Langer, J.S., Phys. Rev. 149 (1966) 301.
- Suzuki, M. and Kubo, R., J. Phys. Soc. Japan 24 (1968) 51.
   Mamada, H. and Takano, F., J. Phys. Soc. Japan 25 (1968) 675.
   Matsudaira, N., Canad, J. Phys. 45 (1967) 2091; J. Phys. Soc. Japan 23 (1967) 232.
   Kawasaki, K. and Yamada, T., Progr. theor. Phys. 39 (1968) 1.
- Felderhof, B. U., Rep. math. Phys. 1 (1970) 215; 2 (1971) 151.
   Felderhof, B. U. and Suzuki, M., Physica 56 (1971) 43.
   Hilhorst, H.J., Suzuki, M. and Felderhof, B. U., Physica 60 (1972) 199.
- Yahata, H. and Suzuki, M., J. Phys. Soc. Japan 27 (1969) 1421.
   Yahata, H., J. Phys. Soc. Japan 30 (1971) 657.
- 5) Van Kampen, N.G., Canad. J. Phys. 39 (1961) 551.
- Kubo, R., Lectures in Theoretical Physics, Vol. I (Boulder, 1958), Interscience Publishers, Inc. (New York, 1959), p. 120.
- 7) Glauber, R.J., J. math. Phys. 4 (1963) 294.
- 8) Kittel, C. and Shore, H., Phys. Rev. 138 (1965) A1165.
- See e.g. Wilkinson, J. H., The Algebraic Eigenvalue Problem, Clarendon Press (Oxford, 1965) section 37, p. 300.
- 10) For a simple discussion see Mattis, D.C., The Theory of Magnetism, Harper and Row (New York, 1965) ch. 6.
- 11) Wilkinson, J.H., op. cit., section 38, p. 300.
- 12) Van Kampen, N.G., J. math. Phys. 2 (1961) 592.
- 13) Nishikawa, K., Progr. theor. Phys. 38 (1967) 305.
- 14) Kubo, R. and Tomita, K., J. Phys. Soc. Japan 9 (1954) 888.
- 15) Casati, G., Physica 46 (1970) 391.
- 16) Van Vianen, H.A.W. and Tjon, J.A., Physica 48 (1970) 497.
- Widder, D. V., The Laplace Transform, Princeton University Press (Princeton, 1946) p. 160, theorem 12a.