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1976 J. Phys. A: Math. Gen. 9 975

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A generalized Fokker-Planck equation for the Ising model

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Received 24 October 1975, in final form 5 February 1976

Abstract. The Fokker-Planck equation is constructed in the space of two variables: s , the long-range order and ϕ , the nearest neighbour correlation function, in the quasi-chemical approximation. This generalizes the equation in the Bragg-Williams approximation earlier presented by two of the authors in which the only variable was s . The master equation is taken as the starting point and expressions are obtained for the transition probabilities. The equations of motion for the mean values of s and ϕ are derived; they behave satisfactorily in an asymptotic manner and yield the thermodynamic values. The time-dependent fluctuations are not given by the approximations used; the fluctuations in equilibrium are derived from the bivariate normal distribution representing the equilibrium state.

1. Introduction and definitions

The Fokker-Planck equation for the Ising model in the Bragg-Williams approximation has recently been analysed in some detail by Bolton and Leng (1973, 1975) and its relation to the Liouville equation established by Goldstein and Scully (1973) and Wang (1973). In the present paper we discuss the Fokker-Planck equation in the Bethe-Peierls or quasi-chemical approximation. This introduces a generalization into the problem which is interesting in its own right and which suggests the structure of the equation for higher approximations. Meijer and Edwards (1969) discussed a master equation in the Bethe-Peierls approximation and showed that the critical slowing down in this approximation is essentially the same as in the Bragg-Williams approximation or molecular field approximation (Suzuki and Kubo 1968). Indeed we should not expect to get new results about the relaxation from these low-order approximations but the interest in their study is to examine the relationship between the time-dependent and the thermodynamic solutions.

In the Bragg-Williams (BW) and mean field approximation (MFA) we have only one function in the description of the problem, the long-range order s , which we define by $s = \langle s_i \rangle$ where $s_i = \pm 1$, $i = 1 \dots N$; to proceed to the higher quasi-chemical approximation, it was found convenient in another problem (Bolton *et al* 1972) to introduce the nearest-neighbour correlation function defined by $\phi = \langle s_i s_j \rangle$. We now expect the Fokker-Planck differential equation to be defined by the time-dependence in an $\{s, \phi\}$ space. We are concerned here with the structure of this differential equation.

In the quasi-chemical approximation, the exact Ising Hamiltonian

$$H = -J \sum_{\langle ij \rangle} s_i s_j - m H_0 \sum_i s_i \quad (1.1)$$

becomes

$$E(s, \phi) = -\frac{1}{2}NzJ\phi - mH_sNs \quad (1.2)$$

where z is the coordination number of the lattice. We define in the usual way (Domb 1960) N_1 as the number of + spins, N_2 as the number of down spins, N_{11} , N_{22} and N_{12} as the numbers of (+ +), (- -) and (+ -) nearest-neighbour bonds respectively; then we have

$$\phi = (N_{11} + N_{22} - N_{12})/\frac{1}{2}zN \quad (1.3)$$

and in terms of s and ϕ , we have

$$N_{11} = \frac{1}{8}zN(1 + 2s + \phi) \quad (1.4)$$

$$N_{22} = \frac{1}{8}zN(1 - 2s + \phi) \quad (1.5)$$

$$N_{12} = \frac{1}{4}zN(1 - \phi). \quad (1.6)$$

To find the degeneracy $\Omega(s, \phi)$ we treat all types of nearest-neighbour pairs (or bonds) as independent; we include (+ -) and (- +) pairs where it is assumed that there are $\frac{1}{2}N_{12}$ of each. Then

$$\Omega(s, \phi) = \mathcal{N}(\frac{1}{2}zN)! / (N_{11})!(\frac{1}{2}N_{12})!(\frac{1}{2}N_{12})!(N_{22})!. \quad (1.7)$$

The normalization factor \mathcal{N} is determined by the condition

$$\sum_{\phi} \Omega(s, \phi) = \Omega(s) = N! / N_1! N_2!$$

which gives

$$\mathcal{N} = \Omega(s) / (\frac{1}{2}zN)! \sum_{\phi} [(N_{11})!(\frac{1}{2}N_{12})!(\frac{1}{2}N_{12})!(N_{22})!]^{-1}. \quad (1.8)$$

This expression is simplified by replacing the summation by the largest term. By differentiating with respect to ϕ it can be shown that the MFA value $\phi = s^2$ maximizes the value of \mathcal{N} . The notation N_{ij}^0 is used to represent N_{ij} with $\phi = s^2$ so that the degeneracy is given by

$$\Omega(s, \phi) = (N! / N_1! N_2!) [(N_{11}^0)! (\frac{1}{2}N_{12}^0)! (\frac{1}{2}N_{12}^0)! (N_{22}^0)!] / [(N_{11})! (\frac{1}{2}N_{12})! (\frac{1}{2}N_{12})! (N_{22})!]. \quad (1.9)$$

2. Transition probabilities

We introduce the function $P(s, \phi; t)$ $ds d\phi$ which represents the probability that the system has instantaneous values in the ranges s to $s + ds$ and ϕ to $\phi + d\phi$. We consider only single-spin reversals. The consequent change in s is $\pm\delta$ and in ϕ , the change is $\pm\Delta$. We write the master equation for the system as

$$\begin{aligned} \tau \frac{\partial P}{\partial t}(s, \phi; t) = & -P(s, \phi; t)[W^+(s, \phi) + W^-(s, \phi)] \\ & + P(s + \delta, \phi + \Delta; t)W^-(s + \delta, \phi + \Delta) + P(s - \delta, \phi - \Delta; t)W^+(s - \delta, \phi - \Delta). \end{aligned} \quad (2.1)$$

The superscripts + and - represent the respective increase and decrease of both the s and ϕ values which result from a spin flipping from down to up (+) and vice versa (-). We define $W^\pm(s, \phi)$ as the transition probabilities for the single spin flips which change s to $s \pm \delta$ and ϕ to $\phi \pm \Delta$. Correspondingly $W^+(s - \delta, \phi - \Delta)$ is the transition probability for the single spin flip which changes $s - \delta$ to s and $\phi - \Delta$ to ϕ , and $W^-(s + \delta, \phi + \Delta)$ is the transition probability for the single spin flip which changes $s + \delta$ to s and $\phi + \Delta$ to ϕ . As in Bolton and Leng, $\delta = 2/N$ and we offer the following way of calculating Δ approximately. We consider a Bethe-Peierls cluster of a given spin and its z neighbours which are recognized as 'edge' spins of the cluster. The probability of an edge spin having the value +1 or -1 may be taken approximately to be the global values N_1/N or N_2/N . If the central spin is down initially, the contribution to N_{12} from this cluster is zN_1/N . Thus the contribution to N_{12} of a reversal of the central spin from down to up is

$$\Delta N_{12} = z(N_2 - N_1)/N = -zs.$$

Using equation (1.6) we have

$$\Delta = -4\Delta N_{12}/zN = 4s/N \tag{2.2}$$

so that on this approximation the changes in s and ϕ are related. We note that this value of Δ would be the dominant term if we chose $\phi = s^2$, which is the MFA value.

If we consider equilibrium then we can use detailed balance in the form

$$P_0(s, \phi)W^+(s, \phi) = P_0(s + \delta, \phi + \Delta)W^-(s + \delta, \phi + \Delta) \tag{2.3}$$

and if we can estimate expressions for W^+ and W^- from the above equation then we can assume that when not in equilibrium, W^+ and W^- have the same structure. The probability P_0 in equation (2.3) is the equilibrium probability given by

$$P_0(s, \phi) = \exp[-\beta F(s, \phi)] \tag{2.4}$$

where $F(s, \phi)$ represents the Helmholtz free energy. Since we define F by

$$F(s, \phi) = E(s, \phi) - kT \ln \Omega(s, \phi) \tag{2.5}$$

we get

$$P_0(s, \phi) = \Omega(s, \phi) \exp[-\beta E(s, \phi)]. \tag{2.6}$$

Substituting this into the detailed balance condition, and putting $H_0 = 0$, we obtain

$$\frac{W^+(s, \phi)}{W^-(s + \delta, \phi + \Delta)} = \frac{\Omega(s + \delta, \phi + \Delta)}{\Omega(s, \phi)} \exp(\frac{1}{2}Na\Delta) \tag{2.7}$$

where $a = \beta zJ$. On substituting for the degeneracy from equation (1.9), the factorials which are a function of s only simplify due to the relations

$$N_1(s \pm \delta) = N_1(s) \pm 1, \quad \text{and} \quad N_2(s \pm \delta) = N_2(s) \mp 1.$$

However, with the present choice of Δ , the quantities N_{11} , N_{22} and N_{12} are not integers in general and the changes in these quantities given by zN_1/N , $-zN_2/N$ and $-zs$ respectively do not have integer values. Simplification of the factorials in equation (2.7) by cancellation is not possible and to make progress we use Stirling's approximation in its lowest order, $\ln N! = N \ln N - N$ if N is large, with an error $O(N^{-1})$. The width of our probability function is expected to be $O(N^{-1/2})$ and if we calculate the second moment this will be $O(N^{-1})$. We should not expect therefore to be able to calculate the second moment satisfactorily by our equations.

The logarithm of both sides of equation (2.7) was taken and Stirling's formula applied. After straightforward but long algebra, we get the following ratio of the transition probabilities:

$$\begin{aligned} & \frac{W^+(s, \phi)}{W^-(s + \delta, \phi + \Delta)} \\ &= \frac{N_2(s)}{N_1(s + \delta)} \left(\frac{1 + 2s + \phi}{1 + 2(s + \delta) + \phi + \Delta} \right)^{\frac{1}{2}zN(1 + 2s + \phi)} \left(\frac{1 - \phi}{1 - \phi - \Delta} \right)^{\frac{1}{2}zN(1 - \phi)} \\ & \times \left(\frac{1 - 2s + \phi}{1 - 2(s + \delta) + \phi + \Delta} \right)^{\frac{1}{2}zN(1 - 2s + \phi)} \left(\frac{1 + 2(s + \delta) + (s + \delta)^2}{1 + 2s + s^2} \right)^{\frac{1}{2}zN(1 + 2s + s^2)} \\ & \times \left(\frac{1 - (s + \delta)^2}{1 - s^2} \right)^{\frac{1}{2}zN(1 - s^2)} \left(\frac{1 - 2(s + \delta) + (s + \delta)^2}{1 - 2s + s^2} \right)^{\frac{1}{2}zN(1 - 2s + s^2)} \left(\frac{1 + (s + \delta)}{1 - (s + \delta)} \right)^z \\ & \times \left(\frac{1 - 2(s + \delta) + \phi + \Delta}{1 + 2(s + \delta) + \phi + \Delta} \right)^{\frac{1}{2}z} \left(\frac{[1 - (\phi + \Delta)]^2}{[1 + 2(s + \delta) + \phi + \Delta][1 - 2(s + \delta) + \phi + \Delta]} \right)^{\frac{1}{2}zs} \\ & \times \left(\frac{[1 + 2(s + \delta) + (s + \delta)^2][1 - 2(s + \delta) + (s + \delta)^2]}{[1 - (s + \delta)^2]^2} \right)^{\frac{1}{2}z(s + 1/N)} \\ & \times \exp[2(as + \beta H_0 m)]. \end{aligned} \tag{2.8}$$

At a similar point in the Bragg-Williams calculation, Bolton and Leng (1973) made choices of W^+ and W^- which, apart from unimportant multiplicative factors, allowed progress to be made describing equilibrium correctly and adequately defining the approach to equilibrium. There seems to be little hope of similar choices from equation (2.8). The only route forward from this equation seemed to be by the simplification $\delta = \Delta = 0$. By rearrangement the expression reduces to

$$\frac{W^+(s, \phi)}{W^-(s, \phi)} = \frac{N_2(s)(1 + s)^z [(1 - \phi)/(1 + 2s + \phi)]^{\frac{1}{2}z(1 + s)} \exp(as + \beta H_0 m)}{N_1(s)(1 - s)^z [(1 - \phi)/(1 - 2s + \phi)]^{\frac{1}{2}z(1 - s)} \exp[-(as + \beta H_0 m)]} \tag{2.9}$$

An alternative and simpler way of deriving equation (2.9), which was pointed out by a referee, is to use the asymptotic expansion

$$\Gamma(x + a)/\Gamma(x + b) = x^{(a-b)}(1 + O(x^{-1})) \quad \text{as } x \rightarrow \infty$$

(Abramowitz and Stegun 1965, chap 6, p 257). It can readily be proved that equation (2.9) is the leading term in the asymptotic expansion of equation (2.7).

We choose the transition probabilities

$$W^+(s, \phi) = \frac{1}{2}N(1 - s)(1 + s)^z [(1 - \phi)/(1 + 2s + \phi)]^{\frac{1}{2}z(1 + s)} \exp(as + \beta H_0 m) \tag{2.10}$$

$$W^-(s, \phi) = \frac{1}{2}N(1 + s)(1 - s)^z [(1 - \phi)/(1 - 2s + \phi)]^{\frac{1}{2}z(1 - s)} \exp[-(as + \beta H_0 m)]. \tag{2.11}$$

There was little to guide our choice beyond a feeling for symmetry and a sense of the propriety of the functions needed to yield the equilibrium values. We note in passing that

$$W^-(s, H_0, \phi) = W^+(-s, -H_0, \phi) \tag{2.12}$$

which can be compared with the similar result from the Bragg-Williams approximation of Bolton and Leng (1973), namely,

$$W^-(s, H_0) = W^+(-s, -H_0). \tag{2.13}$$

3. The generalized Fokker-Planck equation

We can now obtain the Fokker-Planck equation. We need to define $A(s, \phi)$ and $B(s, \phi)$ through

$$A(s, \phi) = W^+(s, \phi) + W^-(s, \phi) \tag{3.1}$$

$$B(s, \phi) = W^+(s, \phi) - W^-(s, \phi) \tag{3.2}$$

and we expand $P(s \pm \delta, \phi \pm \Delta; t)$ and $W^\mp(s \pm \delta, \phi \pm \Delta)$ about (s, ϕ) . Substituting these expansions in the quasi-chemical master equation we get

$$\tau \frac{\partial P(s, \phi; t)}{\partial t} = - \left(\delta \frac{\partial(PB)}{\partial s} + \Delta \frac{\partial(PB)}{\partial \phi} \right) + \frac{1}{2!} \left(\delta^2 \frac{\partial^2(PA)}{\partial s^2} + 2\delta\Delta \frac{\partial^2(PA)}{\partial s \partial \phi} + \Delta^2 \frac{\partial^2(PA)}{\partial \phi^2} \right) + \dots \tag{3.3}$$

In a way similar to that given in Bolton and Leng we can examine the order of magnitude of the terms in equation (3.3) by considering expansions about $s = \sigma$ and $\phi = \eta$, the two values at the centre of the $P_0(s, \phi)$ distribution. Retaining only those terms needed to give correctly the first and second moments of the $P(s, \phi; t)$ we get

$$\tau \frac{\partial P(s, \phi; t)}{\partial t} = - \frac{2}{N} \frac{\partial(PB)}{\partial s} - \frac{4s}{N} \frac{\partial(PB)}{\partial \phi} + \frac{2}{N^2} A \frac{\partial^2 P}{\partial s^2} + \frac{8s}{N^2} A \frac{\partial^2 P}{\partial s \partial \phi} + \frac{8s^2}{N^2} A \frac{\partial^2 P}{\partial \phi^2} \tag{3.4}$$

which is the generalized Fokker-Planck equation sought. As in other such equations the first-order terms essentially describe the 'drift' or the time-evolution of the first moments and the second-order terms essentially describe the 'diffusion' or the time-evolution of the second moments.

We can now obtain the coupled time-dependent equations for the first moments $\langle s(t) \rangle, \langle \phi(t) \rangle$ defined by

$$\begin{aligned} \langle s(t) \rangle &= \int_{-1}^1 d\phi \int_{-1}^1 ds s P(s, \phi; t) \\ \langle \phi(t) \rangle &= \int_{-1}^1 ds \int_{-1}^1 d\phi \phi P(s, \phi; t). \end{aligned} \tag{3.5}$$

The boundary conditions needed are as follows:

$$\begin{aligned} P(\pm 1, \phi; t) &= P(s, \pm 1; t) = 0 \\ \left(\frac{\partial P}{\partial s} \right)_{s=\pm 1, \phi} &= \left(\frac{\partial P}{\partial s} \right)_{s, \phi=\pm 1} = 0 \\ \left(\frac{\partial P}{\partial \phi} \right)_{s=\pm 1, \phi} &= \left(\frac{\partial P}{\partial \phi} \right)_{s, \phi=\pm 1} = 0. \end{aligned} \tag{3.6}$$

We put $H_0 = 0$, and use only the first-order terms of equation (3.4). Performing the double integrations in equations (3.5), integrating by parts and using the boundary conditions we get

$$\tau \frac{\partial \langle s(t) \rangle}{\partial t} = \frac{2}{N} \langle B(s, \phi) \rangle \tag{3.7}$$

and

$$\tau \frac{\partial}{\partial t} \langle \phi(t) \rangle = \frac{4}{N} \langle sB(s, \phi) \rangle. \quad (3.8)$$

Our probability functions are always sharply peaked about their average or most probable value, so that, defining

$$s_0(t) = \langle s(t) \rangle \quad \text{and} \quad \phi_0(t) = \langle \phi(t) \rangle$$

we can replace equation (3.7) by

$$\begin{aligned} \tau \frac{\partial s_0}{\partial t} = C = & (1+s_0)(1-s_0) \{ (1+s_0)^{z-1} [(1-\phi_0)/(1+2s_0+\phi_0)]^{\frac{1}{2}z(1+s_0)} \\ & \times \exp(as_0) - (1-s_0)^{z-1} [(1-\phi_0)/(1-2s_0+\phi_0)]^{\frac{1}{2}z(1-s_0)} \exp(-as_0) \}. \end{aligned} \quad (3.9)$$

Defining $C(s_0, \phi_0)$ as the right hand side of equation (3.9), then

$$\tau \frac{\partial \phi_0}{\partial t} = 2s_0 C(s_0, \phi_0). \quad (3.10)$$

It is straightforward to check that either equation (3.7) or equation (3.8) yields the correct equilibrium condition. We define

$$s_0(\infty) = \sigma \quad \phi_0(\infty) = \eta \quad (3.11)$$

and when $\partial/\partial t = 0$, we have

$$C(\sigma, \eta) = 0$$

whose terms can be rearranged to give

$$\frac{(1-\eta)^2}{(1+2\sigma+\eta)(1-2\sigma+\eta)} = \exp\left(-\frac{4a}{z}\right) \left[\left(\frac{1-\sigma}{1+\sigma}\right)^{2(z-1)} \left(\frac{1+2\sigma+\eta}{1-2\sigma+\eta}\right)^z \right]^{1/z\sigma} \quad (3.12)$$

The thermodynamic route to the equilibrium condition is through the minimization of the free energy $F(s, \phi)$ with respect to s and ϕ . The minimum occurs at $s = \sigma$ and $\phi = \eta$ and the two coupled equations are given by Lee (1971) and Bolton *et al* (1972) after zeroing all terms referring to the spin-phonon coupling; the two equations are

$$(1-\eta)^2/(1+2\sigma+\eta)(1-2\sigma+\eta) = \exp(-4a/z) \quad (3.13)$$

and

$$\left(\frac{1+\sigma}{1-\sigma}\right)^{2(z-1)} \left(\frac{1+2\sigma+\eta}{1-2\sigma+\eta}\right)^z = 1. \quad (3.14)$$

Combining equations (3.13) and (3.14) gives agreement with equation (3.12).

From what has been said earlier about the approximations made in the structure of the transition probabilities, it should not be surprising to learn that no information is given from the present Fokker-Planck equation (3.4) about the second moments of the probability function. A higher approximation would be needed for the transition probabilities before the second moments could be given adequately; the algebra, already lengthy in the present approximation could be prohibitive.

4. Equilibrium fluctuations

Although we cannot get the time-dependence of the second moments from the present Fokker–Planck equation we can readily get them in the equilibrium state, defined by equation (2.4). We rewrite this in terms of small deviations from the equilibrium average values σ and η as a bivariate normal distribution:

$$P_0(s, \phi) = D \exp \left[- \left(\frac{(s - \sigma)^2}{2M_2^s} - \frac{(s - \sigma)(\phi - \eta)M_2^{s\phi}}{M_2^s M_2^\phi} + \frac{(\phi - \eta)^2}{2M_2^\phi} \right) \right] \quad (4.1)$$

where D is the normalization constant and $M_2^{s\phi}$ is the covariance of the distribution (Feller 1968). Expanding equation (2.4) to second order, we make the identifications

$$M_2^s = \beta^{-1} \left(\frac{\partial^2 F}{\partial s^2} \right)_{\sigma, \eta}^{-1} = \left(\frac{zN(1 + \eta)}{(1 + \eta)^2 - 4\sigma^2} - \frac{N(z - 1)}{1 - \sigma^2} \right)^{-1} \quad (4.2)$$

$$M_2^\phi = \beta^{-1} \left(\frac{\partial^2 F}{\partial \phi^2} \right)_{\sigma, \eta}^{-1} = \left(\frac{\frac{1}{2}zN(1 + \eta - 2\sigma^2)}{(1 - \eta^2)(1 + \eta) - 4\sigma^2(1 - \eta)} \right)^{-1} \quad (4.3)$$

$$M_2^{s\phi} = -\beta^{-1} \left(\frac{\partial^2 F}{\partial s \partial \phi} \right)_{\sigma, \eta} \left(\frac{\partial^2 F}{\partial s^2} \right)_{\sigma, \eta}^{-1} \left(\frac{\partial^2 F}{\partial \phi^2} \right)_{\sigma, \eta}^{-1} = \left(\frac{zN\sigma}{(1 + \eta)^2 - 4\sigma^2} \right) M_2^s M_2^\phi. \quad (4.4)$$

The behaviour of these quantities can readily be given in terms of the equilibrium relationships (3.13) and (3.14) between σ and η . The critical temperature T_c is defined by

$$J/kT_c = \frac{1}{2} \ln z/(z - 2).$$

For $T > T_c$, we have $\sigma = 0$ and $\eta = \tanh \beta J$. At T_c , we have

$$\eta_c = 1/(z - 1)$$

and M_2^s diverges as T approaches T_c .

In zero magnetic field, expression (1.2) shows that energy E is proportional to ϕ and since the specific heat C_V is defined by

$$C_V = M_2^E/kT^2$$

we see that $C_V \propto M_2^E$, which remains finite at $T = T_c$. We see from equation (4.4) that the covariance $M_2^{s\phi}$ is zero for $T > T_c$. It diverges as $T \rightarrow T_c^-$.

5. Conclusion

We have shown that we can extend the Fokker–Planck equation in the single dimension s for the Ising model in lowest approximation to a generalized equation in the two dimensions (s, ϕ) . Two approximations had to be made; firstly, we had to put both δ and Δ equal to zero in analysing the ratio of the transition probabilities in the equation and secondly we had to use Stirling’s approximation. Neither are likely to give trouble if we are only concerned with the time-dependence of the mean values of s and ϕ and indeed, our equilibrium condition is exactly that given by thermodynamics. If however we wanted to examine the fluctuations in the time-dependent equations, the two approximations that we have used are not adequate. We know what the fluctuations are

like in equilibrium in this Bethe–Peierls approach to the Ising model; from our experience it seems that the algebra of a successful Fokker–Planck equation could be very heavy.

Acknowledgment

One of us, C A Leng wishes to acknowledge a Commonwealth of Australia Post-graduate Research Award. All the authors acknowledge the cooperative and constructive comments of one referee.

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