Time-Dependent Statistics of the Ising Model

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The individual spins of the Ising model are assumed to interact with an external agency (e.g., a heat reservoir) which causes them to change their states randomly with time. Coupling between the spins is introduced through the assumption that the transition probabilities for any one spin depend on the values of the neighboring spins. This dependence is determined, in part, by the detailed balancing condition obeyed by the equilibrium state of the model. The Markoff process which describes the spin functions is analyzed in detail for the case of a closed N-member chain. The expectation values of the individual spins and of the products of pairs of spins, each of the pair evaluated at a different time, are found explicitly. The influence of a uniform, time-varying magnetic field upon the model is discussed, and the frequency-dependent magnetic susceptibility is found in the weak-field limit. Some fluctuation–dissipation theorems are derived which relate the susceptibility to the Fourier transform of the time-dependent correlation function of the magnetization at equilibrium.

INTRODUCTION

THE statistical study of systems of strongly interacting particles is beset by many problems, largely mathematical in nature. These difficulties have motivated theorists to devote a great deal of effort to devising and studying the simplest sorts of model systems which show any resemblance to those occurring in nature. The property most desired in these models is mathematical transparency. The deeper insights offered by the possibility of exact treatment are intended to compensate for any unrealistic simplifications in the formulation. The first, and most successful of these models is one introduced by Ising[1] in an attempt to explain the ferromagnetic phase transition. While many generalizations of this model have been studied, we may note that the first true understanding of a phase transition in an interacting system was reached by Onsager[2] for the case of the two-dimensional Ising model.

If the mathematical problems of equilibrium statistical mechanics are great, they are at least relatively well-defined. The situation is quite otherwise in dealing with systems which undergo large-scale changes with time. The principles of nonequilibrium statistical mechanics remain in largest measure unformulated. While this lack persists, it may be useful to have in hand whatever precise statements can be made about the time-dependent behavior of statistical systems, however simple they may be.

We have attempted, therefore, to devise a form of the Ising model whose behavior can be followed exactly, in statistical terms, as a function of time. While certain of the assumptions underlying the model are to a degree arbitrary, it is surely one of the simplest ones involving N coupled particles for which exact time-dependent solutions can be found.

The model we shall discuss is a stochastic one. The spins of N fixed particles are represented as stochastic functions of time $\sigma_j(t)$, $(j = 1, \cdots N)$, which are restricted to the values ± 1, and make transitions randomly between these two values. These transitions take place because of the interaction of the spins with an external agency which may be regarded as a heat reservoir. The transition probabilities of the individual spins, however, are assumed to depend on the momentary values of the neighboring spins as well as on the influence of the heat bath. It is for this reason that statistical correlations arise between the values of neighboring spins. The coupling of the spins through their transition probabilities makes it necessary, in mathematical terms, to deal with the entire N-spin system as a unit. The spin functions form a Markoff process of N discrete random variables with a continuous time variable as argument. Fortunately, if the coupling of the spins is not too complicated, the differential equations governing the probabilities may be simplified greatly, making it possible to solve for all of the quantities of immediate physical interest by elementary means.

In the sections that follow, we introduce first the individual spins interacting with the heat bath, then the means by which they are coupled to one another. The description of the behavior of the model

[1] E. Ising, Z. Physik 31, 253 (1925).
[2] L. Onsager, Phys. Rev. 65, 117 (1944).

is then formulated as a matter of solving for the expectation values of the spin functions and of their products. We center the subsequent discussion largely upon explicit solutions for the single-spin and two-spin averages, since most of the interesting properties of the system may be constructed in terms of these. In addition we find the time-delayed spin correlation function, i.e. the average product of two spin variables, each evaluated at a different time. We then describe the model in the presence of a uniform, time-varying magnetic field. Two results of this generalization are a derivation of the complex frequency-dependent magnetic susceptibility for weak fields, and a discussion of fluctuation–dissipation relations which hold when the field-induced departures from equilibrium are small. Our efforts, in the present paper, are confined to treating a one-dimensional model which, as already indicated by the treatment of the Ising model at equilibrium,[2] appears to be a great deal simpler than dealing with the model in two or more dimensions.

SINGLE-SPIN SYSTEM

It may be helpful in introducing our model to begin by discussing the most simple of such systems: a single particle whose interaction with a heat reservoir of some sort causes its spin to flip between the values $\sigma = 1$ and $\sigma = -1$ randomly, but at a known rate. We assume that no magnetic field is present so that neither of the states $\sigma = \pm 1$ is preferred. Then, if the rate per unit time at which the particle makes transitions from either state to the opposite one is written as $\alpha/2$, the probability $p(\sigma, t)$ that the spin takes on the value σ at time t obeys the equation

$$(d/dt)p(\sigma, t) = -\tfrac{1}{2}\alpha p(\sigma, t) + \tfrac{1}{2}\alpha p(-\sigma, t). \quad (1)$$

This equation, or more properly, this pair of equations for $\sigma = \pm 1$, preserves the normalization condition

$$p(1, t) + p(-1, t) = 1. \quad (2)$$

The pair of equations is therefore immediately reducible to a single equation for a single unknown function. A convenient choice of the latter function is the difference of the two probabilities

$$q(t) = p(1, t) - p(-1, t)$$
$$= \sum_{\sigma = -1} \sigma p(\sigma, t), \quad (3)$$

which is simply the expectation value of the spin as a function of time, i.e. if we think of the time-dependent spin variable as a stochastic function

$\sigma(t)$ taking on the values $\sigma = \pm 1$ we have

$$q(t) = \langle \sigma(t) \rangle. \quad (4)$$

The equation obeyed by the mean spin is seen from (1) to be

$$(d/dt)q(t) = -\alpha q(t), \quad (5)$$

so that the mean spin simply decays exponentially with a relaxation time $1/\alpha$ from whatever value it is known to have initially,

$$q(t) = q(0)e^{-\alpha t}. \quad (6)$$

We may regain the individual probabilities $p(\pm 1, t)$ from a knowledge of $q(t)$ by means of the identities (2) and (3) which together yield

$$p(\sigma, t) = \tfrac{1}{2}[1 + \sigma q(t)]. \quad (7)$$

MANY-SPIN SYSTEM

Particles such as the one we have just discussed, each of them responding to a random spin-flipping agency, will form the basic units of the model we wish to describe. We shall assume that these particles are arranged in a regularly spaced linear array which may be closed to form an N-particle ring. The dynamical resemblance between this model and the Ising model rests on the assumption that the individual spins of the ring are not wholly independent stochastic functions. We may, for example, introduce a tendency for a particular spin σ_j ($j = 1 \cdots N$) to correlate with its neighboring spins by assuming that its transition probabilities between the states $\sigma_j = \pm 1$ depend appropriately on the momentary spin values of the other particles. To treat any such model we must consider the entire ring as a unit and introduce a set of 2^N probability functions $p(\sigma_1, \cdots \sigma_N)$, one for each complexion, i.e. each set $\sigma_1, \cdots \sigma_N$ for the ring.

If we let $w_i(\sigma_i)$ be the probability per unit time that the jth spin flips from the value σ_j to $-\sigma_j$, while the others remain momentarily fixed, then we may write the time derivative of the function $p(\sigma_1, \cdots \sigma_N t)$ as

$$\frac{d}{dt} p(\sigma_1, \cdots \sigma_N t) = -\left[\sum_i w_i(\sigma_i)\right] p(\sigma_1, \cdots \sigma_N t)$$
$$+ \sum_i w_i(-\sigma_i) p(\sigma_1, \cdots -\sigma_i, \cdots \sigma_N t), \quad (8)$$

i.e., the complexion $\sigma_1, \cdots \sigma_N$ is destroyed by a flip of any of the spins σ_j, but it may also be created by spin flip from any complexion of the form $\sigma_1, \cdots -\sigma_j, \cdots \sigma_N$. We shall refer to Eq. (8) as the master equation since its solution would con-

tain the most complete description of the system available.

CORRESPONDENCE WITH THE ISING MODEL

We have already mentioned that the transition probabilities $w_i(\sigma_i)$ may be chosen to depend on neighboring spin values as well as on σ_j. If we want, for example, to describe a tendency for each spin to align itself parallel to its nearest neighbors we may choose the probabilities $w_i(\sigma_i)$ to be of the form

$$w_i(\sigma_i) = \tfrac{1}{2}\alpha\{1 - \tfrac{1}{2}\gamma\sigma_i(\sigma_{i-1} + \sigma_{i+1})\}, \qquad (9)$$

which may be seen to take on three possible values

$$w_i(\sigma_i) = \tfrac{1}{2}\alpha(1 - \gamma), \qquad \tfrac{1}{2}\alpha, \qquad \tfrac{1}{2}\alpha(1 + \gamma). \qquad (10)$$

The value $\tfrac{1}{2}\alpha$ corresponds to the case in which the neighboring spins are antiparallel, $\sigma_{i-1} = -\sigma_{i+1}$. When the neighboring spins are parallel to each other the transition probability takes on the value $\tfrac{1}{2}\alpha(1 - \gamma)$ for σ_i parallel to the two of them or $\tfrac{1}{2}\alpha(1 + \gamma)$ for σ_i antiparallel. Clearly as long as γ is positive the parallel configurations will be longer-lived than the antiparallel ones and we shall be dealing with a model having ferromagnetic tendencies. Conversely negative γ will mean a tendency of neighboring spins to remain aligned oppositely, and will describe the antiferromagnetic case. We note, incidently, that $|\gamma|$ may not exceed unity.

The parameter α which occurs in the transition probabilities simply describes the time scale on which all transitions take place. It has, of course, no analog in the familiar discussions of the Ising model at equilibrium. The parameter γ, however, describes the tendency of spins toward alignment and thereby determines the equilibrium state of the present model much as the exchange interaction does in the Ising model. To indicate the quantitative correspondence between the models we write the Hamiltonian for the linear Ising model as

$$\mathcal{3C} = -J \sum_i \sigma_i\sigma_{i+1}. \qquad (11)$$

When the Ising model has reached equilibrium at temperature T, the probability that the jth spin will take on the value σ_j as opposed to $-\sigma_j$ (for a given set of values of the neighboring spins) is just proportional to the Maxwell–Boltzmann factor $\exp(-\mathcal{3C}/kT)$. The ratio of the probabilities $p_i(-\sigma_i)$ and $p_i(\sigma_i)$ corresponding to the two states for the jth spin is therefore

$$\frac{p_i(-\sigma_i)}{p_i(\sigma_i)} = \frac{\exp[-(J/kT)\sigma_i(\sigma_{i-1} + \sigma_{i+1})]}{\exp[(J/kT)\sigma_i(\sigma_{i-1} + \sigma_{i+1})]}. \qquad (12)$$

If the spins other than σ_j are considered as fixed, the stochastic model described by (8) and (9) will approach an equilibrium in which

$$\frac{p_i(-\sigma_i)}{p_i(\sigma_i)} = \frac{w_i(\sigma_i)}{w_i(-\sigma_i)} \qquad (13)$$

$$= \frac{1 - \tfrac{1}{2}\gamma\sigma_i(\sigma_{i-1} + \sigma_{i+1})}{1 + \tfrac{1}{2}\gamma\sigma_i(\sigma_{i-1} + \sigma_{i+1})}. \qquad (14)$$

The exponentials which occur in the ratio (12) may be written in the forms

$$\exp[\pm(J/kT)\sigma_i(\sigma_{i-1} + \sigma_{i+1})]$$

$$= \cosh\left[\frac{J}{kT}(\sigma_{i-1} + \sigma_{i+1})\right]$$

$$\pm \sigma_i \sinh\left[\frac{J}{kT}(\sigma_{i-1} + \sigma_{i+1})\right] \qquad (15)$$

$$= \cosh\left[\frac{J}{kT}(\sigma_{i-1} + \sigma_{i+1})\right]$$

$$\times \left\{1 \pm \tfrac{1}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1})\tanh\frac{2J}{kT}\right\}, \qquad (16)$$

the latter of which is readily checked for the three values the function can take on. The correspondence between the ratios of the equilibrium probabilities (12) and (14) may evidently be made precise by identifying the constant γ as

$$\gamma = \tanh(2J/kT). \qquad (17)$$

We should mention that the particular choice we have made for the way in which the transition probabilities (9) depend on neighboring spin values is motivated more by the desire for simplicity than for generality. There exist other, but less simple, coupling schemes which also yield the same equilibrium states as the Ising model with nearest-neighbor interactions. Some of these are discussed in the Appendix. There exists, furthermore, the possibility that each spin is coupled through the transition probabilities to some or all of its more distant neighbors. We shall mention this possibility further at a later point. For the present we shall continue to deal with the transition probabilities (9) and discuss the mathematical treatment of the master equation based on them.

REDUCTION OF THE PROBABILITY FUNCTION

The functions $p(\sigma_1, \cdots \sigma_N t)$ which satisfy the master equation (8) furnish, as we have noted earlier, the fullest possible description of the system. While

we cannot deny that it would be desirable to know these functions in their entirety we must nevertheless point out that, for N large, they contain vastly more information than we usually require in practice. To answer the most familiar physical questions about the system, in fact, it suffices to know just the probabilities that individual spins or pairs of spins occupy specified states. Alternatively, we need know only the expectation values of spins or the average products of pairs of spins. Most of our attention in the present paper will be devoted to discussing just these functions. However before proceeding to the discussion, it may be helpful to indicate some general relations between the probability functions and the expectation values of products of spin variables.

We define the functions $q_i(t)$ to be the expectation values of the spins $\sigma_i(t)$ regarded as stochastic functions of time:

$$q_i(t) = \langle \sigma_i(t) \rangle \tag{18}$$
$$= \sum_{\{\sigma\}} \sigma_i p(\sigma_1, \cdots \sigma_N t).$$

Here and in future work we designate by a sum over $\{\sigma\}$, a sum carried out over the 2^N values of the set $\sigma_1, \cdots \sigma_N$. The functions $r_{j,k}(t)$ are defined, likewise, as the expectation values of the products $\sigma_i(t)\sigma_k(t)$:

$$r_{j,k}(t) = \langle \sigma_i(t)\sigma_k(t) \rangle$$
$$= \sum_{\{\sigma\}} \sigma_i \sigma_k p(\sigma_1, \cdots \sigma_N t). \tag{19}$$

We note in particular that the "diagonal" expectation values $r_{j,j}$ are identically unity:

$$r_{j,j}(t) = 1. \tag{20}$$

We next construct a general identity relating the probability to the expectation values as follows: Let σ_j and σ_j' be two possibly different values of the jth spin. Then the function $\frac{1}{2}(1 + \sigma_j\sigma_j')$ equals unity for $\sigma_j' = \sigma_j$ and zero for $\sigma_j' = -\sigma_j$. We may therefore construct an identity expressing $p(\sigma_1, \cdots \sigma_N t)$ as a sum over all spins by writing

$$p(\sigma_1, \cdots \sigma_N t) = \frac{1}{2^N}$$
$$\times \sum_{\{\sigma'\}} (1 + \sigma_1\sigma_1') \cdots (1 + \sigma_N\sigma_N')p(\sigma_1', \cdots \sigma_N', t). \tag{21}$$

If we expand the product in the summand of this relation and carry out the indicated summations, we find

$$p(\sigma_1, \cdots \sigma_N, t) = \frac{1}{2^N} \left\{ 1 + \sum_j \sigma_j q_j(t) \right.$$
$$\left. + \sum_{j \neq k} \sigma_j \sigma_k r_{j,k}(t) + \cdots \right\}, \tag{22}$$

which exhibits a general expansion of the probability functions in terms of the expectation values of the spins and their products taken two at a time, three at a time, etc., i.e. the functions 1 and σ form a complete orthogonal basis for the expansion of any function of σ, and (22) is just such an expansion with N independent variables. The relation (7) for a single spin is a trivial example of the expansion.

The reduced probability functions which furnish the probabilities that individual spins or pairs of spins occupy specified states, whatever may be the states of the remaining spins, are defined by

$$p_i(\sigma_i, t) = \sum_{\{\sigma \neq \sigma_i\}} p(\sigma_1, \cdots \sigma_N, t), \tag{23}$$
$$p_{ik}(\sigma_i, \sigma_k, t) = \sum_{\{\sigma \neq \sigma_i, \sigma_k\}} p(\sigma_1, \cdots \sigma_N, t), \tag{24}$$

where the notation is intended to indicate summation over all the spin variables save σ_i in (23) and σ_i and σ_k in (24). If these summations are carried out upon the form (22) for $p(\sigma_1, \cdots \sigma_N, t)$ we find

$$p_i(\sigma_i, t) = \frac{1}{2}\{1 + \sigma_i q_i(t)\}, \tag{25}$$
$$p_{ik}(\sigma_i, \sigma_k, t) = \frac{1}{4}\{1 + \sigma_i q_i(t)$$
$$+ \sigma_k q_k(t) + \sigma_i\sigma_k r_{j,k}(t)\}. \tag{26}$$

It should be clear that by solving for the expectation values of the spins and their products we are beginning a systematic expansion of the probability functions as well as finding the quantities of greatest physical interest.

As a preliminary step to finding the time-dependent equations satisfied by the expectation values, we may write the master equation (8) in the more compact form

$$\frac{d}{dt} p(\sigma_1, \cdots \sigma_N, t)$$
$$= - \sum_m \sigma_m \sum_{\sigma_m'} \sigma_m' w_m(\sigma_m') p(\sigma_1, \cdots \sigma_m', \cdots \sigma_N, t). \tag{27}$$

If we multiply both sides of this relation by σ_k and sum over all values of the σ variables we obtain

$$(d/dt)q_k(t) = -2 \sum \sigma_k w_k(\sigma_k) p(\sigma_1, \cdots \sigma_N, t)$$
$$= -2\langle \sigma_k(t) w_k[\sigma_k(t)] \rangle. \tag{28}$$

Similarly, if both sides of (27) are multiplied by the product $\sigma_j\sigma_k$ (where $j \neq k$) and summed over the σ variables we obtain

$$\frac{d}{dt} r_{j,k}(t)$$

$$= -2 \sum_{\{\sigma\}} \sigma_j \sigma_k \{w_j(\sigma_j) + w_k(\sigma_k)\} p(\sigma_1, \cdots \sigma_N, t)$$

$$= -2\langle \sigma_j(t)\sigma_k(t)\{w_j[\sigma_j(t)] + w_k[\sigma_k(t)]\}\rangle. \quad (29)$$

If we substitute the form (9) for the transition probabilities in (28) we obtain a recursive system of differential equations for the expectation values $q_k(t)$:

$$(d/d\alpha t)q_k(t) = -q_k(t) + \tfrac{1}{2}\gamma\{q_{k-1}(t) + q_{k+1}(t)\}. \quad (30)$$

An analogous system of equations for the expectation values of products of pairs of spins results from the substitution of (9) in (29). For $j \neq k$ we have

$$(d/d\alpha t)r_{j,k}(t) = -2r_{j,k}(t) + \tfrac{1}{2}\gamma\{r_{j,k-1}(t)$$

$$+ r_{j,k+1}(t) + r_{j-1,k}(t) + r_{j+1,k}(t)\}, \quad (31)$$

while for $j = k$, the functions obey the identity (20).

These equations, as we shall see, may be solved quite readily. It is worth noting, however, that the assumption of forms different from (9) for the transition probabilities leads, in many cases, to systems of equations in which the expectation values of products of differing numbers of spins are coupled in each equation. Such systems are considerably less tractable than the present one.

SOLUTION FOR THE AVERAGE SPINS: INFINITE RING

The coupled differential equations (30) are particularly easy to solve for the case of an infinite ring, $N \to \infty$. It is convenient, for this case, to alter slightly the scheme for numbering the spins by labeling a particular spin as the zeroth and designating those to one side of it with positive integers and those to the other side with negative ones. We then construct the generating function

$$F(\lambda, t) = \sum_{k=-\infty}^{\infty} \lambda^k q_k(t), \quad (32)$$

which, according to Eq. (30), satisfies the differential equation

$$(\partial/\partial\alpha t)F(\lambda, t) = -F(\lambda, t) + \tfrac{1}{2}\gamma(\lambda + \lambda^{-1})F(\lambda, t). \quad (33)$$

The solution for the generating function is evidently

$$F(\lambda, t) = F(\lambda, 0) \exp\left[-\alpha t + \tfrac{1}{2}\gamma(\lambda + \lambda^{-1})\alpha t\right], \quad (34)$$

which furnishes us an implicit solution for the $q_k(t)$ in terms of the initial values $q_k(0)$. To make the solution an explicit one we note that one of the factors in (34) is just the generating function for

the Bessel functions of imaginary argument,[3]

$$\exp\left[\tfrac{1}{2}x(\lambda + \lambda^{-1})\right] = \sum_{n=-\infty}^{\infty} \lambda^n I_n(x), \quad (35)$$

where

$$I_n(x) = i^{-n}J_n(ix). \quad (36)$$

Hence the time-dependent generating function is given by

$$F(\lambda, t) = F(\lambda, 0)e^{-\alpha t} \sum_{k=-\infty}^{\infty} \lambda^k I_k(\gamma\alpha t). \quad (37)$$

We consider first the case in which all of the spin expectations q_k vanish initially except for one, which we may choose to be the one at the origin

$$q_k(0) = \delta_{k,0}. \quad (38)$$

Then the initial value of the generating function is just unity, and at later times it is

$$F(\lambda, t) = e^{-\alpha t} \sum_{k=-\infty}^{\infty} \lambda^k I_k(\gamma\alpha t), \quad (39)$$

from which we conclude, by comparing with (32), that the spin expectations are given by

$$q_k(t) = e^{-\alpha t}I_k(\gamma\alpha t). \quad (40)$$

An examination of the functions I_k shows that q_0 decreases steadily to zero as time increases, while the neighboring spin expectations rise from zero to positive values for a while as a form of transient polarization induced by the positive spin at the origin. The functions q_k for spins neighboring the origin rise for times $t \ll k/\gamma\alpha$ as

$$q_k(t) \approx (1/|k|!)(\tfrac{1}{2}\gamma\alpha t)^{|k|}e^{-\alpha t}. \quad (41)$$

They then reach a maximum[4] at a time given, for $k \gg 1$, by $\alpha t \approx k(1 - \gamma^2)^{-\frac{1}{2}}$, and, for much larger times, decrease as

$$q_k(t) \sim (2\pi\gamma\alpha t)^{-\frac{1}{2}}e^{-\alpha(1-\gamma)t}. \quad (42)$$

The most general solution for the spin expectation values, corresponding to an arbitrary set of initial values $q_k(0)$, may clearly be obtained from (40) by linear superposition,

$$q_k(t) = e^{-\alpha t} \sum_{m=-\infty}^{\infty} q_m(0)I_{k-m}(\gamma\alpha t), \quad (43)$$

where we note that the functions I_n for negative

[3] See, for example, G. N. Watson, *Bessel Functions* (Cambridge University Press, Cambridge, England, 1958), pp. 14 and 77.

[4] The locations of the maxima and various other properties of the functions $e^{-\alpha x}I_n(x)$ for $\alpha \geq 1$ are discussed by E. W. Montroll, J. Math and Phys. **25**, 37 (1946).

order are the same as those for positive order, $I_n = I_{-n}$.

AVERAGE SPINS: FINITE RING

A somewhat more general means of treating the set of equations (30) for arbitrary N may be based on a system of normal modes for the spin expectation values q_k. If we seek solutions to Eqs. (30) in the form

$$q_k(t) = A\zeta^k e^{-\nu t}, \qquad (44)$$

where A is a constant, then we have

$$\nu = \alpha\{1 - \tfrac{1}{2}\gamma(\zeta^{-1} + \zeta)\}. \qquad (45)$$

The closure of the N-spin ring requires that the solution (44) be periodic in k with period N, i.e., that $\zeta^N = 1$. Hence there are N roots for ζ of the form

$$\zeta_m = \exp(2\pi i m/N), \quad m = 0, 1, \cdots N - 1, \qquad (46)$$

and for these the eigenvalues ν_m are

$$\nu_m = \alpha\{1 - \gamma\cos(2\pi m/N)\}. \qquad (47)$$

The system of mode functions $q_k^{(m)} = \exp(2\pi i m k/N)$ forms a complete orthogonal basis on the ring. Hence any solution to (30) may be written in the form

$$q_k(t) = \sum_{m=0}^{N-1} A_m e^{(2\pi i m k/N) - \nu_m t}, \qquad (48)$$

where the constants A_m may be solved for in terms of the $q_k(0)$ by using the orthogonality theorem. These constants are

$$A_m = \frac{1}{N} \sum_{l=1}^{N} q_l(0) e^{-2\pi i m l/N}. \qquad (49)$$

The solution for the spin expectation values in terms of their initial values is thus

$$q_k(t) = \frac{1}{N} \sum_{l,m} q_l(0) e^{(2\pi i m/N)(k-l) - \nu_m t}$$
$$= e^{-\alpha t} \sum_{l=1}^{N} \sum_{j=-\infty}^{\infty} q_l(0) I_{k-l+jN}(\gamma\alpha t). \qquad (50)$$

The latter form of the solution is obtained from the former by carrying out the summation over m explicitly. That the solutions may be expressed in this way is obvious from the fact that the problem for a finite ring may be solved by inserting periodic initial values in (43).

A particular consequence of the solution (50) is the fact that the total magnetization always decreases exponentially,

$$\sum_k q_k(t) = e^{-\alpha(1-\gamma)t} \sum_l q_l(0), \qquad (51)$$

a result which corresponds to the known absence of permanent magnetization in the linear Ising model (with interactions restricted to a finite number of neighbors). The net effect of the spin interactions is to reduce the coefficient in the exponent from the α of Eq. (6) to $\alpha(1 - \gamma)$.

SOLUTION FOR ONE SPIN FIXED

It is interesting to investigate the behavior of the spin system when one of the spins is assumed somehow to be fixed or frozen. We shall, for simplicity, consider the infinite ring and let the zeroth spin, the one at the origin, take on the fixed value $\sigma_0 = 1$. Then the differential equations derived earlier for the $q_k(t)$ still hold for $k \neq 0$. In particular, for $k = 1$, we have

$$(d/d\alpha t)q_1(t) = -q_1(t) + \tfrac{1}{2}\gamma\{1 + q_2(t)\}, \qquad (52)$$

while the equations for $k > 1$ assume precisely the form (30). This sequence of equations for $k \geq 1$ is an inhomogeneous one because of the constant term on the right-hand side of (52). It possesses a non-vanishing equilibrium solution, which satisfies the recursion relation

$$q_k = \tfrac{1}{2}\gamma\{q_{k-1} + q_{k+1}\}, \qquad k \neq 0, \qquad (53)$$

where $q_0 = 1$. The solution to such a linear difference equation may be written as

$$q_k = \eta^{|k|}, \qquad (54)$$

where η satisfies the quadratic equation

$$\eta^2 - 2\gamma^{-1}\eta + 1 = 0. \qquad (55)$$

It is worth noting that the same quadratic equation for η holds for negative values of k as for positive values of k, i.e., the equation is unchanged by the substitution of η^{-1} for η. The roots of (55), which are always real, form a reciprocal pair. One member of the pair, $\gamma^{-1}\{1 + (1 - \gamma^2)^{\frac{1}{2}}\}$, always has absolute value greater than unity for $|\gamma| \leq 1$ and therefore is of no use in solving the problem for an infinite ring. The correct root for η has absolute value less than unity and is given by

$$\eta = \gamma^{-1}\{1 - (1 - \gamma^2)^{\frac{1}{2}}\}. \qquad (56)$$

For this value, using the correspondence (17) with the static Ising model, we find

$$\eta = \tanh(J/kT). \qquad (57)$$

The solution (54) exhibits clearly the tendency of any spin, in this case a fixed one, to surround itself

with a "polarization cloud." (In the antiferromagnetic case, $\gamma < 0$, the signs of the induced spins will alternate.) The value of η given by (57) is just the familiar short-range order parameter of the Ising model.

To complete the solution of the time-dependent equations for the $q_k(t)$, with the zeroth spin fixed, we need only note that (54) constitutes a particular solution of the inhomogeneous system. We may add to it any solution to the homogeneous system of equations obtained by requiring q_0 to vanish at all times. Such a boundary condition may easily be satisfied by using the method of images, since the requirement $q_0 = 0$ separates the system into two halves which do not influence each other. (The infinite ring need not be imagined as closed.) If we seek a solution to the homogeneous system of equations in which the q_k assume a particular set of initial values, say v_k for $k > 0$, we may reach a solution for the positive-k half of the system by using the general solution (43) and imagining that the initial values of the q_k at the negative sites are given by $q_{-k}(0) = -v_k$ for $k > 0$, and that we have $q_0(0) = 0$. Interpreted in this way for $k > 0$, the solution (43) may be made to fit the correct initial conditions and yet, since it remains odd at k at all times, meet the boundary condition $q_0(t) = 0$ as well. An analogous imaging procedure solves the equations for negative k as well.

To find the general solution to the time-dependent equations with the zeroth spin fixed we must add together the particular solution (54) for the inhomogeneous system and the general solution, constructed by the method of images, for the homogeneous system, i.e., we add to the solution η^k the solution to the homogeneous system which corresponds for $k > 0$ to the set of initial values $q_k(0) - \eta^k$. The resulting solution for $k > 0$ is

$$q_k(t) = \eta^k + e^{-\alpha t} \sum_{l=1}^{\infty} (q_l(0) - \eta^l)$$
$$\times \{I_{k-l}(\gamma\alpha t) - I_{k+l}(\gamma\alpha t)\}. \quad (58)$$

An analogous solution exists for negative k values. For times $t \gg (\gamma\alpha)^{-1}$, the solutions in all cases decay exponentially to the equilibrium form.

SOLUTION FOR THE SPIN CORRELATIONS

We next turn our attention to the average values of products of pairs of spin variables. The functions $r_{j,k}(t)$ which express these averages obey the two-index system of Eqs. (31) for $j \neq k$, and for $j = k$ obey the identity $r_{j,j} = 1$. We can secure a rapid

insight into the behavior of these functions by simplifying the problem so that they depend, in effect, on only one index. It often happens, in fact, that our knowledge of the initial state of the system is characterized by translational invariance, i.e., our initial knowledge about all of the spins is the same. Then $r_{j,k}(0)$ can only depend on $j - k$, and no other dependence on j or k can be present at later times. In that case it becomes convenient to introduce the abbreviation

$$r_m = r_{k,k+m} \quad (59)$$

for the spin correlation functions. We shall consider this translationally invariant situation first and then return to the more general one presently.

In the uniform case the functions r_m are seen to obey the relations

$$(d/d\alpha t)r_m(t) = -2r_m(t) + \gamma\{r_{m-1}(t) + r_{m+1}(t)\} \quad (60)$$

for $m \neq 0$, and

$$r_0(t) = 1. \quad (61)$$

Aside from a trivial change of a factor of two in the coefficients, this is precisely the sequence of equations we solved in the preceding section, for the single-spin averages with the zeroth spin fixed. The factor of two in the coefficients affects only the time scale in which the functions change. In particular, the equilibrium solution on the infinite chain is again given by

$$r_m = \eta^{|m|}, \quad (62)$$

where η is the short-range order parameter mentioned earlier. The time-dependent solution for arbitrary initial correlations may be constructed immediately from (58). For $m > 0$ we have

$$r_m(t) = \eta^m + e^{-2\alpha t} \sum_{l=1}^{\infty} [r_l(0) - \eta^l]$$
$$\times \{I_{m-l}(2\gamma\alpha t) - I_{m+l}(2\gamma\alpha t)\}. \quad (63)$$

As a particular example of the type of problem to which this result is applicable, we may suppose that the spin system is suddenly subjected to a change of temperature; i.e., after coming to equilibrium with a heat reservoir at temperature T_0, it is suddenly placed in contact with another heat bath at a different temperature T. In that case the initial values of the r_l are given by

$$r_l(0) = \eta_0^l = [\tanh (J/kT_0)]^l, \quad (64)$$

and the way these relax into the equilibrium values at temperature T is shown by (63).

We return now to the general problem of solving

the two-index system of differential equations (31) without the simplifying assumption of translational invariance. The system is an inhomogeneous one because of the condition $r_{k,k}(t) = 1$, which plays a role similar to that of the fixed spin in the preceding section. The translationally invariant equilibrium solution $r_{k,l} = \eta^{|k-l|}$, which we have just discussed, clearly satisfies the system of equations. It can be used as a particular solution to the inhomogeneous system. To this particular solution, we must add a general solution to the homogeneous system obtained by supplementing (31) with the conditions $r_{k,k}(t) = 0$. The solutions to these equations may be obtained and the boundary conditions met by generalizing the methods of the preceding sections to deal with a two-index array $r_{j,k}(t)$, i.e. a matrix, rather than a linear sequence $q_i(t)$.

If, for the moment, we ignore the boundary condition on $r_{k,k}(t)$ and assume that Eqs. (31) hold even for $j = k$, it becomes a simple matter to solve the equations by using a two-parameter generating function analogous to (39). We then find that if all of the initial values of $r_{j,k}(0)$ vanish except one, which is unity, i.e.,

$$r_{j,k}(0) = \delta_{jl}\delta_{km}, \qquad (65)$$

the solution for $r_{j,k}(t)$ is

$$r_{j,k}(t) = e^{-2\alpha t}I_{j-l}(\gamma\alpha t)I_{k-m}(\gamma\alpha t). \qquad (66)$$

Such solutions may be superposed to secure the appropriate initial values and to meet the condition $r_{k,k}(t) = 0$. To satisfy the latter condition, we must generalize to a two-index array the method of images used earlier.

The matrix $r_{j,k}(t)$ is, or course, symmetric. However, it is quite convenient to think of it as if it were antisymmetric. What we shall do is fix our attention, for the moment, on the values of $r_{j,k}(t)$ for $j > k$ and only attempt to deal correctly with these. We assume that these matrix elements take on their correct initial values but that the elements $r_{k,j}(0)$ are given by $-r_{j,k}(0)$ for $j > k$, and that $r_{j,j}(0) = 0$. The matrix $r_{j,k}$ which is thus assumed initially antisymmetric, maintains its antisymmetry at later times and, therefore, always meets the condition $r_{j,j}(t) = 0$. In fact, it satisfies the sequence of equations (31) including, in virtue of its antisymmetry, the equation of the same form for $j = k$. We need not be embarrassed, therefore, by our inclusion of the $j = k$ equations in the arguments leading to (66).

The basic set of solutions we seek, which meets the initial condition (65) and the boundary condition

$r_{j,j}(t) = 0$, is just the solution (66) antisymmetrized in the two indices l and m, i.e., for $j \geq k$ and $l \geq m$

$$r_{j,k}(t) = e^{-2\alpha t}\{I_{j-l}(\gamma\alpha t)I_{k-m}(\gamma\alpha t)$$
$$- I_{j-m}(\gamma\alpha t)I_{k-l}(\gamma\alpha t)\}. \qquad (67)$$

The general solution to the homogeneous system is obtained by superposing the solutions (67). In order to solve the inhomogeneous system with which we began, we must add the particular solution η^{l-k} to the solutions we have just found. The form which satisfies the correct initial conditions for $j \geq k$ is

$$r_{j,k}(t) = \eta^{j-k} + e^{-2\alpha t}\sum_{l>m}[r_{l,m}(0) - \eta^{l-m}]$$

$$\times \{I_{j-l}(\gamma\alpha t)I_{k-m}(\gamma\alpha t) - I_{j-m}(\gamma\alpha t)I_{k-l}(\gamma\alpha t)\}, \qquad (68)$$

which is the general solution for the expectation values of the spin products. When translational invariance holds, this solution may be seen to reduce to (63) by applying the relation

$$I_k(2x) = \sum_{m=-\infty}^{\infty} I_{k+m}(x)I_m(x), \qquad (69)$$

which is a special case of the addition theorem for Bessel functions.[5]

TIME-DELAYED SPIN CORRELATION FUNCTIONS

The functions $r_{j,k}(t)$, which we have discussed up to this point, describe whatever tendency the pairs of spins σ_j and σ_k may have to be correlated in direction, on the average, at a particular instant of time t. Not all of the spin correlations of interest, however, have this instantaneous character. In particular, variation of any one spin at a given instant induces polarizations among its neighbors which only become appreciable after finite intervals of time. To describe correlation effects extending over an interval of length t', we shall discuss the functions $\langle\sigma_j(t)\sigma_k(t + t')\rangle$, i.e. the expectation values of the products of the stochastic spin functions σ_j evaluated at time t, and σ_k evaluated at time $t + t'$.

To evaluate these more general correlation functions we represent the values assumed by the spins at time t as $\sigma_1, \cdots \sigma_N$ and at the later time $t + t'$ as $\sigma_1', \cdots \sigma_N'$. The probability associated with the spin values $\sigma_1, \cdots \sigma_N$ at time t is $p(\sigma_1, \cdots \sigma_N, t)$, i.e., the solution to the master equation which satisfies whatever initial conditions our physical knowledge imposes. In order to carry out the averaging correctly, we must also know the probability associated with the final configuration $\sigma_1', \cdots \sigma_N'$ at time $t + t'$. The question we ask in determining that

[5] Reference 3, p. 361.

probability is rather different from the one answered by $p(\sigma_1, \cdots \sigma_N, t)$, since we assume that the spins are known to have the values $\sigma_1, \cdots \sigma_N$ at time t. The values $\sigma_1, \cdots \sigma_N$ are thus to be regarded as initial spin values in determining the probability of finding $\sigma_1', \cdots \sigma_N'$ at a time t' later. We shall write this conditional probability for finding $\sigma_1', \cdots \sigma_N'$ as $p(\sigma_1, \cdots \sigma_N \mid \sigma_1', \cdots \sigma_N' t)$. The expectation value we seek for the product of two spins may then be constructed by summing over all possible values of the sets $\sigma_1, \cdots \sigma_N$ and $\sigma_1', \cdots \sigma_N'$ as follows:

$$\langle \sigma_j(t)\sigma_k(t+t')\rangle$$
$$= \sum_{\{\sigma\}\{\sigma'\}} p(\sigma_1, \cdots \sigma_N t)\sigma_j p(\sigma_1, \cdots \sigma_N \mid \sigma_1', \cdots \sigma_N' t')\sigma_k'. \tag{70}$$

The part of this summation which is to be carried out over the variables $\sigma_1', \cdots \sigma_N'$ may be regarded simply as the expectation value of the kth spin when the spins are initially $\sigma_1, \cdots \sigma_N$. We may then write

$$\sum_{\{\sigma'\}} p(\sigma_1, \cdots \sigma_N \mid \sigma_1', \cdots \sigma_N', t')\sigma_k' = q_k(t'), \tag{71}$$

where it is understood that the initial values of the q_k are given by $q_k(0) = \sigma_k$. For the case of an infinite chain, the functions $q_k(t')$ are given in terms of these initial values by the general solution (43) as

$$q_k(t') = e^{-\alpha t'} \sum_l \sigma_l I_{k-l}(\gamma\alpha t'). \tag{72}$$

By substituting (71) and (72) into (70) we find

$$\langle \sigma_j(t)\sigma_k(t+t')\rangle$$
$$= e^{-\alpha t'} \sum_{l=-\infty}^{\infty} I_{k-l}(\gamma\alpha t') \sum_{\{\sigma\}} p(\sigma_1, \cdots \sigma_N t)\sigma_j\sigma_l. \tag{73}$$

The summation over $\sigma_1, \cdots \sigma_N$, however, is just the instantaneous correlation $r_{j,k}(t)$ defined by (19). The time-delayed correlation function, therefore, reduces to

$$\langle \sigma_j(t)\sigma_k(t+t')\rangle = e^{-\alpha t'} \sum_{l=-\infty}^{\infty} r_{j,l}(t)I_{k-l}(\gamma\alpha t'), \tag{74}$$

where the functions $r_{j,l}(t)$ are given, in general, by the results of the preceding section.

For the particular case of a system in thermal equilibrium at temperature T, the correlation function depends only on the interval t', i.e.,

$$\langle \sigma_j(t)\sigma_k(t+t')\rangle_T = e^{-\alpha t'} \sum_{l=-\infty}^{\infty} \eta^{|j-k+l|}I_l(\gamma\alpha t'). \tag{75}$$

The term corresponding to $l = k - j$ is the only contribution which would be present if there were

no correlations between spins in the initial state, as would be true, for example, for infinite temperature. The remaining terms of the series describe the stabilizing effects upon the kth spin of the polarizations which exist about it in the initial state. For either sign of γ, the addition of the effects of neighboring spins in (75) makes the correlation function decrease in magnitude more slowly with increasing t'.

In all of our work to date, we have assumed that we are in possession of some knowledge about the system at an initial time $t = 0$, and have sought, in a probabilistic sense, to answer questions about the behavior of the system at later times. Of course, the same questions may be asked in a reversed sense. What may we say, on the basis of knowledge at $t = 0$, about the behavior of the system at negative times? Since the dynamical properties of our model are presumably reversible, there is no need to construct or solve a new master equation. The probabilities are simply even functions of time. The time t is to be construed more generally as $|t|$ in all of the probability functions we have calculated thus far. In particular, the time-dependent spin correlation function (75) may be written for $t = 0$ and arbitrary t' as

$$\langle \sigma_j(0)\sigma_k(t')\rangle_T = e^{-\alpha|t'|} \sum_{l=-\infty}^{\infty} \eta^{|j-k+l|}I_l(\gamma\alpha |t'|). \tag{76}$$

SINGLE SPIN IN A MAGNETIC FIELD

It is not difficult to formulate the equations which describe the behavior of our model when it is placed in a uniform magnetic field. The influence of the magnetic field H, which we suppose is parallel to the axis of spin quantization, is to introduce a preference of the spins for either the $\sigma = 1$ or the $\sigma = -1$ state. For the most simple case, in which only a single spin is present, the transition probability from σ to $-\sigma$ may be written as

$$w(\sigma) = \tfrac{1}{2}\alpha(1 - \beta\sigma).$$

If we equate the ratios of the equilibrium probabilities calculated according to the stochastic model and according to statistical mechanics, we find

$$\frac{p(-\sigma)}{p(\sigma)} = \frac{w(\sigma)}{w(-\sigma)} = \frac{1 - \beta\sigma}{1 + \beta\sigma}$$

$$= \frac{\exp\left[-(\mu H/kT)\sigma\right]}{\exp\left[(\mu H/kT)\sigma\right]}$$

$$= \frac{1 - \sigma \tanh(\mu H/kT)}{1 + \sigma \tanh(\mu H/kT)}, \tag{77}$$

where μ is the magnetic moment associated with the spins or, more concisely, we find the correspondence

$$\beta = \tanh (\mu H/kT). \tag{78}$$

The equation satisfied by the expectation value of the spin is then

$$(d/d\alpha t)q(t) = \beta - q(t). \tag{79}$$

In the work that follows, it will be interesting to be able to discuss the behavior of the spins in time-dependent magnetic fields. Since the arguments of statistical mechanics used in treating the Ising model deal only with constant magnetic fields, we are free in defining the stochastic model to choose any time-dependence of the parameter β which yields (78) when H is constant. The simplest way of defining a time-dependent β is to retain the relation (78) when H depends on time. The solution for the average spins is then

$$q(t) = q(t_0)e^{-\alpha(t-t_0)} + \int_{t_0}^{t} e^{-\alpha(t-t')}\beta(t')\alpha \, dt', \tag{80}$$

where t_0 is a time at which q is known initially.

SPIN SYSTEM IN A MAGNETIC FIELD

To construct a stochastic analog of the Ising model in a magnetic field, we must first find an appropriate set of transition probabilities. To this end we note that the Hamiltonian of the Ising model is

$$\mathcal{K} = -\mu H \sum_{m} \sigma_m - J \sum_{m} \sigma_m \sigma_{m+1}, \tag{81}$$

so that, if the spins other than σ_i are considered as fixed, the ratio of equilibrium probabilities for the states $-\sigma_i$ and σ_i is

$$\frac{p_i(-\sigma_i)}{p_i(\sigma_i)} = \frac{\exp\{-(1/kT)\sigma_i[J(\sigma_{i-1} + \sigma_{i+1}) + \mu H]\}}{\exp\{(1/kT)\sigma_i[J(\sigma_{i-1} + \sigma_{i+1}) + \mu H]\}}$$

$$= \frac{w_i(\sigma_i) \exp[-(\mu H/kT)\sigma_i]}{w_i(-\sigma_i) \exp[(\mu H/kT)\sigma_i]}, \tag{82}$$

where the identities (12) and (13) were used in securing the latter relation. If we write the transition probabilities for the model in a magnetic field as $w_i'(\sigma_i)$, the detailed balancing condition at equilibrium requires

$$\frac{w_i'(\sigma_i)}{w_i'(-\sigma_i)} = \frac{p_i(-\sigma_i)}{p_i(\sigma_i)}$$

$$= \frac{w_i(\sigma_i)[1 - \sigma_i \tanh (\mu H/kT)]}{w_i(-\sigma_i)[1 + \sigma_i \tanh (\mu H/kT)]}. \tag{83}$$

Hence our model will approach the same equilibrium state as the Ising model if we choose

$$w_i'(\sigma_i) = w_i(\sigma_i)[1 - \sigma_i \tanh (\mu H/kT)]$$

$$= w_i(\sigma_i)(1 - \beta\sigma_i)$$

$$= \tfrac{1}{2}\alpha\{1 - \beta\sigma_i + \tfrac{1}{2}\gamma(\beta - \sigma_i)(\sigma_{i-1} + \sigma_{i+1})\}. \tag{84}$$

The difference-differential equations satisfied by the average spins and the average products are easily constructed by means of (28) and (29). For the average spins we find the sequence of equations

$$(d/d\alpha t)q_k(t) = -q_k(t) + \beta$$
$$+ \tfrac{1}{2}\gamma[q_{k-1}(t) + q_{k+1}(t)]$$
$$- \tfrac{1}{2}\beta\gamma[r_{k-1,k}(t) + r_{k,k+1}(t)], \tag{85}$$

which differs from the sequence (30) considered earlier by the inclusion of the inhomogeneous term β and, more importantly, through the inclusion of the pair-correlation terms $r_{k-1,k}$ and $r_{k,k+1}$. The equations for the pair correlation are likewise found to contain terms proportional to other correlation functions, i.e., the single-spin expectations and the expectation of the product of three spins. Such equations appear, because of their mixed structure, to be essentially more difficult to solve than those treated earlier. It is not difficult, however, to solve them in the limit of weak magnetic fields, $\mu H \ll kT$, and by doing so we are able to discuss the time-dependent magnetic susceptibility of the system.

In the weak-field limit, the parameter β is proportional to the magnetic field, $\beta = \mu H/kT$. The first-order changes of the averages $q_k(t)$ may be found from Eqs. (85) by using as a zeroth approximation for the functions $r_{k-1,k}$ and $r_{k,k+1}$ the solution (68) derived for them in our earlier work. The equations for the $q_k(t)$ become in this way an inhomogeneous sequence, with the inhomogeneous terms proportioned to H. The solution of these equations is simplified considerably if we assume that the model is in thermal equilibrium to zeroth order in H, i.e., that the field induces only small departures from equilibrium. In that case we have

$$r_{k-1,k} = r_{k,k+1} = \eta, \tag{86}$$

which is independent of k, and Eqs. (85) reduce to the sequence

$$\frac{d}{d\alpha t} q_k = -q_k + \tfrac{1}{2}\gamma(q_{k-1} + q_{k+1}) + \beta(1 - \gamma\eta). \tag{87}$$

We shall assume, as before, that the definition of β holds for time-dependent magnetic fields as well as stationary ones. The inhomogeneous term in (87) may also be written, by using Eq. (55), as

$$\beta(1 - \gamma\eta) = \frac{\mu H(t)}{kT}\frac{1 - \eta^2}{1 + \eta^2}. \qquad (88)$$

The sequence of Eqs. (87) differs from the sequence (52), which we solved earlier, only by the inclusion of this inhomogeneous term. Since the term is independent of k, the particular solution required may be chosen independent of k as well. Finding the particular solution is then a matter of treating the simplest of first-order linear differential equations. The general solution to the sequence (87) for an infinite chain is

$$q_k(t) = e^{-\alpha(t - t_0)} \sum_l q_l(t_0) I_{k-l}[\gamma\alpha(t - t_0)]$$

$$+ \frac{\mu}{kT}\frac{1 - \eta^2}{1 + \eta^2} \int_{t_0}^{t} e^{-\alpha(1-\gamma)(t-t')} H(t')\alpha\, dt', \quad (89)$$

where again we have let t_0 be the initial time. Since the model is assumed to be in thermal equilibrium before the magnetic field is turned on at time t_0, the initial values of the q_l may be taken to vanish. The spin expectations therefore all have the value given by the integral term of (89).

We now introduce the stochastic magnetization function

$$M(t) = \mu \sum_k \sigma_k(t), \qquad (90)$$

whose average value is given by the sum

$$\langle M(t)\rangle = \mu \sum_k q_k(t). \qquad (91)$$

If we let the initial time recede into the past, $t_0 \to -\infty$, the average magnetization obtained by summing (89) becomes

$$\langle M(t)\rangle = \frac{\mu^2 N}{kT}\frac{1 - \eta^2}{1 + \eta^2} \int_{-\infty}^{t} e^{-\alpha(1-\gamma)(t-t')} H(t')\alpha\, dt'. \quad (92)$$

For the case of a magnetic field which varies harmonically, $H(t) = H_0 e^{-i\omega t}$, we may define a complex, frequency-dependent magnetic susceptibility $\chi(\omega)$ via the relation

$$\langle M(t)\rangle = \chi(\omega)H_0 e^{-i\omega t}. \qquad (93)$$

The susceptibility is then given by

$$\chi(\omega) = \frac{\mu^2 N}{kT}\frac{1 - \eta^2}{1 + \eta^2}\frac{\alpha}{\alpha(1 - \gamma) - i\omega}$$

$$= \frac{\mu^2 N}{kT}\frac{1 + \eta}{1 - \eta}\frac{\alpha(1 - \gamma)}{\alpha(1 - \gamma) - i\omega}. \qquad (94)$$

In particular, in the low-frequency limit $\omega \to 0$, we find the static susceptibility

$$\chi(0) = \frac{\mu^2 N}{kT}\frac{1 + \eta}{1 - \eta} = \frac{\mu^2 N}{kT}\exp\frac{2J}{kT}, \qquad (95)$$

which is the familiar result furnished by the Ising model.

FLUCTUATION–DISSIPATION THEOREMS

It is interesting to note that our result (94) for the magnetic susceptibility is closely related to the result (76) for the time-dependent correlation function. If we sum the correlation functions (76) over the indices j and k by means of the generating function (35), and multiply by μ^2, we find the time-dependent correlation function for the magnetization,

$$\langle M(0)M(t')\rangle_T = \mu^2 N \frac{1 + \eta}{1 - \eta} e^{-\alpha(1-\gamma)|t'|}. \qquad (96)$$

The Fourier transform of this function is

$$\int_{-\infty}^{\infty} \langle M(0)M(t')\rangle_T e^{i\omega t'}\, dt'$$

$$= \mu^2 N \frac{1 + \eta}{1 - \eta}\frac{2\alpha(1 - \gamma)}{\alpha^2(1 - \gamma)^2 + \omega^2}$$

$$= \frac{2kT}{\omega}\,\mathrm{Im}\,\chi(\omega), \qquad (97)$$

i.e., the imaginary, or dissipative part of the magnetic susceptibility is proportional to the Fourier transform of the time-dependent magnetization correlation function. We thus have in hand a particularly simple example of a fluctuation–dissipation relation. Although the derivation we have given depends on the explicit evaluation of the functions involved, analogous relations are known to hold for a wide class of mechanical systems. These relations are derived from statistical mechanics by discussing the way in which perturbations of the Liouville equation affect the distribution function or density matrix and the expectation values derived from them. Since the model we are discussing, on the other hand, is a stochastic one, our equations do not follow the dynamics of the spin variables in detail. In place of the quantum-mechanical Liouville equation we have the master equation, which has altogether different properties. Our model, nevertheless, does permit the statement of a number of simple identities analogous to the fluctuation–dissipation theorems of statistical mechanics, but differing from them slightly in form. Since these relations may be of use in finding the effect of a weak field upon the average values of quite general functions of the spin variables, we shall derive them here.

We denote the change of any quantity A induced

by the presence of the weak magnetic field by the increment symbol ΔA. The change of the transition probabilities according to (84) is then

$$\Delta w_i(\sigma_i) = w_i'(\sigma_i) - w_i(\sigma_i)$$
$$= -(\mu H/kT)\sigma_i w_i(\sigma_i). \quad (98)$$

The first-order changes of the quantities involved in the master equation (27) are related by

$$\frac{d}{dt}\Delta p(\sigma_1', \cdots \sigma_N', t)$$
$$= -\sum_i \sigma_i' \sum_{\sigma_i''} \sigma_i'' \{\Delta w_i(\sigma_i'')p(\sigma_1', \cdots \sigma_i'', \cdots \sigma_N', t)$$
$$+ w_i(\sigma_i'')\Delta p(\sigma_1', \cdots \sigma_i'', \cdots \sigma_N', t)\}. \quad (99)$$

Now if $p(\sigma_1', \cdots \sigma_N' \mid \sigma_1, \cdots \sigma_N t)$ is a conditioned probability function in the sense described earlier, i.e., it satisfies the unperturbed master equation and reduces to $\prod_i \delta_{\sigma_i \sigma_i'}$ for $t = 0$, then it constitutes a Green's function for the sequence of Eqs. (99). If the initial time is $-\infty$, the solution to (99) may be written as

$$\Delta p(\sigma_1, \cdots \sigma_N, t) = -\sum_{\{\sigma'\}} \sum_i \sigma_i' \sum_{\sigma_i''} \sigma_i''$$
$$\times \int_{-\infty}^t \Delta w_i(\sigma_i'', t')p(\sigma_1', \cdots \sigma_i'', \cdots \sigma_N', t')$$
$$\times p(\sigma_1', \cdots \sigma_N' \mid \sigma_1, \cdots \sigma_N, t - t') dt'. \quad (100)$$

We next substitute the expression (98) for the increment of the transition probabilities into (100) and sum explicitly over the values of σ'', finding

$$\Delta p(\sigma_1, \cdots \sigma_N, t) = \frac{\mu}{kT} \sum_{\{\sigma'\}} \sum_i \sigma_i'$$
$$\times \int_{-\infty}^t H(t')\{w_i(\sigma_i', t')p(\sigma_1', \cdots \sigma_i', \cdots \sigma_N', t')$$
$$+ w_i(-\sigma_i', t')p(\sigma_1', \cdots -\sigma_i', \cdots \sigma_N, t')\}$$
$$\times p(\sigma_1', \cdots \sigma_N' \mid \sigma_1, \cdots \sigma_N, t - t') dt'. \quad (101)$$

The detailed balancing relation (83) assures us that the two products within the curly brackets of (101) are equal, i.e. that the probability increment may be simplified to the form

$$\Delta p(\sigma_1, \cdots \sigma_N, t)$$
$$= \frac{2\mu}{kT} \sum_i \sum_{\{\sigma'\}} \int_{-\infty}^t H(t')p(\sigma_1', \cdots \sigma_N', t')\sigma_i' w_i(\sigma', t')$$
$$\times p(\sigma_1', \cdots \sigma_N' \mid \sigma_1, \cdots \sigma_N, t - t') dt'. \quad (102)$$

To evaluate the change induced by the magnetic field in the expectation value of any function of the

σ variables, $F(\sigma_1, \cdots \sigma_N)$, we have only to multiply Eq. (102) through by F and sum over spins σ_i. The integrand on the right-hand side may then be recognized as an equilibrium-state average of a product of three stochastic functions. Expressed in this way, the change of the average value of F becomes

$$\Delta\langle F[\sigma_1(t), \cdots \sigma_N(t)]\rangle$$
$$= \frac{2\mu}{kT} \int_{-\infty}^t \sum_i \langle \sigma_i(t')w_i[\sigma_i(t)]F[\sigma_1(t), \cdots \sigma_N(t)]\rangle_T$$
$$\times H(t') dt'. \quad (103)$$

In particular, when the transition probabilities are given by (9) we find more simply

$$\Delta\langle F[\sigma_1(t), \cdots \sigma_N(t)]\rangle$$
$$= \frac{\mu}{kT}\alpha(1 - \gamma) \int_{-\infty}^t \sum_i \langle \sigma_i(t')F[\sigma_1(t), \cdots \sigma_N(t)]\rangle_T$$
$$\times H(t') dt'. \quad (104)$$

If the function F is taken to be the magnetization, we find that it obeys the relation

$$\Delta\langle M(t)\rangle = \langle M(t)\rangle$$
$$= \frac{1}{kT}\alpha(1 - \gamma) \int_{-\infty}^t \langle M(t')M(t)\rangle_T H(t') dt'. \quad (105)$$

Since the equilibrium state is stationary, the thermal average in the integrand can only depend on $t - t'$. Hence for the case of a harmonic field $H(t) = H_0 e^{-i\omega t}$, we find

$$\chi(\omega) = \frac{1}{kT}\alpha(1 - \gamma) \int_0^\infty \langle M(0)M(t)\rangle_T e^{i\omega t} dt. \quad (106)$$

The foregoing relations are rather similar in structure to the complex forms of the fluctuation-dissipation theorems of statistical mechanics, and furnish us with similar information. They differ from those relations, however, in two respects illustrated by comparing (97) and (106). The former equation relates the imaginary part of the susceptibility to the transform of the correlation function, while the latter relates the real part to it with a different proportionality constant. Although both types of relation hold true for the model at hand, it is interesting to see how the difference between them arises. For this purpose let us consider the stochastic function

$$L(t) = -2\mu \sum_m \sigma_m(t)w_m(\sigma_m, t). \quad (107)$$

The expectation value of L is the time derivative of the average magnetization. To see this, we use

(28) to write

$$\langle L(t) \rangle = \mu \sum_m \frac{d}{dt} q_m(t) = \frac{d}{dt} \langle M(t) \rangle. \quad (108)$$

The function $L(t)$ itself, however, is not the time derivative of $M(t)$. If it were, the substitution of $\dot{M}(t)$ for it in (103) would lead to precisely the relations furnished by discussions based on the Liouville equation. The relations we find instead are evidently quite similar in content.

ALTERNATIVE METHOD AND GENERALIZATION

It may be of interest to mention briefly another way of studying Markoff processes, one rather different from the preceding discussion. The 2^N values of the probability function $p(\sigma_1, \cdots \sigma_N, t)$ may be regarded as the components of a vector $\mathbf{p}$. Then by suitably defining the elements of a matrix M, we may write the master equation (27) in the form

$$(d/dt)\mathbf{p} = M\mathbf{p}, \quad (109)$$

which suggests that p is a superposition of eigenvectors $\mathbf{p}^{(s)}$ which satisfy

$$M\mathbf{p}^{(s)} = -\nu_s\mathbf{p}^{(s)}. \quad (110)$$

One eigenvector, at least, is quite well-known to us. The probability distribution for the Ising model at equilibrium, the normalized Maxwell–Boltzmann distribution, corresponds to the eigenvalue $\nu = 0$. It is

$$p^{(0)}(\sigma_1, \cdots \sigma_N) = Z^{-1} \exp [(J/kT) \sum_l \sigma_l\sigma_{l+1}], \quad (111)$$

where Z, the normalizing factor, is the partition function.

Other eigenvectors may be sought by multiplying $\mathbf{p}^{(0)}$ by sums of products of spin variables with undetermined coefficients. For example, if we write

$$p^{(1)}(\sigma_1, \cdots \sigma_N, t) = \sum_i a_i(t)\sigma_i p^{(0)}(\sigma_1, \cdots \sigma_N), \quad (112)$$

we find that the condition that this form satisfy (109) is that the functions $a_i(t)$ satisfy the same sequence of equations (30) as we discussed earlier in connection with $q_i(t)$. The mode functions ζ_m^k, where ζ_m is given by (46) therefore furnish us with N different eigenvectors corresponding to roots ν_m given by (47).

The eigenvectors which are constructed by multiplying $\mathbf{p}^{(0)}$ by higher-order polynomials in $\sigma_1, \cdots \sigma_N$, are somewhat more complicated in form, and will be discussed in a later publication. The eigenvalues

to which they correspond are fairly simple, however. The eigenvectors which are formed from the products of rth degree polynomials with $\mathbf{p}^{(0)}$ have eigenvalues

$$\nu = \nu_{m_1} + \nu_{m_2} + \cdots + \nu_{m_r}, \quad (113)$$

where the ν_{m_i} are given by (47), and the set of integers $m_1, \cdots m_r$ is selected from $0, 1 \cdots N - 1$ with no repetitions. The number of such eigenvalues is given by the binomial coefficient $\binom{N}{r}$. The full set of 2^N eigenvalues is obtained by allowing r to range from 0 to N.

In particular, the largest eigenvalue is obtained for $r = N$ and is $\nu = N$. The eigenvector for this case is simply proportional to

$$p^{(N)}(\sigma_1, \cdots \sigma_N, t) = \prod_{j=1}^{N} \sigma_j e^{-N\alpha t}. \quad (114)$$

All of the foregoing discussion has been restricted to the case of nearest-neighbor coupling among spins in order to make contact with the familiar studies of the Ising model. The coupling may be extended to include the first n nearest neighbors by introducing the transition probability

$$w_i(\sigma_i) = \tfrac{1}{2}\alpha\left\{1 - \tfrac{1}{2}\sigma_i \sum_{l=1}^{n} \gamma_l(\sigma_{i-l} + \sigma_{i+l})\right\}, \quad (115)$$

where $\sum_l |\gamma_l| \leq 1$. The methods of the preceding sections deal equally with the equations which follow from this more general type of coupling. The only significant change is that the quadratic equation, (55), for the short-range order is replaced by an equation of $2n$th degree which has n roots $\eta_1, \cdots \eta_n$ with absolute value less than unity. The equilibrium solution for the average spins, when the zeroth spin is fixed, is then an expression of the form

$$q_k = \sum_{j=1}^{n} c_j \eta_j^k, \quad (116)$$

where the coefficients c_j must be determined from the condition $q_0 = 1$ and the equations for $q_1, \cdots q_{n-1}$. These spin averages then determine the equilibrium spin correlations $r_{j,k}$ in precisely the way described earlier.

APPENDIX

We have already noted that other forms of the transition probability than (9) are capable of bringing the stochastic model to the same equilibrium state as the Ising model. The condition that such a transition probability $w_i(\sigma_i)$ must satisfy is that the ratio $w_i(\sigma_i)/w_i(-\sigma_i)$ be equal to the equilibrium probability ratio (12). If we assume that $w_i(\sigma_i)$ depends symmetrically on the two neighboring spins σ_{i-1} and σ_{i+1} as well as on σ_i, then the condition just mentioned may be regarded as a functional equation for the transition probability. Its most general solution is given by the form

$$w_i(\sigma_i) = \tfrac{1}{2}\alpha\{1 + \delta\sigma_{i-1}\sigma_{i+1}$$
$$- \tfrac{1}{2}\gamma(1 + \delta)\sigma_i(\sigma_{i-1} + \sigma_{i+1})\}, \quad (117)$$

in the absence of any magnetic field. In this form the parameter γ must still be identified with the constant (17), but the parameter δ has no analog in the discussions of the Ising model at equilibrium, and may evidently be chosen arbitrarily. It was assumed to vanish in our discussions of the time-dependent model since its presence materially complicates the equations for the spin expectation values.