ANALYTIC AND COMPUTATIONAL STUDIES OF SPIN GLASSES

BY

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A thesis submitted for the degree of Doctor of Philosophy in the University of London and the Diploma of Membership of the Imperial College of Science and Technology

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February 1985

ABSTRACT

The Sherrington-Kirkpatrick and the nearest-neighbour X-Y spin-glass models are studied.

The effect of a small uniform symmetry breaking field on the infinite-ranged Sherrington-Kirkpatrick Ising spin-glass model is discussed. It is shown that the off-diagonal contributions to the fluctuation-dissipation formula vanish for a symmetric distribution of interactions and the limit of zero field. This contradicts the result of Young and Kirkpatrick based on numerical evidence for small samples.

The dynamics of the Sherrington-Kirkpatrick spin-glass are investigated. Below the critical temperature this model exhibits non-ergodic behaviour. Consequently, in order to obtain time-dependent correlation functions it is necessary to average over the initial states with a Boltzmann weight. This necessitates the use of "replicas". It is shown that in Parisi's scheme the "dynamical" Edwards-Anderson order parameter is given by $q(x = 1)$, whereas the statistical mechanics order parameter is given by $\int_0^1 q(x)dx$. The result for the statistical mechanics order parameter implies that there is no violation of the fluctuation-dissipation theorem once an average over samples is performed. It is also shown that the system in general keeps its memory of the initial state for all time. However, this memory is "lost" if one makes a replica symmetric ansatz for the order parameters. This illustrates the connection between replica symmetry breaking and non-ergodicity.

The nearest neighbour X-Y spin-glass in both two- and three-dimensions is investigated by Monte Carlo simulation. In two-

dimensions it is shown that the results are consistent with a zero-temperature phase transition; the spin-glass susceptibility, the correlation length and the average relaxation time all diverge as a power law in T^{-1} as $T \to 0$. The exponents γ_{SG}, η_{SG}, ν_{SG} and $\nu_{SG} z_{SG}$ are estimated. Although in three-dimensions the data is consistent with any of the three possibilities investigated, a zero-temperature transition, a finite temperature transition or an LCD of 3, the second case is marginally favoured over the other two. Estimates for the critical exponents are given in all of the three possibilities.

DEDICATION

This thesis is dedicated to the memory of my grandfather

Mr. Jainti Prasad Jain

ACKNOWLEDGMENTS

I should like to thank my supervisor Dr. A.P. Young for his continual guidance, encouragement and assistance throughout the past three years.

I am also grateful to Professor A. Houghton who, during his sabbatical leave from Brown University (U.S.A.), checked the calculations presented in Chapter III.

My thanks also go to the Science and Engineering Research Council (U.K.) for supporting my computations on the Distributed Array Processor (DAP) at Queen Mary College, London. Mr. K. Smith of the DAP support unit is thanked for helping in the programming of the DAP.

The Imperial College Computer Centre is also thanked for providing computing facilities.

Finally, financial assistance in the form of a research studentship from the Science and Engineering Research Council (U.K.) is gratefully acknowledged.

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ABBREVIATIONS

a.c. - Alternating current.

DAP - Distributed array processor.

d.c. - Direct current.

EA - Edwards and Anderson (1975).

FC - Field-cooled.

FDT - Fluctuation-dissipation theorem.

IRM - Isothermal remanent magnetisation.

LCD - Lower critical dimension.

LRT - Linear response theory.

MCS - Monte Carlo step.

MFT - Mean field theory.

nn - Nearest neighbour.

RKKY - Ruderman, Kittel, Kasuya and Yosida.

SK - Sherrington and Kirkpatrick (1975).

TAP - Thouless, Anderson and Palmer (1977).

TRM - Thermoremanent magnetisation.

UCD - Upper critical dimension.

YK - Young and Kirkpatrick (1982).

ZFC - Zero-field-cooled.

CHAPTER I

INTRODUCTION

Section A: Spin-Glasses

1. Spin-glass systems

The canonical spin-glasses are dilute magnetic alloys of a non-magnetic host metal and a magnetic impurity. The impurities (typically 1 to 10 atomic per cent) are quenched, that is frozen, into the host. Examples of spin-glasses are (the host is underlined): AuFe, AuMn, AgMn, CuMn,... . The magnetic spins, which are distributed randomly in the host, interact with each other by polarizing the conduction electrons around them. This is the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [Ruderman & Kittel 1954; Kasuya 1956; Yosida 1957], J_{ij}:

$$J_{ij} \sim \frac{1}{(k_F R_{ij})^3} \text{ Cos } 2k_F R_{ij}, \qquad (1.1)$$

where k_F is the Fermi wavevector of the host metal and R_{ij} is the distance between sites i and j. As can be seen from Figure 1.1a, the RKKY interaction oscillates in sign with distance. Hence, depending upon the separation, the coupling between two given spins can be either ferromagnetic ($J_{ij} > 0$) or antiferromagnetic ($J_{ij} < 0$). Since the positions of the impurity ions within the host are completely disordered, the magnetic interactions, too, will be distributed randomly, that is there will be "competition" among the interactions. Both disorder and competition between couplings are believed to be the main prerequisites for spin-glass behaviour.

Many insulating systems such as $Eu_xSr_{1-x}S$ also exhibit the characteristics of spin-glasses. In this system the Eu ions and Sr ions are distributed randomly on a face centred cubic lattice, x% of the sites being occupied by the Eu ions. Although this time the magnetic interactions, which take place between the Eu ions, are short-ranged, there is competition between the nearest neighbour (nn) couplings (ferromagnetic) and the next nearest neighbour couplings (antiferromagnetic). Spin-glass behaviour has been observed for $0.13 \leqslant x \leqslant 0.5$ [Maletta & Felsch 1980]; larger concentrations of Eu ions give rise to a ferromagnetic phase while the percolation threshold is reached at lower concentrations.

It should be noted that spin-glass behaviour is not confined to magnetic systems [Fischer 1983]. For example, both dilute ferroelectrics and a mixture of ortho- and parahydrogen crystals also show the characteristics of spin-glasses.

2. Properties of spin-glasses

Spin-glass behaviour was first observed by Canella and Mydosh (1972). They found a "cusp", that is non-analyticity, in the a.c. susceptibility of AuFe at a well defined "freezing" temperature, T_g, suggesting that the system undergoes a phase transition. The magnetic specific heat, on the other hand, is a smooth function of the temperature, there being no anomaly at T_g. Also, neutron diffraction experiments [Arrot 1965] indicate the absence of long-range magnetic order below T_g. Further, when the frequency, ν, at which the a.c. susceptibility measurements are performed is varied, there is a shift in T_g to lower temperatures as ν tends to zero [see Figure 1.1b]. Experimentalists actually measure

the relative shift in T_g per decade of frequency: $(1/T_g)(\Delta T_g/\Delta \log_{10} \nu)$. As we can see from Table 1.1, this quantity appears to be nonuniversal for RKKY systems.

Table 1.1

THE DYNAMIC BEHAVIOUR OF SOME RKKY SYSTEMS

System	$(1/T_g)(\Delta T_g/\Delta \log_{10} \nu)$ x 10^{-3}	Reference
AuMn	4.5 ± 0.4	Mulder et al. (1982)
CuMn	5.0 ± 0.7	Mulder et al. (1981a)
AgMn	6 ± 2	Tholence (1981)
PdMn	11 - 15	Mulder et al. (1981b)
NiMn	18	Goldfarb and Patton (1981)

Since a d.c. measurement of the susceptibility is performed on a time scale τ one can regard it as an a.c. measurement at a frequency $\nu \sim 1/\tau$. Hence, one could argue that if τ were infinite (or, equivalently, ν were zero) the "cusp" would vanish and the "phase transition" is simply a non-equilibrium manifestation. One can extract a dynamic exponent $\nu_{SG} z_{SG}$ from the quantity tabulated in Table 1.1. Assuming a zero-temperature transition, Binder and Young (1984) estimate that

$$\nu_{SG} z_{SG} \simeq 5\text{-}9 \quad \text{for NiMn, PdMn}$$

$$\simeq 20 \quad \text{for AuMn, CuMn, AgMn.} \qquad (1.2)$$

Bontemps et al. (1984) have investigated the insulating spin-glass $Eu_{0.4}Sr_{0.6}S$. They find that ($T_c \equiv T_g$)

$$\text{for } T_c = 0, \quad \nu_{SG} z_{SG} = 8 \tag{1.3a}$$

while

$$\text{for } T_c = 1.5K, \quad \nu_{SG} z_{SG} = 7. \tag{1.3b}$$

However, there is also evidence for a phase transition from recent measurements of the non-linear susceptibility, $\chi_{n\ell}$. In Table 1.2 we compare some experimental results for the exponents γ_{SG} and β_{SG} with the mean field values; see Chapter IV for the definitions of the exponents and their values in the Sherrington-Kirkpatrick (SK) model [Sherrington & Kirkpatrick 1975].

Table 1.2

SOME EXPERIMENTAL DATA

System	T_c(K)	β_{SG}	γ_{SG}	Reference
SK	-	1	1	Sherrington and Kirkpatrick (1975)
AuFe	11.8	0.9	1.2±0.2	Taniguchi et al. (1983)
AgMn	37.4	-	1.5±0.5	Monod and Bouchiat (1982)
CuMn (0.25%)	3.53	1	3.65±0.35	Berton et al. (1982)
(1%)	10.05	0.75±0.25	3.25±0.10	Omari et al. (1983)
(4.6%)	26.25	1.1±0.2	3.4±0.4	Barbara et al. (1981, 1982)
AlGd	15.51	0.6±0.1	2.7±0.1	Barbara et al. (1981, 1982)
$CsNiFeF_6$	5.35	1.3	3.0±0.5	Pappa et al. (1984)
Mn-alumina	2.95	1.4±0.1	3.1±0.1	Beauvillain et al. (1984)

Although some of the experimental values for γ_{SG} are close to the mean field prediction, the majority are consistent with $\gamma_{SG} \simeq 3$.

Below T_g spin-glasses exhibit hysteresis and their field dependent properties are influenced by the history of the system. In particular, one has to distinguish between "field-cooled" (FC) and "zero-field-cooled" (ZFC) situations. If one cools the system down to a temperature T ($< T_g$) through T_g in a magnetic field, h, one obtains the FC magnetisation and the FC susceptibility. On the other hand, if the system is first cooled in a zero field and the field is then subsequently applied, one obtains the ZFC magnetisation and ZFC susceptibility. If one now switches the field off one obtains the "thermoremanent magnetisation" (TRM) in the FC case and the "isothermal remanent magnetisation" (IRM) in the ZFC case. The FC behaviour is believed to correspond to the equilibrium properties of the system as time dependent effects in it are very difficult to detect, whereas the ZFC values tend logarithmically towards the FC ones. Further, there is evidence [Chamberlin et al. 1982; Yeshuru et al. 1982; Bontemps et al. 1983] for a "transition line" in the h-T plane below which the above features become prominent.

The experimental properties of spin-glasses are reviewed by Rammel and Souletie (1982) and Fischer (1983); also see the Proceedings of the Heidelberg Colloquium on Spin Glasses (1983).

Section B: The Edwards-Anderson Model

In the experimental spin-glasses discussed above, although the magnetic ions are situated at random throughout the host lattice, there is a well-defined interaction. Edwards and Anderson (1975) proposed a theoretical model - the EA model - of spin-glasses in which one works with a well-defined lattice and the site-randomness is replaced by bond-randomness. The Hamiltonian of the EA model for Ising spins is given by

$$H = - \sum_{<ij>} J_{ij} S_i S_j , \qquad (1.4)$$

where the spins $S_i (= \pm 1)$ occupy every site, $i = 1,\ldots,N$, of a regular lattice (for example, a square lattice in 2D) and the quenched bonds J_{ij}, which act between nearest neighbours only, are selected from either a Gaussian, (4.15), or a binary, (4.16), distribution.

Although most theoretical work has been concerned with the Hamiltonian (1.4), one can also consider Heisenberg spins and planar spins [see Chapter IV]. The majority of experimental spin-glasses are "Heisenberg-like" but with the additional feature of anisotropy. The anisotropy can convert such systems to "Ising-like" (ZnMn) or "X-Y-like" (CdMn) [Albrecht et al. 1982].

As either of the distributions mentioned above leads to a mixture of negative and positive bonds, the EA model contains the essential ingredients for a spin-glass: disorder and "frustration".

One refers to the smallest closed loop of bonds on a lattice as a plaquette (that is, for a two-dimensional square lattice the plaquettes are squares). We show in Figure 1.2 how the competition

between the bonds can give rise to "frustrated" plaquettes. (For simplicity, Figure 1.2 is restricted to 2D with $|J_{ij}| = 1$.) The frustration of a plaquette is summarised in the "frustration function" Φ [Toulouse 1977] (see Figure 1.2 for notation):

$$\Phi = \text{SIGN}\,(J_{ij}J_{jk}J_{k\ell}J_{\ell m})$$

$$= -1 \quad \text{for a frustrated plaquette}$$

$$= +1 \quad \text{otherwise.} \qquad (1.5)$$

Hence, a plaquette is frustrated whenever it contains an odd number of negative bonds.

Since, on average, half of the plaquettes in the two-dimensional $\pm J$ model will be frustrated, its ground state is highly degenerate [Binder & Kinzel 1981]. On the other hand, the ground state for the model with a Gaussian bond distribution is only doubly degenerate; although these two models probably belong to different universality classes [Morgenstern & Binder 1980a; Cheung & McMillan 1983a,b], they both have a zero temperature transition [Young 1983, 1984; McMillan 1983, 1984b,c; Bray and Moore 1984].

The Hamiltonian and the frustration function are both gauge invariant under the transformation

$$S_i' = \eta_i S_i \qquad (\eta_i = \pm 1; \quad i = 1,\ldots,N)$$

$$J_{ij}' = \eta_i J_{ij} \eta_j. \qquad (1.6)$$

We can apply this transformation to the Mattis model [Mattis 1976] which contains disorder but no frustration and for which

$$J_{ij} = J\eta_i\eta_j \qquad (\eta_i = \pm 1; \quad J > 0). \tag{1.7}$$

So we see that the disorder in this model is trivial in the sense that it can be "gauged" away. This emphasises the necessity for both disorder and frustration in order to obtain spin-glass behaviour.

As a possible order parameter Edwards and Anderson (1975) suggested the long time limit of the autocorrelation function:

$$q_{EA} = \lim_{t\to\infty} N^{-1} \sum_{i=1}^{N} \langle\langle S_i(0)S_i(t)\rangle_T\rangle_J \tag{1.8}$$

where $S_i(t)$ in the i-th spin at time t, $\langle \ldots \rangle_T$ denotes a thermal average and $\langle \ldots \rangle_J$ an average over the bond distribution. It was suggested that the spin-glass phase is associated with "freezing" of the spins in random positions on long time-scales, that is q_{EA} is non-zero.

The theoretical problem, although simple to formulate, is extremely difficult to solve. We now discuss the mean field theory of Ising spin-glasses.

Section C: Mean Field Theory of Spin-Glasses

1. The Parisi solution

For a pure ferromagnet mean field theory is defined by the solution of the corresponding infinite-range model. This motivated Sherrington and Kirkpatrick (1975) to propose an analogous model - the SK model - for Ising spin-glasses; mean field theory for spin-glasses is identified as the solution of the SK model.

The Hamiltonian of the SK model is given in Chapter II (see equation (2.1)). As the disorder is quenched, in order to evaluate the interaction-averaged free-energy per spin, F, one needs to

average the logarithm of the partition function, Z, over the bond distribution. One achieves this by using "replicas" (Boltzmann's constant is set to unity):

$$-F/T = \lim_{N\to\infty} N^{-1} \langle \ln Z \rangle_J \tag{1.9}$$

$$= \lim_{N\to\infty} \lim_{n\to 0} \left\{ \frac{\langle Z^n \rangle_J - 1}{Nn} \right\} \tag{1.10}$$

$$= \lim_{N\to\infty} \lim_{n\to 0} \left\{ \frac{\langle \prod_{\alpha=1}^{n} Z^\alpha \rangle_J - 1}{Nn} \right\} \tag{1.11}$$

where Z^α ($\alpha = 1,\ldots,n$) are n identical, non-interacting replicas. [For a discussion on replicas see Chapter III.] Performing the bond average appearing in (1.11) results in couplings between spins in different replicas. This method leads to replica-dependent order parameters, $q^{\alpha\beta}$:

$$q^{\alpha\beta} = N^{-1} \sum_{i=1}^{N} \langle S_i^\alpha S_i^\beta \rangle \qquad (\alpha \neq \beta) \tag{1.12}$$

where $\langle \ldots \rangle$ denotes an average in replica space and S_i^α is the ith spin in replica α. In their original "replica-symmetric" solution SK (1975) found, on making the naive assumption that

$$q^{\alpha\beta} = q \qquad \text{(for all } \alpha \neq \beta\text{)}$$

$$= N^{-1} \sum_{i=1}^{N} \langle \langle S_i \rangle_T^2 \rangle_J \quad , \tag{1.13}$$

the statistical mechanics order parameter, a transition at $T = T_c = J$. However, it was subsequently discovered that the SK solution is unstable below the Almeida-Thouless line in the h-T plane [Pytte & Rudnick 1978; Almeida & Thouless 1978]; see Figure 1.3a.

The instability of the SK solution in the spin-glass regime means that the replica-symmetric ansatz is invalid and one has to break the symmetry explicitly. The initial attempts [Bray & Moore 1978; de Dominicis & Garel 1979; Blandin et al. 1980] failed to resolve the instability. Eventually, Parisi (1979, 1980 a,b,c) proposed a scheme which in effect associated an infinite number of order parameters with the spin-glass phase, that is an order parameter function $q(x)$, where $0 \leqslant x \leqslant 1$; de Dominicis and Kondor (1983) have checked the stability of the Parisi solution.

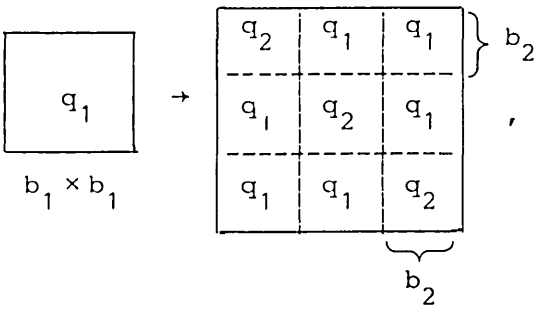
In the Parisi scheme the elements $q^{\alpha\beta}$ of the $n\times n$ matrix $(q^{\alpha\beta})$ are evaluated from a hierarchical parametrization generated from the replica-symmetric SK matrix. Schematically, one starts at the zeroth level by setting

$$(q_0^{\alpha\beta}) = \underbrace{\boxed{q_0}}_{n\times n} \tag{1.14}$$

where q_0 is the SK solution. One then divides the nxn matrix into $\{(n/b_1)\times(n/b_1)\}$ sub-matrices of size $b_1\times b_1$ and changes the elements of the diagonal sub-matrices from q_0 to q_1:

$$(q_0^{\alpha\beta}) \rightarrow (q_1^{\alpha\beta}) = \begin{array}{|c|c|c|} \hline q_1 & q_0 & q_0 \\ \hline q_0 & q_1 & q_0 \\ \hline q_0 & q_0 & q_1 \\ \hline \end{array} \quad \begin{matrix} \} b_1 \\ \\ \\ \\ \underbrace{\qquad}_{b_1} \end{matrix} \tag{1.15}$$

The above transformation is now repeated on just the diagonal matrices, leaving the off-diagonal ones untouched:



(1.16)

thereby generating $(q_2^{\alpha\beta})$. One repeats the process on each successive set of diagonals, with the constraint

$$n \geqslant b_1 \geqslant b_2 \geqslant \ldots \geqslant b_k \geqslant 1 \ , \tag{1.17}$$

which becomes

$$0 \leqslant b_1 \leqslant b_2 \leqslant \ldots \leqslant b_k \leqslant 1 \tag{1.18}$$

on taking the $n \to 0$ limit.

Parisi (1979) then defined

$$b_i = i/(k+1) \qquad i = 1,\ldots,k$$

$$q_i = q(x) \qquad b_i < x < b_{i+1} \tag{1.19}$$

which gives the Parisi order parameter function, $q(x)$, in the continuum limit:

$$\lim_{k\to\infty} q_i = q(x), \qquad 0 \leqslant x \leqslant 1. \tag{1.20}$$

See Figure 1.3b for a sketch of $q(x)$ in zero field. We shall return later to the physical interpretation of the dummy variable x.

An alternative, complementary, analysis of the SK model was

carried out by Thouless et al. (TAP) (1977) who wrote down a set of N mean field equations (TAP equations) for the thermal expectation value, $m_i = \langle S_i \rangle_T$ $(i = 1,\ldots,N)$:

$$m_i = \tanh\left(\beta \sum_j J_{ij} m_j + \beta h - m_i \beta^2 \sum_j J_{ij}^2 (1 - m_j^2)\right) \qquad (1.21)$$

where $\beta = 1/T$. In (1.21) one subtracts the "feedback" term - the field induced at site i by the spin S_i itself - from the total mean field at site i. The TAP equations have an enormous number, $\langle N_s \rangle_J$, of solutions [Bray & Moore 1980a; de Dominicis et al. 1980; Edwards & Tanaka 1980]:

$$\langle N_s \rangle_J \sim e^{\alpha(T)N} \qquad (1.22)$$

where

$$\text{for } h \to 0,\ \alpha(T) \sim 0.2 \text{ as } T \to 0$$
$$\sim 0 \quad \text{as } T \to T_c. \qquad (1.23)$$

The TAP solutions are separated by free energy barriers that diverge in the thermodynamic limit [Bray & Moore 1981; Mackenzie 1982; Mackenzie & Young 1982, 1983]. As a consequence the SK model is non-ergodic in the spin-glass regime [Young 1981; Toulouse 1982].

The non-ergodicity of the SK model means that one can define many order parameters in the low temperature phase; in particular, one has to distinguish between time averages and statistical mechanics averages [de Dominicis & Young 1983a]. Thus, the two order parameters - q_{EA} and q (see (1.8) and (1.13)) - introduced above are, in general, not the same.

The existence of many equilibrium states in the SK model recently led Houghton et al. (1983a) and Parisi (1983) to a physical interpretation of the Parisi variable x. One first defines the thermal expectation value of site i in state 's' by m_i^s and the overlap by

$$q^{ss'} = N^{-1} \sum_{i=1}^{N} m_i^s m_i^{s'} \; ; \tag{1.24}$$

$p(q,\{J_{ij}\})$, the probability distribution for two solutions to have an overlap q, is given by

$$p(q,\{J_{ij}\}) = \sum_{s,s'} p^s p^{s'} \delta(q^{ss'} - q) \tag{1.25}$$

where the probability for the pure state 's' is given by [de Dominicis & Young 1983a]

$$p^s = e^{-\beta F\{m^s\}} \Big/ \sum_s e^{-\beta F\{m^s\}} \tag{1.26}$$

and here $F\{m^s\}$ is the TAP free energy. Then, the derivative of the inverse Parisi function, that is dx(q)/dq, turns out to be

$$\frac{dx}{dq} = \langle p(q,\{J_{ij}\}) \rangle_J \tag{1.27}$$

$$= p(q). \tag{1.28}$$

The Edwards-Anderson order parameter, q_{EA}, which describes ordering in one state averaged over all states is given by

$$q_{EA} = \langle N^{-1} \sum_{s,i} p^s (m_i^s)^2 \rangle_J \tag{1.29}$$

$$= \langle \sum_s p^s q^{ss} \rangle_J \; , \tag{1.30}$$

whereas the statistical mechanics order parameter, q, which includes interference between different states is given by

$$q = \left\langle N^{-1} \sum_i \left(\sum_s p^s m_i^s \right)^2 \right\rangle_J \tag{1.31}$$

$$= \left\langle \sum_{s,s'} p^s p^{s'} q^{ss'} \right\rangle_J . \tag{1.32}$$

It is surprising that the overlap distribution, $p(q,\{J_{ij}\})$, depends on the particular set of interactions, $\{J_{ij}\}$, in question [Young et al. 1984], that is, it fluctuates from sample to sample. Although this observation does not affect experimentally observable quantities such as the magnetization and energy, it does have a consequence for the uniform susceptibility, $\chi(N,h,T)$.

Now, $\chi(N,h,T)$, which is defined by (2.10), is given by

$$\chi(N,h,T) = \left\langle \chi(N,h,T,\{J_{ij}\}) \right\rangle_J . \tag{1.33}$$

We show in Chapter II that in the symmetry broken situation ($N \to \infty$, $h \to 0$) for a symmetric distribution $\{J_{ij}\}$ only the $i = j$ terms contribute to (1.33):

$$\lim_{h\to 0} \lim_{N\to\infty} \chi(N,h,T) = \frac{1 - q}{T} . \tag{1.34}$$

(1.34) is trivial for $h \equiv 0$ but is not obvious a priori if the thermodynamic limit is taken first. Young et al. (1984) show that the 'lack of self-averaging' in the SK spin-glass results in the invalidity of the Fluctuation Dissipation Theorem (FDT) for a single sample, that is

$$\lim_{h\to 0}\lim_{N\to\infty} \chi(N,h,T,\{J_{ij}\}) \neq \frac{1-q}{T} , \tag{1.35}$$

although it does hold once an average over samples is performed.

2. The Sompolinsky solution

By introducing dynamics into the problem Sompolinsky (1981) proposed a solution of the SK model which was free of replicas. Subsequently it was shown that one could obtain the thermodynamics predicted by Sompolinsky (1981) via a replica symmetry-breaking approach analogous to that of Parisi's [de Dominicis et al. 1981, 1982]. This time one starts at the zeroth level by setting

$$(q_0^{\alpha\beta}) = \begin{array}{|c|c|c|} \hline q_0 & r_o & r_0 \\ \hline r_0 & q_0 & r_0 \\ \hline r_0 & r_0 & q_0 \\ \hline \end{array} \quad \begin{matrix} \overbrace{}^{b_1} \\ \\ \\ \end{matrix} \quad \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} b_1 \qquad n \times n \tag{1.36}$$

and then carries out the Parisi scheme outlined above on both sub-matrices q_0 and r_0.

In the Sompolinsky (1981) solution [Sompolinsky & Zippelius 1981, 1982] one derives equations valid in the thermodynamic limit via the saddle point method and then incorporates the fluctuations which occur in a finite system. However, it is not apparent whether one is justified in using the saddle point equations since the fluctuations occur only for finite N; it is possible that this is the source of the discrepancy with the results we obtain in Chapter III.

In his theory Sompolinsky (1981) proposed a 'dynamical' interpretation of the variable x. He assumed that there is a distribution of energy barries E_a:

$$E_a < E_b \quad \text{for} \quad a > b \ . \tag{1.37}$$

The energy barriers give rise to a distribution of relaxation times t_i:

$$t_i \sim e^{E_i/T} \tag{1.38}$$

which are parametrized in a <u>decreasing</u> order by an arbitrary parameter x ($0 \leqslant x \leqslant 1$), that is, if $x_1 > x_2$ then $t_{x_1} < t_{x_2}$. Further, one also assumes that $t_{x_2}/t_{x_1} \to \infty$ in this thermodynamic limit, all of the relaxation times diverging in this limit.

The Sompolinsky (1981) theory is characterised by two order parameters: $q(x)$ and $\Delta(x)$. The order parameter

$$q(x) = N^{-1} \sum_{i=1}^{N} \langle S_i(0) S_i(t_x) \rangle \ , \tag{1.39}$$

where $\langle \ldots \rangle$ indicates an average over all earlier time-scales, measures those correlations which persist at the time-scale t_x. Consequently, $q(x)$ is a monotonically increasing function with a maximum value at $x = 1$, for which

$$q(1) = q_{EA}, \tag{1.40}$$

the Edwards-Anderson order parameter. Statistical mechanics averages, on the other hand, are obtained on time-scales longer than the longest relaxation time and so, according to Sompolinsky (1981), the statistical mechanics order parameter, q, is given by

$$q = q(0). \tag{1.41}$$

The second order parameter, $\Delta(x)$, introduced by Sompolinsky (1981) measures the anomalous response of the system due to the crossing of infinitely high (in the thermodynamic limit) energy barriers. Thus, $\Delta(x)$ is a monotonically decreasing function of x with

$$\Delta(x \to 1) = 0 \tag{1.42}$$

and

$$\Delta(x \to 0) = \Delta \neq 0. \tag{1.43}$$

The anomaly, Δ, vanishes everywhere above the Almeida-Thouless (1978) line in the h-T plane.

Sompolinsky's (1981) solution is mathematically identical to that of Parisi's (1979, 1980a,b,c) under the gauge transformation

$$x \to X = \frac{-d\Delta(x)}{dx} \Big/ \frac{dq(x)}{dx} \tag{1.44}$$

$$= - \frac{d\Delta}{dq} \tag{1.45}$$

[de Dominicis et al. 1981; Elderfield 1984].

So, according to Sompolinsky (1981), the spin-glass regime is characterised by the appearance of both an Edwards-Anderson order parameter, q_{EA}, and an anomaly, Δ. As a consequence, it was claimed that the FDT breaks down in the low temperature phase [Sompolinsky (1981); Sompolinsky & Zippelius 1981, 1982] even when an average over samples is performed (see previous sub-section).

In Chapter III we argue that the non-ergodicity of the SK spin-glass invalidates the conventional techniques used in dynamics. In particular, in order to obtain the correct equilibrium behaviour

one needs to insert 'by hand' an initial Boltzmann distribution. However, as we show in Chapter III, this necessitates the use of replicas. Consequently, one needs to break the replica symmetry in the spin-glass phase. We go on to argue that the FDT does, in fact, hold once one performs an average over samples. So, whereas Sompolinsky and Zippelius (1981, 1982) introduced an anomaly, Δ, in order to stabilise their solution at low temperatures, we have to break the symmetry among the replicas.

As mentioned above, we shall consider an initial canonical (Boltzmann) distribution in Chapter III. De Dominicis and Young (1983b) have shown that Equation (1.41) holds if the initial distribution differs slightly from a canonical one. This would appear to indicate that Sompolinsky's (1981) solution is valid under non-equilibrium conditions.

We now discuss two- and three-dimensional Ising spin-glasses.

Section D: Short-Range Spin-Glasses

1. The two-dimensional Ising spin-glass

The EA model - see Equation (1.4) - on a square lattice was investigated by Morgenstern and Binder (1979, 1980a). Using a numerically exact transfer matrix approach they showed that there was no transition at any finite temperature.

As was discussed above, it was suggested by Morgenstern and Binder (1980a) that the $\pm J$ model probably belongs to a different universality class from the model with a continuous bond distribution, the two models having different values for the critical exponents. This was subsequently confirmed by Cheung and McMillan

(1983a,b) who combined the ideas of finite size scaling with those of transfer matrix.

Young (1983, 1984) and McMillan (1983) have also performed Monte Carlo simulations of the 2D Ising spin-glass. Once again they agree with the previous conclusions that there is no finite temperature transition.

Both of the techniques mentioned above involve extrapolations from relatively high temperatures to zero temperature. This problem was avoided by Bray and Moore (1984) and McMillan (1984b,c) who worked at zero temperature. By considering the scaling of effective couplings with the linear dimension of the samples they found that the model with Gaussian bonds has a zero-temperature transition.

Below, in Table 1.3, we compare the various values obtained for the static exponents γ_{SG}, ν_{SG} and η_{SG} [the exponents are defined in Chapter IV].

Bray and Moore (1984) have argued that an "effective" temperature-dependent exponent, $\nu_{SG}^{eff}(T)$, increases as T is lowered. This would explain the larger values obtained by Bray and Moore (1984) and McMillan (1984b,c) as they worked at $T = 0$.

Young (1983, 1984) and McMillan (1983) have also studied the dynamical behaviour of the ±J model. The quantity of interest, the average relaxation time τ, is defined in Chapter IV. Young (1983, 1984) finds that the characteristic energy barriers, ΔE, are temperature-dependent, behaving like T^{-1} as $T \to 0$. McMillan (1983), on the other hand, finds that $\Delta E \to 14.16J$ (a constant) as $T \to 0$. Nemoto and Takayama's (1983) analysis of the model with Gaussian bonds is consistent with the Young (1983, 1984) result.

Table 1.3

STATIC EXPONENTS FOR THE TWO-DIMENSIONAL ISING SPIN-GLASS

T_c/J	γ_{SG}	ν_{SG}	η_{SG}	Reference	
0	4.1	2.75	-	Young (1983, 1984)	±J
0.10±0.25	-	2.64±0.23	0.28±0.04	McMillan (1983)	±J
0	-	-	0.4±0.1	Morgenstern & Binder (1980a)	±J
0.02±0.11	-	2.59±0.13	-	Cheung & McMillan (1983a)	±J
0.05±0.05	-	2.96±0.22	0*	Cheung & McMillan (1983b)	continuous bond distribution
0	-	3.4±0.1	0*	Bray & Moore (1984a)	continuous bond distribution
0	-	2.6 3.56±0.06 3.27±0.16	0*	McMillan (1984a,b,c)	continuous bond distribution

* For continuous bond distributions there is a discontinuity in the Edwards-Anderson order parameter at $T_c = 0$; the system goes from a disordered state for $T > 0$ to a state with non-zero order parameter. Hence, $\beta_{SG} = 0$ and $\eta_{SG} = 2 - d = 0$ [Kinzel & Binder 1983; Binder & Young 1984] - See Chapter IV.

So, although one can explain the two-dimensional Ising spin-glass by a zero temperature transition [Binder & Young 1984], there is some controversy regarding its dynamical behaviour.

In Chapter IV we present the results of Monte Carlo simulations performed on the analogous X-Y spin-glass with a discrete distribution of bonds. We find that there is a zero temperature transition and estimate the exponents for such a transition to be smaller than those given in Table 1.3. Further, unlike the Ising case, we find no evidence for energy barriers; the system relaxes by "ordinary" critical slowing down [Hohenberg & Halperin 1977].

2. The three-dimensional Ising spin-glass

The Ising spin-glass on a cubic lattice has been far more controversial than the two-dimensional case.

At first the transfer matrix calculations [Morgenstern & Binder 1980b] and Monte Carlo simulations [Young 1984] for the three-dimensional Ising spin-glass were also interpreted in terms of a zero temperature transition [Binder & Young 1984]. However, as Morgenstern and Binder (1980b) were restricted to rather small sizes (the largest being $4 \times 4 \times 10$) they could not rule out a finite T_c in an infinite system; Young's (1984) data was, in fact, also consistent with a transition at a finite temperature.

On applying their analysis of the two-dimensional model, both McMillan (1984c) and Bray and Moore (1984a) suggest that there is a phase transition at a finite temperature in three dimensions. Recently, a value for T_c has been evaluated by extending the calculations to finite temperatures [McMillan 1984d; Bray & Moore 1984b]. This work is restricted to samples with small

linear dimension L; whereas McMillan (1984d) worked with $3 \leqslant L \leqslant 6$, Bray and Moore (1984a,b) were confined to $2 \leqslant L \leqslant 4$.

On performing Monte Carlo simulations both Bhatt and Young (1984) ($3 \leqslant L \leqslant 20$) and Ogielski and Morgenstern (1984) ($16 \leqslant L \leqslant 64$) have also found evidence for a transition at a finite temperature in the three-dimensional Ising spin-glass with ±J bonds.

In Table 1.4 we summarise the results obtained to date for the critical temperature and critical exponents.

Table 1.4

ESTIMATES OF THE TRANSITION TEMPERATURE AND CRITICAL EXPONENTS FOR THE THREE-DIMENSIONAL ISING SPIN-GLASS

T_c/J	γ_{SG}	ν_{SG}	η_{SG}	$\nu_{SG}z_{SG}$	Reference	
1.15±0.15	-	1.3 ± 0.3	- 0.3±0.2	-	Bhatt and Young (1984)	±J
1.22±0.04	-	1.12±0.12	0.07±0.07	5.2±0.2	Ogielski and Morgenstern (1984)	±J
1.0 ± 0.2	-	1.8 ± 0.5	-	-	McMillan (1984d)	Gaussian bond distribution
0.85	-	3.1	-	-	Bray and Moore (1984b)	Gaussian bond distribution

It is not clear as to why Bray and Moore's (1984b) value for ν_{SG} is much larger than the others in Table 1.4.

Interpolation between two and three dimensions predicts a Lower Critial Dimensionality (LCD) of about 2.6 [McMillan 1984c]. Although the Monte Carlo simulations of Ogielski and Morgenstern (1984) favour a finite T_c, they are unable to rule out completely

the possibility of an LCD of three. [See Chapter IV for a discussion on the LCD.]

Thus, it would appear that the LCD for Ising spin-glasses is certainly less than or equal to three.

In Chapter IV we discuss the results of Monte Carlo simulations performed on a 16×16×16 X-Y spin-glass with ±J bonds. Although we are unable to decide conclusively between the three possibilities we investigate ($T_c = 0$, $T_c \neq 0$ and LCD = 3), we marginally favour a transition at $T_c \simeq 0.45J$. We also give estimates for the various critical exponents on assuming that $T_c = 0.45J$, $T_c = 0$ and that the LCD = 3.

CHAPTER II

BROKEN SYMMETRY IN THE SHERRINGTON-KIRKPATRICK SPIN-GLASS

Section A: The Sherrington-Kirkpatrick Model

Sherrington and Kirkpatrick (1975) proposed an infinite-ranged model (SK model) for Ising spin-glasses whose solution it was hoped would provide a mean field theory for the corresponding short-ranged Edwards-Anderson (EA) model [Edwards & Anderson 1975].

The Hamiltonian of the SK model in a uniform external field is given by

$$H = - \sum_{i<j} J_{ij} S_i S_j - h \sum_{i=1}^{N} S_i , \qquad (2.1)$$

where $S_i = \pm 1$ are Ising spins at sites i (i = 1,2,...,N), h is the uniform magnetic field and the interactions $\{J_{ij}\}$ between any distinct pair of sites (i,j) are independent and identically distributed quenched random variables. This distribution is assumed to be Gaussian with zero mean and variance J^2/N, that is

$$P(J_{ij}) = \left(\frac{N}{2\pi} \right)^{1/2} \frac{1}{J} e^{-NJ_{ij}^2/2J^2} . \qquad (2.2)$$

The variance of the distribution is scaled by the number of spins, N, to ensure that the free energy is extensive, that is proportional to N. The SK model is discussed extensively in Chapter I. The rest of this chapter is restricted to J = 1.

In this case, when h = 0 there is a transition to a spin-glass state in the thermodynamic limit ($N \to \infty$) at a temperature

$T_c = 1$ (in units where Boltzmann's constant is set equal to unity) [Sherrington & Kirkpatrick 1975]. In the original "replica-symmetric" solution as proposed by Sherrington and Kirkpatrick (1975) the spin-glass state is completely determined by the conventional statistical mechanics order parameter, q, defined by

$$q = \frac{1}{N} \sum_{i=1}^{N} \langle \langle S_i \rangle_T^2 \rangle_J \ , \qquad (2.3)$$

where $\langle \ldots \rangle_T$ indicates a thermal (ensemble) average for a given set of interactions and $\langle \ldots \rangle_J$ indicates an average over the bond distribution $\{J_{ij}\}$. The "replica-symmetric" solution was subsequently found to be incorrect as it implies a negative entropy at low temperature, which is impossible for an Ising system [Kirkpatrick & Sherrington 1978]. In fact, the SK solution is unstable in the spin-glass phase with respect to fluctuations below the Almeida-Thouless line in the h-T plane (h magnetic field, T temperature) [Pytte & Rudnick 1978; Almeida & Thouless 1978].

Thouless et al. (1977) heuristically derived a set of N mean field equations for the site magnetisations, m_i, for a given set of J_{ij} (TAP equations) for the SK spin-glass using a method which avoided replicas. Below T_c the TAP equations have an exponentially large number of solutions [Bray & Moore 1980a; de Dominicis et al. 1980; Tanaka & Edwards 1980]. Bray and Moore (1981) argued that for these solutions to be independent they would have to be separated by free energy barriers that diverge in the thermodynamic limit.

Monte Carlo simulations of this model [Mackenzie 1982; Mackenzie & Young 1982, 1983] indicate that in the low temperature phase one has a spectrum of barrier heights, giving rise to a spectrum of

relaxation times. τ, the time required for properties to equilibrate within one half of phase space, and N, the system size, are related by: $T \ln \tau \propto N^{1/4}$ (here T is the temperature). See figure 2.1 for a schematic representation of the free energy in phase space.

The numerical work outlined above is in qualitative agreement with the analytic approaches of Sompolinsky (1981) and Hertz (1983). Using Langevin dynamics these two authors have suggested that below T_c there is a distribution of relaxation times, each of which is much longer than the previous one and all of which diverge in the thermodynamic limit.

Hence, if one interprets the TAP solutions as the metastable states in phase space separated by free energy barriers whose heights diverge in the thermodynamic limit, below the transition temperature the SK model is non-ergodic [Young 1981; Toulouse 1982], that is an infinite system will be trapped in a particular valley in phase space. As a consequence, one has to distinguish between time-averages which are evaluated from fluctuations in one phase and statistical mechanics averages which include contributions from all phases with a suitable weight [de Dominicis & Young 1983a].

Although a similar problem of non-ergodicity arises in the pure ferromagnet below the transition temperature, in that case there are just two stable solutions separated by time-reversal symmetry, whereas in the spin-glass there are many. The non-trivial non-ergodicity of the SK model makes its solution highly complex.

As mentioned above, the original "replica-symmetric" solution of Sherrington and Kirkpatrick (1975) is incorrect in the spin-glass phase. Although various tentative attempts were made to break the replica symmetry [Bray & Moore 1978; de Dominicis & Garel 1979; Blandin et al. 1980], it was Parisi (1979, 1980a,b,c) who managed to break

the permutation group symmetry among the replicas and suggested that the spin-glass phase should be characterized, not by a single order parameter, but by an order parameter function $q(x)$, $0 \leqslant x \leqslant 1$. [Parisi's solution is discussed in Chapter I.]

Although at the time Parisi offered no explanation as to what the dummy variable, x, could be, Houghton et al. (1983a) and Parisi (1983)[see Chapter I] have suggested that one should interpret dx/dq as the probability distribution for suitable weighted TAP solutions [de Dominicis & Young 1983a] to have an overlap q.

De Dominicis and Young (1983a) also argued that in the replica-symmetry broken situation one should evaluate statistical mechanics averages by averaging over all distinct replicas. In particular, this implies that

$$q = \int_0^1 q(x)\, dx, \tag{2.4}$$

where q, the statistical mechanics order parameter, is defined by (2.3).

Furthermore, in Parisi's (1980c) theory

$$T\chi(T) = 1 - \int_0^1 q(x)\, dx, \tag{2.5}$$

where $\chi(T)$, the uniform susceptibility, is defined by (2.10) below. Parisi claimed that $\chi(T) = 1$ in the replica-symmetry broken situation. Thus, combining (2.4) and (2.5) one has

$$q = 1 - T, \qquad 0 \leqslant T \leqslant 1. \tag{2.6}$$

An alternative interpretation of Parisi's x was proposed by Sompolinsky (1981) using Langevin dynamics. [Sompolinsky's solution is discussed

in Chapter I.] Subsequently, Sompolinsky's solution turned out to be mathematically identical to that of Parisi's under a suitable gauge transformation [de Dominicis et al. 1982; Elderfield 1984].

In the "dynamical solution" there are many monotonically decreasing timescales, τ_x, all of which diverge in the thermodynamic limit. In this approach [Sompolinsky 1981]

$$q(x) = \frac{1}{N} \sum_{i=1}^{N} \langle S_i(0)\, S_i(\tau_x) \rangle, \qquad (2.7)$$

where the average is over all timescales shorter than τ_x. According to Sompolinsky (1981) q(x) is a measure of the correlations which persist at the timescale τ_x. As statistical mechanics averages are evaluated on timescales longer than the longest relaxation time, in this interpretation of x, one has

$$q = \lim_{x \to 0} q(x) = q(0). \qquad (2.8)$$

Furthermore, Sompolinsky (1981) suggested that in the replica-symmetry broken situation q(0) is zero, that is

$$q = 0, \qquad 0 \leqslant T \leqslant 1. \qquad (2.9)$$

So, the two interpretations of x give widely differing predictions for q below T_c. In Section B evidence is presented which appears to rule out (2.9).

Another quantity which has been the subject of some controversy is the uniform susceptibility, $\chi(N,h,T)$, defined by

$$T\chi(N,h,T) = \frac{1}{N} \sum_{i,j=1}^{N} \langle\langle S_i S_j \rangle_T - \langle S_i \rangle_T \langle S_j \rangle_T \rangle_J \ . \qquad (2.10)$$

For a symmetric distribution of interactions $\{J_{ij}\}$ (such as the one defined by (2.2)) and $h \equiv 0$ time-reversal symmetry (that is, $S_i \to -S_i$ for all sites i) of the Hamiltonian (2.1) ensures that $\langle S_i \rangle_T = 0$ and (2.10) reduces trivially to

$$T\chi(T) \equiv \lim_{N\to\infty} \lim_{h\to 0} T\chi(N,h,T) = \lim_{N\to\infty} T\chi(N,0,T) = 1. \qquad (2.11)$$

However, as with the ferromagnet, one can restrict the thermal average to include states in the vicinity of just one of the two degenerate ground states by applying a small symmetry breaking field, h.

It has been claimed [Fischer 1976] that the off-diagonal ($i \neq j$) terms in (2.10) vanish even in the symmetry broken situation, leading to the Fischer relation [Fischer 1976]:

$$T\chi(T) = 1 - q \qquad (2.12)$$

where

$$\chi(T) \equiv \lim_{h\to 0} \lim_{N\to\infty} \chi(N,h,T). \qquad (2.13)$$

On the other hand, Bray and Moore (1980b) gave a replica-symmetry breaking argument which implied the break-down of Linear Response Theory (LRT) in the spin-glass phase and consequently the invalidity of both (2.10) and (2.12). Yet another possibility was raised by Young and Kirkpatrick (1982) who argued on the basis of exact statistical mechanics that although LRT is valid (that is, (2.10) holds), the Fischer

relation (2.12) breaks down below T_c. They noted that the order of limits in (2.11) and (2.13) are interchanged and argued that in the symmetry broken situation the off-diagonal ($i \neq j$) terms to (2.10) give a finite contribution.

In Section B it is shown that both (2.10) and (2.12) hold in the spin-glass state.

So, as statistical mechanics averages have to be evaluated in the presence of a symmetry breaking field, q in (2.3) is defined by

$$q = \lim_{h \to 0} \lim_{N \to \infty} q(N,h), \tag{2.14a}$$

where

$$q(N,h) = \frac{1}{N} \sum_{i=1}^{N} \langle\langle S_i \rangle_T^2 \rangle_J \ . \tag{2.14b}$$

Although the present discussion is restricted to a uniform symmetry breaking field, it also applies to an arbitrary random staggered field, h_i, uncorrelated with the interaction $\{J_{ij}\}$. As one is dealing with discrete Ising spins it is natural to assume a binary distribution of fields, that is

$$h_i = \tau_i h, \tag{2.15a}$$

where

$$P(\tau_i) = \frac{1}{2} \delta(\tau_i - 1) + \frac{1}{2} \delta(\tau_i + 1). \tag{2.15b}$$

Then, as Young and Kirkpatrick (1982) noticed, the Hamiltonian expressed in terms of the new variables

$$S_i' = \tau_i S_i \quad , \tag{2.16a}$$

$$S_j' = \tau_j S_j \quad , \tag{2.16b}$$

$$J_{ij}' = \tau_i \tau_j J_{ij} \quad , \tag{2.16c}$$

is identical to (2.1).

The case of interaction-dependent fields conjugate to one of the two ground states will not be considered.

The order of limits as indicated in (2.14a) is not very suitable for numerical calculations as one is restricted to relatively small values of N. For any given finite system of size N the symmetry breaking field has to be greater than a critical field, h*, before one can take the thermodynamic limit. h* has to be large enough to suppress the time-reversed state with negative magnetization. YK (1982) argued that because low-energy states in the spin-glass phase have a magnetization of order $N^{1/2}$ in order to overcome thermal fluctuations one needs to set

$$h^* = T/\sqrt{N} \quad , \tag{2.17}$$

where Boltzmann's constant is set equal to unity.

As $h \to 0$ at the end, in the symmetry broken situation one requires

$$h^* \ll h \ll 1. \tag{2.18}$$

Hence the limits in (2.14a) correspond to

$$\frac{h}{h^*} \to \infty \text{ and } h \ll 1. \tag{2.19}$$

In Sections B and C there is a detailed analysis of (2.10) under the conditions imposed by (2.19).

As YK (1982) pointed out, it is possible to define an order parameter which is not automatically zero by time-reversal symmetry in the absence of a field. They suggested the correlation function $q^{(2)}$, defined by

$$q^{(2)} = \frac{1}{N(N-1)} \sum_{i \neq j} \langle\langle S_i S_j \rangle_T^2 \rangle_J \ . \tag{2.20}$$

The material in this chapter has also been discussed in Young and Jain (1983).

Section B: The Cumulant Expansion

The uniform susceptibility, defined by (2.10), is given by

$$T\chi(N,h,T) = 1 - q(N,h) + (1 - \frac{1}{N}) q^{O-D}(N,h), \tag{2.21}$$

where q(N,h) is defined by (2.14b) and the off-diagonal contribution, $q^{O-D}(N,h)$, is defined by

$$q^{O-D}(N,h) = \frac{1}{N-1} \sum_{i \neq j} \langle\langle S_i S_j \rangle_T - \langle S_i \rangle_T \langle S_j \rangle_T \rangle_J . \tag{2.22}$$

However, the uniform susceptibility is also given by [Stanley 1971]

$$T\chi(N,h,T) = - T \left\langle \frac{\partial^2 F(N,h,T)}{\partial h^2} \right\rangle_J \tag{2.23a}$$

where F is the free energy per spin defined by

$$F(N,h,T) = -\frac{T}{N} \ln Z\{N,h,T\} \tag{2.23b}$$

and here Z is the partition function given by

$$Z\{N,h,T\} = \sum_{\{S_i=\pm 1\}} e^{-H/T}. \quad \text{(Boltzmann's constant=1)} \tag{2.23c}$$

In (2.23c) H denotes the Hamiltonian defined by (2.1). Let H_0 denote the Hamiltonian with h = 0 and Z_0 the corresponding partition function, that is,

$$Z_0 \equiv Z\{N,0,T\} = \sum_{\{S_i=\pm 1\}} e^{-H_0/T}. \tag{2.24}$$

Substituting (2.23c) into (2.23b) one gets for the free energy

$$F(N,h,T) = -\frac{T}{N} \ln\left(\sum_{\{S_i=\pm 1\}} e^{-H/T} \right)$$

$$= -\frac{T}{N} \ln\left(\sum_{\{S_i=\pm 1\}} e^{-\beta H_0}.e^{+hM/T} \right), \quad (\beta = 1/T) \tag{2.25}$$

since from (2.1)

$$H = H_0 - h\sum_{i=1}^{N} S_i$$

$$\equiv H_0 - hM. \tag{2.26}$$

So the symmetry breaking field couples to the total magnetization $M \left(= \sum_{i=1}^{N} S_i\right)$.

Expanding the second exponential in (2.25) we get

$$F(N,h,T) = -\frac{T}{N}\ln\left(\sum_{\{S_i=\pm1\}} e^{-H_0/T}\left\{1 + h(\frac{M}{T}) + \ldots + \frac{h^r}{r!}(\frac{M}{T})^r + \ldots\right\}\right)$$

$$= -\frac{T}{N}\ln\left(Z_0\left\{1 + h\langle\frac{M}{T}\rangle_T + \ldots + \frac{h^r}{r!}\langle(\frac{M}{T})^r\rangle_T + \ldots\right\}\right)$$

$$= -\frac{T}{N}\ln Z_0 - \frac{T}{N}\ln\left(\sum_{n=0}^{\infty}\frac{h^n}{n!}\langle(\frac{M}{T})^n\rangle_T\right), \qquad (2.27)$$

where $\langle\ldots\rangle_T$ denotes a statistical mechanics average in <u>zero field</u>. Now, expanding the second term in (2.27) in terms of a cumulant expansion [Beyer 1968] one gets

$$F(N,T,h) = -\frac{T}{N}\ln Z_0 - \frac{T}{N}\sum_{n=1}^{\infty}\frac{h^n}{n!}\langle(\frac{M}{T})^n\rangle_{C_0}, \qquad (2.28)$$

where $\langle\ldots\rangle_{C_o}$ denotes a cumulant (statistical mechanics) average evaluated in zero field. Substituting (2.28) into (2.23a) the uniform susceptibility becomes

$$T\chi(N,h,T) = \frac{1}{N}\sum_{n=0}^{\infty}\frac{h^n}{n!}\langle\langle MM(\frac{M}{T})^n\rangle_{C_o}\rangle_J . \qquad (2.29)$$

Thus, defining

$$\langle\langle S_iS_j\rangle_C\rangle_J = \sum_{n=0}^{\infty} C_n\frac{h^n}{n!}, \quad C_n = \langle\langle S_iS_j(\frac{M}{T})^n\rangle_{C_0}\rangle_J , \qquad (2.30)$$

where $\langle\ldots\rangle_C$ denotes a cumulant average, one has from (2.29) that

$$T\chi(N,h,T) = \frac{1}{N}\sum_{i,j=1}^{N}\langle\langle S_iS_j\rangle_C\rangle_J$$

$$= \frac{1}{N}\sum_{i=j} \langle\langle S_i S_j\rangle_C\rangle_J + \frac{1}{N}\sum_{i\neq j} \langle\langle S_i S_j\rangle_C\rangle_J \ . \qquad (2.31)$$

So, from (2.21) and (2.31) we get

$$1-q(N,h) = \frac{1}{N}\sum_{i=j} \langle\langle S_i S_j\rangle_C\rangle_J$$

$$= \langle\langle S_i S_i\rangle_C\rangle_J \qquad (2.32a)$$

and

$$q^{O-D}(N,h) = \frac{1}{N-1}\sum_{i\neq j} \langle\langle S_i S_j\rangle_C\rangle_J$$

$$= N\langle\langle S_i S_j\rangle_C\rangle_J \ , \quad (i \neq j) \qquad (2.32b)$$

since there are N(N-1) off-diagonal terms. Using definitions (2.30) in (2.32a) and (2.32b) one gets

$$1-q(N,h) = \sum_{n=0}^{\infty} a_n \frac{h^n}{n!} \ , \quad a_n = \langle\langle S_i S_i (\frac{M}{T})^n\rangle_{C_0}\rangle_J \qquad (2.33a)$$

and

$$q^{O-D}(N,h) = N\sum_{n=0}^{\infty} b_n \frac{h^n}{n!} \ , \ b_n = \langle\langle S_i S_j (\frac{M}{T})^n\rangle_{C_0}\rangle_J \ . \ (i \neq j) \qquad (2.33b)$$

We now pick out the terms that are going to dominate (2.33a) and (2.33b) in the thermodynamic limit. We look at (2.33a) first, in particular the coefficients a_n. Now, as $M = \sum_{k=1}^{N} S_k$,

$$a_n = \langle\langle S_i S_i (\frac{M}{T})^n\rangle_{C_0}\rangle_J$$

$$= \frac{1}{T^n}\langle\langle S_i S_i \Big(\sum_{k=1}^{N} S_k\Big)^n\rangle_{C_0}\rangle_J$$

$$= \frac{1}{T^n} \langle\langle S_i S_i \sum_{k_1,\ldots,k_n=1}^{N} S_{k_1} S_{k_2} \ldots S_{k_n} \rangle_{C_0} \rangle_J \quad , \; n=0,1,\ldots \; . \tag{2.34}$$

Since time-reversal symmetry requires each site in (2.34) to occur an even number of times for the cumulant average to be non-zero, the coefficients of odd powers of h in (2.33a) vanish, that is,

$$a_{2n+1} = 0, \quad n = 0,1,2,\ldots \tag{2.35}$$

and (2.34) becomes

$$a_{2n} = \frac{1}{T^{2n}} \langle\langle S_i S_i \sum_{k_1,\ldots,k_{2n}=1}^{N} S_{k_1} S_{k_2} \ldots S_{k_{2n}} \rangle_{C_0} \rangle_J \; ,$$

$$n = 0,1,\ldots \; . \tag{2.36}$$

When each site in (2.36) occurs just twice the number of independent summations is maximised and we obtain the dominant contribution to a_{2n}. Hence, we need to divide the spins $S_{k_1}, S_{k_2}, \ldots, S_{k_{2n}}$ into n pairs. As there are (2n-1)!!* ways of dividing 2n objects into n pairs, one has from (2.36)

$$a_{2n} = \frac{(2n-1)!!}{T^{2n}} \langle\langle S_i S_i \Big(\sum_{k_1=k_2} S_{k_1} S_{k_2} \Big) \Big(\sum_{k_3=k_4} S_{k_3} S_{k_4} \Big) \ldots \Big(\sum_{\substack{k_{2n-1} \\ =k_{2n}}} S_{k_{2n-1}} S_{k_{2n}} \Big) \rangle_{C_o} \rangle_J$$

$$= \frac{(2n)!}{2^n n! T^{2n}} \langle\langle S_i S_i (NS_{k_1} S_{k_1})(NS_{k_3} S_{k_3}) \ldots (NS_{k_{2n-1}} S_{k_{2n-1}}) \rangle_{C_0} \rangle_J$$

$$= \frac{(2n)!}{2^n n!} \left(\frac{N}{T^2} \right)^n \langle\langle S_1 S_1 S_2 S_2 \ldots S_{n+1} S_{n+1} \rangle_{C_0} \rangle_J \tag{2.37}$$

---

* $m!! \equiv m.(m-2).(m-4)\ldots 3.1$

where we have re-defined the suffixes into a more convenient form. Combining (2.37) with (2.33a) and using (2.17) [$h^* = T/\sqrt{N}$] one has

$$f(x) \equiv 1 - q(N,h)$$

$$= \sum_{n=0}^{\infty} \frac{A_{2n}}{2^n n!} x^{2n} , \qquad x = \frac{h}{h^*} \tag{2.38a}$$

where

$$A_{2n} = \langle\langle S_1 S_1 S_2 S_2 \ldots S_{n+1} S_{n+1} \rangle_{C_0} \rangle_J \quad . \tag{2.38b}$$

So, in the symmetry broken situation

$$\lim_{x \to \infty} f(x) = 1 - q, \tag{2.39}$$

where q is given by (2.14a) and (2.14b).

The calculation of (2.33b), the coefficient b_n, is similar to the one outlined above, although there are minor differences. Once again time-reversal symmetry requires that

$$b_{2n+1} = 0, \qquad n = 0,1,2,\ldots \quad . \tag{2.40}$$

Furthermore, as $i \neq j$, $b_0 = 0$ also. Hence, from (2.33b) one has

$$b_{2n} = \frac{1}{T^{2n}} \langle\langle S_i S_j \sum_{\ell_1,\ldots,\ell_{2n}=1}^{N} S_{\ell_1} S_{\ell_2} \ldots S_{\ell_{2n}} \rangle_{C_0} \rangle_J ,$$

$$n = 1,2,\ldots \quad . \tag{2.41}$$

This time one of the spins from "$S_{\ell_1} S_{\ell_2} \ldots S_{\ell_{2n}}$" has to be paired with S_i and another with S_j; there are (2n)(2n-1) ways of doing this. As there are (2n-3)!! ways of dividing 2n-2 spins into n-1 pairs, one gets from (2.41) that

$$b_{2n} = \frac{(2n)(2n-1)!!}{T^{2n}} \langle\langle \left(S_i \sum_{\ell_1=i} S_{\ell_1}\right)\left(S_j \sum_{\ell_2=j} S_{\ell_2}\right)\left(NS_{\ell_3} S_{\ell_3}\right) \ldots \left(NS_{\ell_{2n-1}} S_{\ell_{2n-1}}\right)\rangle_{C_0}\rangle_J$$

$$= \frac{(2n)(2n)!}{2^n n! N}\left(\frac{N}{T^2}\right)^n \langle\langle S_1 S_1 S_2 S_2 \ldots S_{n+1} S_{n+1}\rangle_{C_0}\rangle_J \qquad (2.42)$$

where once again the suffixes have been re-defined. Combining (2.42) with (2.33b) and using (2.17) [$h^* = T/\sqrt{N}$] we get

$$g(x) \equiv q^{O-D}(N,h)$$

$$= \sum_{n=1}^{\infty} \left(\frac{A_{2n}}{2^n n!}\right) 2n x^{2n}, \qquad x = \frac{h}{h^*} \qquad (2.43)$$

where A_{2n} is defined by (2.38b) and in the symmetry broken situation

$$\lim_{x\to\infty} g(x) = q^{O-D}, \qquad (2.44)$$

the off-diagonal contribution.

We see from (2.38a) and (2.43) that in fact

$$g(x) = x \frac{df}{dx} . \qquad (2.45)$$

Now, if we suppose that

$$f(x) = 1 - q + Ax^{-\lambda} \qquad (2.46)$$

where A is an arbitrary constant and λ is a positive constant, so that in the symmetry broken situation we retrieve (2.39), we have from (2.45) that

$$g(x) = - A\lambda x^{-\lambda}. \tag{2.47}$$

Hence

$$\begin{aligned} q^{O-D} &= \lim_{h\to 0} \lim_{N\to\infty} q^{O-D}(N,h) \\ &= \lim_{x\to\infty} g(x) = 0. \end{aligned} \tag{2.48}$$

This shows that the off-diagonal contribution vanishes below T_c, that is, from (2.21)

$$\begin{aligned} \lim_{h\to 0} \lim_{N\to\infty} T\chi(N,h,T) &= \lim_{h\to 0} \lim_{N\to\infty} \{1 - q(N,h)\} \\ &\quad + \lim_{h\to 0} \lim_{N\to\infty} \{(1 - \tfrac{1}{N})q^{O-D}(N,h)\} \\ &= 1 - q, \end{aligned} \tag{2.49}$$

where we have used (2.39) and (2.48).

As was mentioned above, YK(1982) concluded on the basis of numerical data that $q^{O-D} \neq 0$. YK (1982), however, did not evaluate q by applying a field and taking the limits as in (2.14a) because the order there is unsuitable for numerical work. Since the magnetic field suppresses states with a negative magnetization, YK (1982) suggested that its role could be mimicked by simply omitting these

states from the thermal average. It was then claimed that the order of limits on such a restricted average ($\langle \ldots \rangle_R$: thermal average restricted to states with a positive magnetization) is irrelevant, that is, if we define

$$q^R(N,h) = \frac{1}{N} \sum_{i=1}^{N} \langle \langle S_i \rangle_R^2 \rangle_J \ , \tag{2.50a}$$

then

$$q = q^R$$

$$= \lim_{h \to 0} \lim_{N \to \infty} q^R(N,h) = \lim_{N \to \infty} \lim_{h \to 0} q^R(N,h)$$

$$= \lim_{N \to \infty} q^R(N,0). \tag{2.50b}$$

However, in view of the above calculation it appears that the order of limits in (2.50b) cannot be interchanged. A possible variation of $q(N,h)$ and $q^R(N,h)$ with h is shown in figure 2.2. So all one can actually say is that

$$q > q^R > 0, \tag{2.51}$$

where the last inequality is based on numerical work [YK 1982; Mackenzie & Young 1983; Mackenzie 1982].

We note that (2.51) disagrees with the Sompolinsky claim, (2.9), that $q = 0$ in the spin-glass phase.

Section C: A Single Order Parameter Ansatz

In general the cumulants (2.38b) appearing in the expansion (2.38a) involve complicated correlation functions. The first two coefficients are the simplest and are evaluated below. Now, (2.38a) is

$$f(x) = A_0 + \frac{A_2}{2} x^2 + \ldots + \frac{A_{2r}}{2^r r!} x^{2r} + \ldots$$

where

$$A_{2r} = \langle\langle S_1 S_1 S_2 S_2 \ldots S_{r+1} S_{r+1} \rangle_{C_0} \rangle_J \,. \tag{2.52}$$

By definition (see (2.27) and (2.28))

$$\sum_{n=0}^{\infty} \langle X^n \rangle_T \frac{\lambda^n}{n!} = \exp\left\{ \sum_{n=1}^{\infty} \langle X^n \rangle_{C_0} \frac{\lambda^n}{n!} \right\}, \tag{2.53}$$

where we define $\langle X^0 \rangle_T \equiv 1$, λ is a dummy variable which keeps track of the terms and X denotes S_i. So, one can extract the cumulants by expanding the right-hand side of (2.53) and then equating the coefficients of powers of λ. Noting that once again the coefficients of all odd powers of λ vanish, the first three non-zero terms in (2.53) are

$$\begin{aligned} 1 + \langle X^2 \rangle_T \frac{\lambda^2}{2!} + \langle X^4 \rangle_T \frac{\lambda^4}{4!} + \ldots &= 1 + \left\{ \langle X^2 \rangle_{C_0} \frac{\lambda^2}{2!} + \langle X^4 \rangle_{C_0} \frac{\lambda^4}{4!} + \ldots \right\} \\ &\quad + \frac{1}{2!} \left\{ \langle X^2 \rangle_{C_0} \frac{\lambda^2}{2!} + \ldots \right\}^2 + \ldots \\ &= 1 + \langle X^2 \rangle_{C_0} \frac{\lambda^2}{2!} + \left\{ \langle X^4 \rangle_{C_0} + 3 \langle X^2 \rangle_{C_0} \langle X^2 \rangle_{C_0} \right\} \frac{\lambda^4}{4!} + \ldots \end{aligned} \tag{2.54}$$

Thus

$$\langle x^2 \rangle_{C_0} = \langle x^2 \rangle_T$$

and

$$\langle x^4 \rangle_{C_0} = \langle x^4 \rangle_T - 3 \langle x^2 \rangle_T \langle x^2 \rangle_T \ . \tag{2.55}$$

Hence, we have from (2.52) and (2.55) that

$$A_0 = \langle \langle S_1 S_1 \rangle_{C_0} \rangle_J$$

$$= \langle \langle S_1 S_1 \rangle_T \rangle_J = 1 \tag{2.56}$$

and that

$$A_2 = \langle \langle S_1 S_1 S_2 S_2 \rangle_{C_0} \rangle_J$$

$$= \langle \langle S_1 S_1 S_2 S_2 \rangle_T - \langle S_1 S_1 \rangle_T \langle S_2 S_2 \rangle_T - 2 \langle S_1 S_2 \rangle_T^2 \rangle_J$$

$$= 1 - 1 - 2 \langle \langle S_1 S_2 \rangle_T^2 \rangle_J$$

$$= - 2 q^{(2)}, \tag{2.57}$$

where we have used definition (2.20) for the order parameter $q^{(2)}$.

Thus, substituting (2.56) and (2.57) into (2.38a) we get that

$$1 - q(N,h) = 1 - q^{(2)} x^2 + \ldots \tag{2.58}$$

$$\Rightarrow q(N,h) = q^{(2)}x^2 + \ldots, \tag{2.59}$$

and from (2.43) that

$$g(x) = q^{O-D}(N,h) = -\,2q^{(2)}x^2 + \ldots\ . \tag{2.60}$$

Now, Bray and Moore (1980) have shown that

$$q^{(2)} = 1 - 2T\left|U(T)\right|, \tag{2.61}$$

where U(T) is the interaction-averaged internal energy. (2.61) is obtained by integrating by parts over J_{ij} in order to perform explicitly the configuration average. There is convincing evidence [Kirkpatrick & Sherrington 1978, Mackenzie 1982, Mackenzie & Young 1983] that $q^{(2)}$ is non-zero below T_c. Hence g(x) is non-monotonic, that is, although

$$\lim_{x\to 0} g(x) = \lim_{x\to\infty} g(x) = 0, \tag{2.62}$$

g(x) is finite for intermediate values of x.

In the symmetry broken situation there is no obvious relationship between the order parameters which appear in the expansion (2.59). We can, however, sum the expansions (2.59) and (2.60) if we make a single order parameter ansatz. With such an ansatz one first assumes that the spins $S_1 \ldots S_{n+1}$ are indistinguishable and then expands out the cumulant average, noting that the thermal average of a product of odd number of spins is zero and that of an even number is unity. Consequently, the A_{2n}'s - see (2.38b) - become

$$A_{2n} = \langle\langle S_1 S_1 S_2 S_2 \ldots S_{n+1} S_{n+1} \rangle_{C_0} \rangle_J$$

$$\equiv \langle\langle SSSS \ldots SS \rangle_{C_0} \rangle_J \mu^{n+1}$$

$$= C_{n+1} \mu^{n+1} \qquad n = 1,2,\ldots, \tag{2.63a}$$

where

$$C_n = \langle S^{2n} \rangle_{C_0} \tag{2.63b}$$

is simply the 2nth cumulant average of a single free spin and the dummy variable μ keeps track of the coefficients. Note that by self-consistency $\mu \equiv q$ in the symmetry broken situation - see Equation (2.85) below.

Consider first A_2 which is given by (2.57). Now, with a single order parameter ansatz this becomes

$$A_2 = C_2 \mu^2 \tag{2.64a}$$

with

$$C_2 = \langle S^4 \rangle_{C_0}$$

$$= \langle S^4 \rangle_T - 3 \langle S^2 \rangle_T \langle S^2 \rangle_T$$

$$= -2, \tag{2.64b}$$

where we have used (2.55) to evaluate the cumulant average. So, in the symmetry broken situation

$$\Lambda_2 = - 2q^2. \tag{2.65}$$

On comparing (2.57) and (2.65) we see that with a single order parameter ansatz one has that

$$q^{(2)} = q^2. \tag{2.66}$$

In general we have from (2.38a) and (2.63a) that

$$q(N,h) = - \sum_{n=1}^{\infty} \frac{C_{n+1}}{2^n n!} \mu^{n+1} x^{2n}, \quad x = h/h^*$$

$$= \mu \tilde{f}(\mu^{1/2} x) \tag{2.67a}$$

where

$$\tilde{f}(x) = - \sum_{n=1}^{\infty} \frac{C_{n+1}}{2^n n!} x^{2n} . \tag{2.67b}$$

Likewise from (2.43) and (2.63a)

$$q^{O-D}(N,h) = \mu \tilde{g}(\mu^{1/2} x) \tag{2.68}$$

where

$$\tilde{g}(x) = x \frac{d\tilde{f}}{dx} . \tag{2.69}$$

To calculate the C_n's we consider the problem of a single spin, S, in a random field h. The Hamiltonian for this trivial system is

$$H = - hs. \tag{2.70}$$

The distribution of the field h is assumed to be Gaussian, that is

$$p(h) = \frac{1}{\Delta\sqrt{2\pi}} \; e^{-\frac{1}{2}h^2/\Delta^2} \tag{2.71}$$

where Δ is the standard deviation of the distribution.

We repeat the above calculation for this simple system. The analogues of (2.31) and (2.32a) are

$$T\tilde{\chi}(h,T) = \langle\langle SS\rangle_C\rangle_h \tag{2.72}$$

$$= 1 - \tilde{q}(\Delta) \tag{2.73}$$

where $\langle \ldots\rangle_h$ denotes an average over the distribution of h, that is (2.71), and the analogue of (2.30) is

$$\langle\langle SS\rangle_C\rangle_h = \sum_{n=0}^{\infty} \frac{\langle S^{n+2}\rangle_{C_0}}{n!} \langle(\frac{h}{T})^n\rangle_h \tag{2.74}$$

where the cumulant on the right-hand side of (2.74) is once again that of a single spin in zero field. Hence, from (2.72), (2.73) and (2.74) one has that

$$\tilde{q}(\Delta) = -\sum_{n=1}^{\infty} \frac{C_{n+1}}{(2n)!} \langle(\frac{h}{T})^{2n}\rangle_h \,, \tag{2.75}$$

where we have dropped the first term (= 1) and noted once again that the coefficients of odd powers of h vanish. Now

$$\langle(\frac{h}{T})^{2n}\rangle_h = \frac{1}{\Delta\sqrt{2\pi}}\int_{-\infty}^{+\infty}(\frac{h}{T})^{2n} \; e^{-h^2/2\Delta^2} \; dh$$

$$= (\frac{\Delta}{T})^{2n} \frac{(2n)!}{2^n n!} \,, \tag{2.76}$$

where we have used

$$\int_{-\infty}^{\infty} x^{2n}\, e^{-ax^2}\, dx = \frac{(2n-1)!!}{2^n\, a^n}\sqrt{\frac{\pi}{a}} \tag{2.77}$$

[Beyer 1968, p. 631].

Thus, one sees from (2.67b), (2.75) and (2.76) that if we identify $x = \frac{\Delta}{T}$

$$\tilde{f}(x) = \tilde{q}(\Delta). \tag{2.78}$$

But for this single spin problem

$$\tilde{q}(\Delta) = \langle \langle S \rangle_T^2 \rangle_h$$

$$= \frac{1}{\Delta\sqrt{2\pi}} \int_{-\infty}^{+\infty} \langle S \rangle_T^2\, e^{-h^2/2\Delta^2}\, dh, \tag{2.79}$$

where

$$\langle S \rangle_T = \sum_{\{S=\pm 1\}} S e^{hS/T} \Big/ \sum_{\{S=\pm 1\}} e^{hS/T}$$

$$= \tanh(h/T). \tag{2.80}$$

Hence,

$$\tilde{q}(\Delta) = \frac{1}{\Delta\sqrt{2\pi}} \int_{-\infty}^{\infty} \tanh^2(h/T)\, e^{-h^2/2\Delta^2}\, dh \tag{2.81}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tanh^2(xy) e^{-y^2/2}\, dy, \qquad \left\{ \begin{array}{l} y = h/\Delta \\ x = \Delta/T. \end{array} \right\} \tag{2.82}$$

Thus, from (2.78) and (2.82)

$$\tilde{f}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tanh^2(xy)\, e^{-y^2/2}\, dy. \tag{2.83}$$

In the symmetry broken situation

$$\lim_{x\to\infty} \tilde{f}(x) = 1 \tag{2.84}$$

and consequently from (2.67a)

$$\lim_{h\to 0}\lim_{N\to\infty} q(N,h) = \mu \equiv q \tag{2.85}$$

by self-consistency. Further, from (2.69)

$$\lim_{x\to\infty} \tilde{g}(x) = 0 \tag{2.86}$$

and, of course, for the sum we have that

$$\lim_{x\to\infty}\{\tilde{f}(x) + \tilde{g}(x)\} = 1. \tag{2.87}$$

We can easily obtain the leading correction in (2.83). For

$$\begin{aligned}
\tilde{f}(x) &= 1 - \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \operatorname{sech}^2(xy)\, e^{-y^2/2}\, dy \\
&= 1 - \frac{1}{x\sqrt{2\pi}}\int_{-\infty}^{+\infty} \operatorname{sech}^2\eta\, e^{-\eta^2/2x^2}\, d\eta, \qquad xy = \eta \\
&\simeq 1 - \frac{1}{x\sqrt{2\pi}}\int_{-\infty}^{+\infty} \operatorname{sech}^2\eta\, d\eta, \qquad e^{-\eta^2/2x^2} \simeq 1 \quad \text{for } x >> 1 \\
&= 1 - \frac{1}{x}\sqrt{\frac{2}{\pi}} \quad .
\end{aligned} \tag{2.88}$$

As a consequence, the leading correction to $\tilde{g}(x)$ is

$$\begin{aligned}
\tilde{g}(x) &= x\tilde{df}/dx \qquad \text{(from (2.69))} \\
&\simeq \frac{1}{x}\sqrt{\frac{2}{\pi}} \quad .
\end{aligned} \tag{2.89}$$

We see from (2.88) and (2.89) that the leading correction cancels in the sum $\tilde{f} + \tilde{g}$. Consequently, it - the sum - approaches its asymptotic value much faster than either $\tilde{f}$ or $\tilde{g}$ approach theirs. This is shown explicitly in Figure 2.3 where all three functions are plotted.

Section D: Conclusions

The effect of a small uniform symmetry breaking field on the SK spin-glass was discussed. Both the diagonal, 1-q(N,h), and the off-diagonal, $q^{O-D}(N,h)$, contributions to the uniform susceptibility are given by scaling functions:

$$1 - q(N,h) = f(h/h^*) \tag{2.90}$$

and

$$q^{O-D}(N,h) = g(h/h^*), \quad h^* = T/\sqrt{N} \tag{2.91}$$

with

$$g(x) = x \frac{df}{dx}, \qquad x = h/h^*. \tag{2.92}$$

Hence, in the spin-glass phase ($h/h^* \to \infty$, $h << 1$)

$$\lim_{x\to\infty} f(x) = 1 - q, \tag{2.93}$$

$$\lim_{x\to\infty} g(x) = 0 \tag{2.94}$$

and

$$T\chi(T) = 1 - q. \tag{2.95}$$

The above result is in contrast to the numerical work of YK (1982) who evaluated an order parameter, q^R, restricted to states with a positive magnetization and interpreted this as q. In fact, one can only say that

$$q > q^R > 0. \tag{2.96}$$

On making a single order parameter ansatz a closed form was derived for q(N,h), that is

$$q(N,h) = \frac{q}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tanh^2(xy) e^{-y^2/2}\, dy, \quad x = \frac{h}{h^*}\sqrt{q} \quad . \tag{2.97}$$

CHAPTER III

ROLE OF INITIAL CONDITIONS IN THE DYNAMICS OF THE SHERRINGTON-KIRKPATRICK SPIN-GLASS

Section A: Introduction

1. The Sherrington-Kirkpatrick spin-glass and replicas

The Hamiltonian of the SK spin-glass discussed in the previous chapter is given by

$$H = -\sum_{i<j} J_{ij} S_i S_j - \sum_{i=1}^{N} h_i S_i, \tag{3.1}$$

where $S_i = \pm 1$ are Ising spins at sites i ($i = 1,2,\ldots,N$), h_i is an external magnetic field and the interactions $\{J_{ij}\}$ are independent and identically distributed quenched random variables drawn from a Gaussian distribution, that is

$$P(J_{ij}) = \left(\frac{N}{2\pi}\right)^{\frac{1}{2}} \frac{1}{J} \; e^{\frac{-NJ_{ij}^2}{2J^2}} . \tag{3.2}$$

The SK spin-glass has a transition in zero field in the thermodynamic limit ($N \to \infty$) at a temperature $T_c = J$ (in units where Boltzmann's constant is set equal to unity) [Sherrington & Kirkpatrick 1975]. Now, the interaction-dependent free energy per spin is given by

$$F(\{J_{ij}\}) = -\lim_{N\to\infty} TN^{-1} \ln Z(\{J_{ij}\}) \tag{3.3}$$

where the partition function, Z, is given by

$$Z(\{J_{ij}\}) = \sum_{\{S_i=\pm 1\}} e^{-\beta H(S_i)}, \qquad \beta = 1/T. \tag{3.4}$$

As the free energy is a self-averaging quantity, we can simplify the problem by evaluating the interaction-averaged free-energy, F, that is

$$F = - \lim_{N\to\infty} TN^{-1} \langle \ln Z \rangle_J \tag{3.5}$$

$$= - \lim_{N\to\infty} TN^{-1} \int_{-\infty}^{+\infty} \prod_{i<j} \ln Z(\{J_{ij}\}) P(J_{ij}) dJ_{ij}, \tag{3.6}$$

where $\langle \ldots \rangle_J$ indicates an average over the bond distribution (3.2). So, the trace over the random degrees of freedom requires the averaging of ln Z. In the original static SK solution [Sherrington & Kirkpatrick 1975] this was achieved by the use of replicas. In this scheme one first notes that

$$\langle \ln Z \rangle_J = \lim_{n\to 0} n^{-1} (\langle Z^n \rangle_J - 1) \tag{3.7}$$

and then evaluates the average over Z^n by writing for integral n

$$Z^n = \prod_{\alpha=1}^{n} Z^{\alpha} \tag{3.8}$$

where Z^{α} ($\alpha = 1,2,\ldots,n$) are n identical, non-interacting replicas of the same real system with the same interactions $\{J_{ij}\}$. Thus

$$F = - \lim_{N\to\infty} \lim_{n\to 0} T(Nn)^{-1} \int_{-\infty}^{+\infty} \prod_{i<j} \left(\prod_{\alpha=1}^{n} Z(\{J_{ij}\})^{\alpha} - 1 \right) P(J_{ij}) dJ_{ij}. \tag{3.9}$$

In order to evaluate (3.9) one needs to interchange the order of limits and, in fact, below T_c the symmetry among the replicas is broken [Parisi 1979, 1980 a,b,c]. In this approach the statistical

mechanics order parameter, q, is defined by

$$q = N^{-1} \sum_{i=1}^{N} \langle\langle S_i \rangle_T^2 \rangle_J \ , \tag{3.10}$$

where $\langle \ldots \rangle_T$ denotes a thermal average. Now

$$\begin{aligned} q &= N^{-1} \sum_{i=1}^{N} \langle\langle S_i \rangle_T^2 \rangle_J \\ &= N^{-1} \sum_{i=1}^{N} \langle (\sum_{\{S_i^{\alpha_0}=\pm 1\}} S_i^{\alpha_0} e^{-\beta H^{\alpha_0}}/Z)(\sum_{\{S_i^{\beta_0}=\pm 1\}} S_i^{\beta_0} e^{-\beta H^{\beta_0}}/Z) \rangle_J \ . \end{aligned} \tag{3.11}$$

In (3.11) α_0 and β_0 are any distinct pair of replicas and H^α denotes the Hamiltonian in a given replica, that is

$$H^\alpha = - \sum_{i<j} J_{ij} S_i^\alpha S_j^\alpha - \sum_{i=1}^{N} h_i S_i^\alpha \ . \tag{3.12}$$

As the random interactions appear both in the numerator and the denominator in (3.11), we multiply the right-hand side by z^{n-2}/z^{n-2} and let n tend to zero. Thus,

$$q = \lim_{n\to 0} N^{-1} \sum_{i=1}^{N} \langle \prod_{\alpha=1}^{n} \sum_{\{S_i^\alpha = \pm 1\}} S_i^{\alpha_0} S_i^{\beta_0} e^{-\beta \sum_{\alpha=1}^{n} H^\alpha} / Z^n \rangle_J \tag{3.13}$$

$$= N^{-1} \sum_{i=1}^{N} \langle S_i^{\alpha_0} S_i^{\beta_0} \rangle \ , \quad \langle \ldots \rangle \equiv \text{'average in replica space'}$$

$$= q^{\alpha_0 \beta_0} \quad (\alpha_0 \neq \beta_0) \ . \tag{3.14}$$

Since the effective Hamiltonian, H^{eff}, defined by

$$H^{\text{eff}} = \sum_{\alpha=1}^{n} H^\alpha , \tag{3.15}$$

is replica symmetric, de Dominicis and Young (1983a) have argued that in the replica symmetry broken situation one should average over all distinct replicas. This means that

$$q = \lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} q^{\alpha\beta} \tag{3.16}$$

$$= \int_0^1 q(x)\, dx \tag{3.17}$$

on making Parisi's ansatz for $q^{\alpha\beta}$ in replica space. In fact, Parisi's theory [which is discussed in Chapter I] predicts that

$$T\,\chi\,(T) = 1 - \int_0^1 q(x)\, dx \tag{3.18}$$

where $\chi(T)$ is the uniform susceptibility. Since the Fluctuation-Dissipation Theorem (FDT) implies that

$$T\,\chi\,(T) = 1 - q, \tag{3.19}$$

we see from (3.17) that there is no contradiction with Parisi's theory if the latter is correctly interpreted. Young et al. (1984) have shown that the FDT holds only if one performs an average over samples, and not for each sample separately [see Chapter I for further details]. As in the present work we shall always perform such an average over samples, one requires the FDT to hold.

Since the use of replicas cannot be justified a priori, an alternative dynamical approach was proposed by de Dominicis (1978). In this scheme one utilises the functional-integral formalism of Martin et al. (1973). Starting from an arbitrary spin configuration

at an initial time, t_0, one formally integrates the equation of motion to derive an interaction-dependent path integral, $\tilde{Z}$. As de Dominicis (1978) observed, since $\tilde{Z}$ is normalised to unity it can be averaged directly over the random degrees of freedom, leaving a bond-averaged generating function from which dynamic correlation functions can be evaluated. Consequently, there is no need to introduce replicas.

The time-dependent correlation function, C(t), is defined by

$$C(t_1 - t_2) = N^{-1} \sum_{i=1}^{N} \langle\langle S_i(t_1) S_i(t_2) \rangle_T \rangle_J \qquad (3.20a)$$

where $S_i(t_1)$ is the i-th spin at time t_1 and the linear-response function, G(t), is given by

$$G(t_1 - t_2) = N^{-1} \sum_{i=1}^{N} \frac{\partial \langle\langle S_i(t_1) \rangle_T \rangle_J}{\partial(\beta h_i(t_2))}, \quad t_1 > t_2. \qquad (3.20b)$$

The Fourier transforms are given by

$$C(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} C(t)\, dt; \quad C(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega t} C(\omega)\, d\omega \qquad (3.20c)$$

$$G(\omega) = \int_{0}^{\infty} e^{i\omega t} G(t)\, dt; \quad G(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega t} G(\omega)\, d\omega \qquad (3.20d)$$

The Edwards-Anderson (1975) order parameter, q_{EA}, is given by the time-persistent part of C(t), that is

$$q_{EA} = \lim_{t\to\infty} \lim_{N\to\infty} C(t) \,. \qquad (3.21)$$

The dynamics of spin-glass was first investigated by Sompolinsky (1981) whose solution is characterized by a spectrum of monotonically

decreasing timescales, τ_x ($0 \leqslant x \leqslant 1$), all of which diverge in the thermodynamic limit. Sompolinsky's theory predicts that

$$q_{EA} = q(1) \tag{3.22}$$

since $x = 1$ corresponds to the shortest timescale, whereas statistical mechanics averages, which include interference between different phases, are evaluated on timescales longer than the longest relaxation time. Thus, according to Sompolinsky,

$$q = q(0). \tag{3.23}$$

We see from (3.18), (3.19) and (3.23) that Sompolinsky's results violate the FDT. In the subsequent sections of this chapter an alternative - which does NOT violate the FDT in the sense discussed above and in Chapter I - to Sompolinsky's theory is proposed.

We shall assume throughout that the thermodynamic limit ($N \to \infty$) is taken before any other. Although we shall introduce dynamics into the SK spin-glass, we want to extract information concerning the statics of the system.

2. Langevin dynamics

As all spin operators, S_i, commute with the Hamiltonian, (3.1), and consequently are constant in time, the Ising system defined by (3.1) contains no intrinsic dynamics. Hence, one needs to introduce external perturbations in order to investigate the time evolution of the system in question. It was Glauber (1963) who first suggested that one could mimic the non-magnetic degrees of freedom

(for example, lattice vibrations) of a physical system by regarding each spin of the idealised system as being in contact with a local heat bath, the latter inducing the spin to "flip" spontaneously. In Glauber Dynamics the heat bath is implicit in the stochastic nature of the model.

Rather than work with (3.1), we employ a 'soft-spin' version of the SK model [Wilson & Fisher 1972]. In this case one allows the spins to assume continuous values ($-\infty < \sigma_i < +\infty$) and the Hamiltonian is given by

$$H = - \sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_{i=1}^{N} h_i\sigma_i + T \sum_{i=1}^{N} (\frac{r}{2}\sigma_i^2 + \frac{u}{4}\sigma_i^4) \qquad (3.24)$$

with $r < 0$ and $u > 0$. Thus, the partition function, (3.4), now becomes

$$Z(\{J_{ij}\}) = \int_{-\infty}^{+\infty} \prod_i e^{\beta(\sum_{i<j} J_{ij}\sigma_i\sigma_j + \sum_{i=1}^{N} h_i\sigma_i)} W(\sigma_i)d\sigma_i \qquad (3.25)$$

where the weighting factor, $W(\sigma_i)$, is given by

$$W(\sigma_i) = \prod_i e^{-(\frac{r}{2}\sigma_i^2 + \frac{u}{4}\sigma_i^4)}. \qquad (3.26)$$

One retrieves the Ising ($\sigma_i = \pm 1$) system at the end of the calculation by

i) setting $r = -u$, and (3.27a)

ii) then letting $u \to \infty$. (3.27b)

Under (3.27a) and (3.27b) it is easy to show that

$$W(\sigma_i) = \prod_i \delta(\sigma_i^2 - 1), \qquad (3.28)$$

the desired result.

The dynamics of (3.24) is assumed to be governed by a Langevin equation:

$$\Gamma^{-1} \frac{\partial \sigma_i}{\partial t} = \frac{-\delta(\beta H)}{\delta \sigma_i} + \xi_i(t), \tag{3.29}$$

where Γ is a kinetic coefficient which sets the microscopic timescale (time is measured in units of Γ^{-1}) and $\xi_i(t)$ is a Gaussian random noise satisfying

$$\langle \xi_i(t) \rangle = 0 \tag{3.30a}$$

and

$$\langle \xi_i(t_1)\xi_j(t_2) \rangle = 2\Gamma^{-1}\delta_{ij}\delta(t_1 - t_2). \tag{3.30b}$$

Equations (3.24), (3.29), (3.30a) and (3.30b) describe a purely relaxational time-dependent Ginzburg-Landau model of the SK spin-glass [Ma 1976].

(3.29) is a phenomenological equation, obtained from analogy with the Brownian motion of a simple harmonic oscillator [Wang and Uhlenbeck 1945]. The effect of the thermal reservoir has been approximated by a frictional force and a fluctuating force. $-\delta(\beta H)/\delta\sigma_i$ simulates a 'damping term' normally met in mechanics, whereas the random noise, $\xi_i(t)$, replaces the non-magnetic degrees of freedom.

As we want to generate equilibrium correlation functions in the thermodynamic limit for $t \to \infty$, it is crucial to know how $P(\{\sigma_i\},t)$, the probability density function of finding the system in state $\{\sigma_i\}$ at time t, evolves with time. Now, if we start the system off at some initial time, t_0, the probability density at some later time, t_1, is given by

$$P(\{\sigma_i\},t_1) = \int_{-\infty}^{+\infty} P((\{\sigma_i\},t_1)|(\{\sigma_i\},t_0))P(\{\sigma_i\},t_0)d(\{\sigma_i\},t_0) \tag{3.31}$$

and, of course, we require the normalization condition

$$\int_{-\infty}^{+\infty} P(\{\sigma_i\},t_1)d(\{\sigma_i\},t_1) = 1. \tag{3.32}$$

The conditional probability density mentioned in (3.31) is defined below by (3.43). It can be shown [Graham 1973] that P satisfies a Fokker-Planck equation:

$$\frac{\partial P}{\partial t} + \sum_{i=1}^{N} \frac{\partial J_i}{\partial \sigma_i} = 0 \tag{3.33}$$

where the probability current, J_i, is given by

$$J_i = -\frac{\partial(\beta H)}{\partial \sigma_i} P - \frac{\partial P}{\partial \sigma_i} . \tag{3.34}$$

Clearly, (3.33) is just the analogue of the familiar continuity equation. Now, for an equilibrium probability density one requires that

$$\frac{\partial P}{\partial t} = 0. \tag{3.35}$$

Hence, from (3.33) one has that

$$\sum_{i=1}^{N} \partial J_i/\partial \sigma_i = 0. \tag{3.36}$$

This is trivially satisfied if

$$P \propto e^{-\beta H}. \tag{3.37}$$

Consequently the dynamics will generate an equilibrium probability distribution for $t \to \infty$ [Ma 1976]. As we shall see in the following sub-section, for spin-glasses one needs to take great care with (3.31).

3. Functional integral formalism

As the random noise is assumed to have a Gaussian distribution, (3.30a) and (3.30b), its path probability density, $\omega\{\xi_i\}$, is given by

$$\omega(\{\xi_i\} : t_0 \leqslant t \leqslant t_f) = M^{-1} \exp[-\frac{\Gamma}{4} \sum_{i=1}^{N} \int_{t_0}^{t_f} \xi_i^2(t)\, dt] \qquad (3.38)$$

where t_0 is some initial time and t_f is a later time, and

$$M = \int D[\xi_i] \exp[-\frac{\Gamma}{4} \sum_{i=1}^{N} \int_{t_0}^{t_f} \xi_i^2(t)\, dt] \qquad (3.39)$$

$$(\int D[\xi_i] \equiv \int_{-\infty}^{+\infty} \prod_{i,t} d\xi_i(t))$$

is a normalization constant. The path probability density is actually defined by discretizing $[t_0, t_f]$; further technical details can be found in Appendix I.

Rather than solving the Langevin equation, (3.29), for σ_i in terms of ξ_i and then averaging over the latter with weight (3.38), we evaluate a path probability density, $W\{\sigma_i\}$, for σ_i [Martin et al. 1973; Janssen 1976; Bausch et al. 1976; de Dominicis and Peliti 1978; de Dominicis 1978]. Since

$$\omega(\{\xi_i\} : t_0 \leqslant t \leqslant t_f) D[\xi_i] = W(\{\sigma_i\} : t_0 \leqslant t \leqslant t_f) D[\sigma_i] \qquad (3.40)$$

$$(D[\xi_i] \equiv \prod_{i,t} d\xi_i(t))$$

we have from (3.29) and (3.38) that

$$W(\{\sigma_i\} : t_0 \leqslant t \leqslant t_f) = M^{-1} \exp[-\frac{\Gamma}{4} \sum_{i=1}^{N} \int_{t_0}^{t_f} (\Gamma^{-1} \frac{\partial \sigma_i}{\partial t} + \frac{\delta(\beta H)}{\delta \sigma_i})^2 dt] . J[\sigma_i]$$

(3.41)

where $J[\sigma_i]$ is the functional Jacobian arising from the above transformation. In Appendix I it is shown that

$$J[\sigma_i] = \exp[\frac{\Gamma}{2} \sum_{i=1}^{N} \int_{t_0}^{t_f} \frac{\delta^2(\beta H)}{\delta \sigma_i^2} \, dt]. \tag{3.42}$$

The conditional probability density, (3.31), discussed in Section A.2 is defined by

$$P((\{\sigma_i\},t_1)|(\{\sigma_i\},t_0)) \equiv \int_{(\{\sigma_i\},t_0)}^{(\{\sigma_i\},t_1)} W(\{\sigma_i\} : t_0 \leqslant t \leqslant t_1) \, D[\sigma_i];$$

(3.43)

here one integrates over all paths between the boundaries.

The exponent appearing in (3.41) can be linearized via a Gaussian transformation* [Martin et al. 1973; Janssen 1976; Bausch et al. 1976]:

$$W(\{\sigma_i\} : t_0 \leqslant t \leqslant t_f) = (2\pi)^{-N/2} |\det A|^{1/2} \int \exp L\{\sigma_i, i\hat{\sigma}_i\} \, D[i\hat{\sigma}_i]$$

(3.44b)

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* Wilson and Kogut (1974), Eqn. (3.5):

$$e^{\frac{1}{2} \sum_{i,j}^{N} \beta_i \Delta_{ij} \beta_j} = (2\pi)^{-N/2} |\det A|^{\frac{1}{2}} \int_{-\infty}^{+\infty} d\alpha_1 \ldots d\alpha_n \, e^{\{-\frac{1}{2} \sum_{i,j}^{N} \alpha_i A_{ij} \alpha_j \pm \sum_{i=1}^{N} \beta_i \alpha_i\}}$$

with $\sum_{K=1}^{N} \Delta_{iK} A_{Kj} = \delta_{ij}$ (3.44a)

where

$$L\{\sigma_i, i\hat{\sigma}_i\} = \sum_{i=1}^{N} \int_{t_0}^{t_f} [i\hat{\sigma}_i(t)\{\Gamma^{-1} i\hat{\sigma}_i(t) - (\Gamma^{-1} \frac{\partial \sigma_i}{\partial t} + \frac{\delta(\beta H)}{\delta \sigma_i})\} + V\{\sigma_i\}]dt, \tag{3.45}$$

$$A_{ij} = -2\Gamma^{-1} \delta_{ij} \qquad (1 \leqslant i,j \leqslant N) \tag{3.46}$$

$$\text{and} \quad V\{\sigma_i\} = \frac{\Gamma}{2} \frac{\delta^2(\beta H)}{\delta \sigma_i^2} \tag{3.47}$$

is the term arising from the functional Jacobian (3.42).

The physical significance of the auxiliary field, $i\hat{\sigma}_i(t)$, is discussed below.

One now defines a generating functional, $\tilde{Z}$, by [de Dominicis 1976; Janssen 1976]

$$\tilde{Z}\{J_{ij}, \ell_i, \hat{\ell}_i\} = (2\pi)^{-N/2} |\det A|^{1/2} \int \exp\{L\{\sigma_i, i\hat{\sigma}_i\} + \sum_{i=1}^{N} \int_{t_0}^{t_f} (\ell_i(t)\sigma_i(t) + \hat{\ell}_i(t) i\hat{\sigma}_i(t))dt\} D[\sigma_i] D[i\hat{\sigma}_i], \tag{3.48}$$

from which one can obtain the cumulants:

$$\langle \langle i\hat{\sigma}_{i_1}(t_1) \ldots \sigma_{i_m}(t_m) \rangle_C \rangle_J = \left\langle \frac{\delta^m \ln \tilde{Z}}{\delta \hat{\ell}_{i_1}(t_1) \ldots \delta \hat{\ell}_{i_m}(t_m)} \right\rangle_J \Bigg|_{\hat{\ell}_{i_1} = \ldots = \ell_{i_m} = 0} \tag{3.49}$$

where $\langle \ldots \rangle_C$ denotes a cumulant average [see Chapter II for a discussion on cumulants]. We see from (3.39), (3.41), (3.44b) and (3.48) that

$$\tilde{Z}\{J_{ij}, \ell_i = \hat{\ell}_i = 0\} = 1. \tag{3.50}$$

This led de Dominicis (1978) to argue that one could perform the quenched average appearing in (3.49) directly on $\tilde{Z}$. Indeed, Sompolinsky and Zippelius (1981, 1982) have performed just such a calculation for the SK spin-glass.

As was explained in Chapters I and II, there is considerable numerical [YK 1982; Mackenzie 1982; Mackenzie & Young 1982, 1983] and analytic [Sompolinsky 1981; Hertz 1983] evidence to suggest that the SK spin-glass is non-ergodic below T_c [Young 1981; Toulouse 1982]. Thus, if the system starts in an arbitrary state at time t_i, earlier than t_0, it will stay trapped in that phase, unable to sample any other. Consequently, the system will not be in equilibrium at t_0 and a Boltzmann distribution has to be imposed at this initial time. So for the SK spin-glass one needs to perform explicitly the integral appearing in (3.31).

Hence, rather than the generating functional, one sees from (3.31),(3.43), (3.44) and (3.48) that one should consider

$$Z\{J_{ij},\ell_i,\hat{\ell}_i\} = \int \tilde{Z}\{J_{ij},\ell_i,\hat{\ell}_i\}\, e^{-\beta H[\sigma_i(t_0)]}\, D[\sigma_i(t_0)]. \qquad (3.51)$$

As the generating functional is normalized to unity, (3.50), $Z\{J_{ij},\ell_i = \hat{\ell}_i = 0\}$ is just the partition function. Cumulants, (3.49), are now given by differentiating ln Z with respect to external sources:

$$\langle\langle i\hat{\sigma}_{i_1}(t_1)\ldots\sigma_{i_m}(t_m)\rangle_C\rangle_J = \left\langle \frac{\delta^m \ln Z}{\delta\hat{\ell}_{i_1}(t_1)\ldots\delta\hat{\ell}_{i_m}(t_m)} \right\rangle_J \Bigg|_{\hat{\ell}_{i_1}=\ldots=\ell_{i_m}=0} \qquad (3.52)$$

Unfortunately, because Z is not normalized to unity, the bond average has to be performed on ln Z and one is once again forced to introduce

replicas. We see from (3.7) and (3.52) that the quantity of interest is now $\langle Z^n \rangle_J$, where n, the number of replicas, is eventually taken to be zero and Z is given by (3.51).

We are interested in the correlation function:

$$C^{\alpha\beta}(t - t') = N^{-1} \sum_{i=1}^{N} \langle \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \rangle_L \tag{3.53}$$

where $\langle \ldots \rangle_L$ denotes an average with respect to a Lagrangian symmetric in replica space (see next section), and α,β refer to replicas. Since from (3.24), (3.45) and (3.48) $\hat{\ell}_i$ mimics the role of an applied magnetic field, $i\hat{\sigma}_i(t)$ acts as a response field $\partial/\partial(\hat{\ell}_i(t))$. Consequently, the linear-response function is given by (once again introducing replica indices)

$$G^{\alpha\beta}(t - t') = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial \langle \sigma_i^{\alpha}(t) \rangle_L}{\partial(\hat{\ell}_i^{\beta}(t'))} \tag{3.54a}$$

$$= N^{-1} \sum_{i=1}^{N} \langle i\hat{\sigma}_i^{\beta}(t')\sigma_i^{\alpha}(t) \rangle_L \qquad t > t' \tag{3.54b}$$

(Note: where β appears as a multiplicative factor it stands for $1/T$). One now identifies

$$C(t - t') = \lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{N} C^{\alpha\alpha}(t - t') \tag{3.55a}$$

and

$$G(t - t') = \lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{N} G^{\alpha\alpha}(t - t'). \tag{3.55b}$$

Order parameters, $q^{\alpha\beta}$, are defined in replica space by

$$q^{\alpha\beta} = \lim_{\substack{N\to\infty \\ n\to 0 \\ t\to\infty}} C^{\alpha\beta}(t), \tag{3.56a}$$

that is,

$$C^{\alpha\beta}(t) = \tilde{C}^{\alpha\beta}(t) + q^{\alpha\beta} \tag{3.56b}$$

where

$$\lim_{t\to\infty} \tilde{C}^{\alpha\beta}(t) = 0. \tag{3.56c}$$

In Appendix II it is shown that the FDT in the present context is given by

$$\tilde{C}(\omega) = \frac{2}{\omega} \operatorname{Im} G(\omega) \tag{3.57}$$

where the Fourier transforms are given by (3.20c,d) and the (Ising) static limit of (3.57) is (3.19).

The rest of this chapter is concerned with the consequences of the above approach.

The contents of this chapter have also appeared in Houghton, Jain and Young (1983a,b).

Section B: Evaluation of an Effective Lagrangian

As mentioned in the previous section, we are interested in $\langle Z^n \rangle_J$. Now, by definition

$$\langle Z^n \rangle_J = \int_{-\infty}^{+\infty} \prod_{i<j} P(J_{ij}) Z^n\{J_{ij}, \ell_i, \hat{\ell}_i\} \, dJ_{ij} \tag{3.58a}$$

$$= \int_{-\infty}^{+\infty} \prod_{i<j} \prod_{\alpha=1}^{n} P(J_{ij})\ Z^{\alpha}\{J_{ij}, \ell_i, \hat{\ell}_i\}\ dJ_{ij} \tag{3.58b}$$

$$= (2\pi)^{-nN/2}\ |\det A|^{n/2} \int_{-\infty}^{+\infty} \prod_{i<j} P(J_{ij}) \exp\left\{ \sum_{\alpha=1}^{n} \left(L\{\sigma_i^{\alpha}, i\hat{\sigma}_i^{\alpha}\} \right.\right.$$

$$\left.\left. + \sum_{i=1}^{N} \int_{t_0}^{t_f} (\ell_i^{\alpha}(t)\sigma_i^{\alpha}(t) + \hat{\ell}_i^{\alpha}(t) i\hat{\sigma}_i^{\alpha}(t))dt - \beta H^{\alpha}[\sigma_i(t_0)] \right) \right\}$$

$$. dJ_{ij} D[\sigma_i^{\alpha}] D[i\hat{\sigma}_i^{\alpha}] D[\sigma_i^{\alpha}(t_0)], \tag{3.59}$$

where we have made use of (3.8), (3.24), (3.48) and (3.51); from (3.24) and (3.45)

$$L\{\sigma_i^{\alpha}, i\hat{\sigma}_i^{\alpha}\} = \sum_{i=1}^{N} \int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) \left\{ \Gamma^{-1} i\hat{\sigma}_i^{\alpha}(t) - \left(\Gamma^{-1} \frac{\partial \sigma_i^{\alpha}}{\partial t} + \frac{\delta(\beta H^{\alpha})}{\delta \sigma_i^{\alpha}} \right) \right\} dt$$

$$+ V\{\sigma_i^{\alpha}(t)\}$$

$$= \sum_{i=1}^{N} \int_{t_0}^{t_f} \left[i\hat{\sigma}_i^{\alpha}(t) \left\{ -\Gamma^{-1} \frac{\partial \sigma_i^{\alpha}}{\partial t} - r\sigma_i^{\alpha}(t) - u(\sigma_i^{\alpha}(t))^3 \right.\right.$$

$$\left.\left. + \beta h_i(t) + \Gamma^{-1} i\hat{\sigma}_i^{\alpha}(t) \right\} + V\{\sigma_i^{\alpha}(t)\} \right] dt$$

$$+ \beta \sum_{i=1}^{N} \int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) \times \frac{\delta(\sum_{k<j} J_{kj} \sigma_k^{\alpha}(t)\sigma_j^{\alpha}(t))}{\delta \sigma_i^{\alpha}(t)} dt \tag{3.60}$$

and

$$-\beta H^{\alpha}[\sigma_i(t_0)] = \beta \sum_{i<j} J_{ij} \sigma_i^{\alpha}(t_0)\sigma_j^{\alpha}(t_0) + \beta \sum_{i=1}^{N} h_i \sigma_i^{\alpha}(t_0)$$

$$- \sum_{i=1}^{N} \left\{ \frac{r}{2} (\sigma_i^{\alpha}(t_0))^2 + \frac{u}{4} (\sigma_i^{\alpha}(t_0))^4 \right\}. \tag{3.61}$$

Since from (3.24) and (3.47) we have that

$$V\{\sigma_i^\alpha(t)\} = \frac{\Gamma}{2}\,(r + 3u(\sigma_i^\alpha(t))^2), \tag{3.62}$$

we see from (3.59) and (3.61) that the 'Lagrangian' contains a purely local part, $L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$, given by

$$\begin{aligned} L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\} = \sum_{\alpha,i}\Bigg[\int_{t_0}^{t_f}\Bigg\{ & i\hat{\sigma}_i^\alpha(t)\{-\Gamma^{-1}\frac{\partial\sigma_i^\alpha}{\partial t} - r\sigma_i^\alpha(t) - u(\sigma_i^\alpha(t))^3 \\ & + \beta h_i(t) + \Gamma^{-1} i\hat{\sigma}_i^\alpha(t)\} + V\{\sigma_i^\alpha(t)\} \\ & + (\ell_i^\alpha(t)\sigma_i^\alpha(t) + \hat{\ell}_i^\alpha(t) i\hat{\sigma}_i^\alpha(t))\Bigg\}\,dt \\ & - \left\{\frac{r}{2}\,(\sigma_i^\alpha(t_0))^2 + \frac{u}{4}\,(\sigma_i^\alpha(t_0))^4 - \beta h_i \sigma_i^\alpha(t_0)\right\}\Bigg] \end{aligned} \tag{3.63}$$

and an interaction-dependent part, $R\{J_{ij}, \sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$, given by

$$\begin{aligned} R\{J_{ij}, \sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\} = \beta\sum_\alpha \Bigg(& \sum_{i=1}^{N}\int_{t_0}^{t_f} i\hat{\sigma}_i^\alpha(t) \times \frac{\delta\left(\sum_{k<j} J_{kj}\sigma_k^\alpha(t)\sigma_j^\alpha(t)\right)}{\delta\sigma_i^\alpha(t)}\,dt \\ & + \beta\sum_{i<j} J_{ij}\sigma_i^\alpha(t_0)\sigma_j^\alpha(t_0)\Bigg) \end{aligned} \tag{3.64}$$

$$\begin{aligned} = \sum_{i<j} J_{ij}\Bigg\{\beta\sum_\alpha\Bigg[\int_{t_0}^{t_f} & \{i\hat{\sigma}_i^\alpha(t)\sigma_j^\alpha(t) + i\hat{\sigma}_j^\alpha(t)\sigma_i^\alpha(t)\}\,dt \\ & + \sigma_i^\alpha(t_0)\sigma_j^\alpha(t_0)\Bigg]\Bigg\}\,. \end{aligned} \tag{3.65}$$

The interaction-dependent part of (3.59) has to be integrated over the random degrees of freedom. Hence we evaluate

$$e^{\bar{R}} = \int_{-\infty}^{+\infty} \prod_{i<j} P(J_{ij}) \exp R\{J_{ij},\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}, \tag{3.66}$$

where $P(J_{ij})$ is given by (3.2) and $R\{J_{ij},\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$ is given by (3.65). (3.66) is evaluated by 'completing the square':

$$e^{\bar{R}} = \int_{-\infty}^{+\infty} \prod_{i<j} \left(\frac{N}{2\pi J^2}\right)^{1/2} \exp\left\{ \frac{-NJ_{ij}^2}{2J^2} + \left(\beta \sum_\alpha \left[\int_{t_0}^{t_f} \{i\hat{\sigma}_i^\alpha(t)\sigma_j^\alpha(t) + i\hat{\sigma}_j^\alpha(t)\sigma_i^\alpha(t)\}dt \right.\right.\right.$$

$$\left.\left.\left. + \sigma_i^\alpha(t_0)\sigma_j^\alpha(t_0)\right]\right) J_{ij}\right\} dJ_{ij} \tag{3.67}$$

$$= \prod_{i<j} \exp \frac{J^2\beta^2}{2N} \left\{ \sum_\alpha \left[\int_{t_0}^{t_f} \{i\hat{\sigma}_i^\alpha(t)\sigma_j^\alpha(t) + i\hat{\sigma}_j^\alpha(t)\sigma_i^\alpha(t)\}dt + \sigma_i^\alpha(t_0)\sigma_j^\alpha(t_0)\right]\right\}^2$$

(3.68)

(Note that we have used (3.44a) in deriving (3.68)). Since

$$\sum_{i<j}\left\{ \sum_\alpha \left[\int_{t_0}^{t_f} \{i\hat{\sigma}_i^\alpha(t)\sigma_j^\alpha(t) + i\hat{\sigma}_j^\alpha(t)\sigma_i^\alpha(t)\}dt + \sigma_i^\alpha(t_0)\sigma_j^\alpha(t_0) \right]\right\}^2$$

$$= 2\sum_{i<j} \sum_{\alpha,\beta} \left[\int_{t_0}^{t_f}\int_{t_0}^{t_f} \left\{i\hat{\sigma}_i^\alpha(t)i\hat{\sigma}_i^\beta(t')\sigma_j^\alpha(t)\sigma_j^\beta(t') + i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t')\sigma_j^\alpha(t)i\hat{\sigma}_j^\beta(t')\right\}dtdt'\right.$$

$$\left. + 2\int_{t_0}^{t_f} i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t_0)\sigma_j^\alpha(t)\sigma_j^\beta(t_0)dt + \frac{1}{2}\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\sigma_j^\alpha(t_0)\sigma_j^\beta(t_0)\right], \tag{3.69}$$

we get from (3.59), (3.63), (3.68) and (3.69) that

$$\langle Z^n \rangle_J = (2\pi)^{-nN/2} \left|\det A\right|^{n/2} \int \exp\Big\{ L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$$

$$+ \frac{\beta^2 J^2}{N} \sum_{\substack{i<j \\ \alpha,\beta}} \Big[\int_{t_0}^{t_f}\int_{t_0}^{t_f} \Big(i\hat{\sigma}_i^\alpha(t) i\hat{\sigma}_i^\beta(t') \sigma_j^\alpha(t)\sigma_j^\beta(t')$$

$$+ i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t')\sigma_j^\alpha(t) i\hat{\sigma}_j^\beta(t') \Big) dt dt'$$

$$+ 2\int_{t_0}^{t_f} i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t_0)\sigma_j^\alpha(t)\sigma_j^\beta(t_0)dt + \frac{1}{2}\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\sigma_j^\alpha(t_0)\sigma_j^\beta(t_0) \Big] \Big\}$$

$$\cdot D[\sigma_i^\alpha] D[i\hat{\sigma}_i^\alpha] D[\sigma_i^\alpha(t_0)], \qquad (3.70)$$

where $L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$, the purely local part, is given by (3.63). Thus, by integrating out the exchange interactions we have introduced four-spin couplings which are non-local in time and between different replicas. Following Sompolinsky and Zippelius (1981,1982), we decouple these four-spin interactions by using (3.44a). We first re-write (3.44a) in a more convenient form:

$$\exp\Big\{ \frac{1}{2} \sum_{a,b=1}^{M} X_a \Delta_{ab} X_b \Big\} = (2\pi)^{-M/2} \left|\det \Delta\right|^{-1/2} \int_{-\infty}^{+\infty} \prod_{a=1}^{M} dY_a \exp\Big\{ -\frac{1}{2} \sum_{a,b=1}^{M} Y_a \Delta_{ab}^{-1} Y_b$$

$$+ \sum_{a=1}^{M} X_a Y_a \Big\} . \qquad (3.71)$$

The first of the four quartic interactions appearing in (3.70) is

$$\exp\Big\{ \frac{\beta^2 J^2}{N} \sum_{\substack{i<j \\ \alpha,\beta}} \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^\alpha(t) i\hat{\sigma}_i^\beta(t')\sigma_j^\alpha(t)\sigma_j^\beta(t')\, dt\, dt' \Big\}$$

$$= \prod_{\alpha,\beta} \exp\Big\{ \frac{\beta^2 J^2}{2N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} \Big[\sum_{i\neq j} i\hat{\sigma}_i^\alpha(t) i\hat{\sigma}_i^\beta(t')\sigma_j^\alpha(t)\sigma_j^\beta(t') \Big] dt\, dt' \Big\} \qquad (3.72)$$

$$= \prod_{\alpha,\beta} \exp\left\{\frac{\beta^2 J^2}{8N} \int_{t_0}^{t_f}\int_{t_0}^{t_f}\left\{ \left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') + \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t')\right)^2 \right.\right.$$

$$\left. - \left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') - \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t')\right)^2 \right\} dt\, dt'$$

$$\left. - \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t')\, dt\, dt' \right\} . \quad (3.73)$$

Writing

$$X^{\alpha\beta} = \sum_{i=1}^{N} \iint \left\{ i\sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') + \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \right\} dt\, dt' \quad (3.74a)$$

and

$$\Delta \equiv \frac{\beta^2 J^2}{4N} \frac{\partial}{\partial t} \frac{\partial}{\partial t'} , \quad (3.74b)$$

the first term of (3.73) becomes

$$\exp\left\{\frac{\beta^2 J^2}{8N} \iint \left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') + \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t')\right)^2 dt\, dt' \right\}$$

$$\equiv \exp\left\{\frac{1}{2} X^{\alpha\beta} \Delta X^{\alpha\beta}\right\} \qquad \text{(definition)} \quad (3.75)$$

$$= \left(\frac{2N}{\pi\beta^2 J^2}\right)^{1/2} \int_{-\infty}^{+\infty} D[Y^{\alpha\beta}] \exp\left\{ -\frac{1}{2} Y^{\alpha\beta} \Delta^{-1} Y^{\alpha\beta} + X^{\alpha\beta} Y^{\alpha\beta} \right\} \quad (3.76)$$

$$\equiv \left(\frac{2N}{\pi\beta^2 J^2}\right)^{1/2} \int_{-\infty}^{+\infty} D[Y^{\alpha\beta}] \exp\left\{ \frac{-2N}{\beta^2 J^2} \iint \{Y^{\alpha\beta}(t,t')\}^2 dt\, dt' \right.$$

$$\left. + \sum_{i=1}^{N} \iint \left\{ i\sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') + \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \right\} Y^{\alpha\beta}(t,t')\, dt\, dt' \right\} , \quad (3.77)$$

where we have used (3.71) and defined

$$\Delta^{-1} \equiv \frac{4N}{\beta^2 J^2} \left(\frac{\partial}{\partial t'}\right)^{-1} \left(\frac{\partial}{\partial t}\right)^{-1} \quad ; \tag{3.78}$$

defining

$$\tilde{X} = \sum_{i=1}^{N} \iint \left(i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') - \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \right) dt\, dt' \tag{3.79}$$

and

$$\tilde{\Delta} \equiv \frac{-\beta^2 J^2}{4N} \frac{\partial}{\partial t} \frac{\partial}{\partial t'}, \tag{3.80}$$

the second term of (3.73) becomes

$$\exp\left\{\frac{-\beta^2 J^2}{8N} \iint \left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') - \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \right)^2 dt\, dt'\right\}$$

$$= \left(\frac{2N}{\pi\beta^2 J^2}\right)^{1/2} \int_{-\infty}^{+\infty} D[\tilde{Y}^{\alpha\beta}] \exp\left\{ \frac{-2N}{\beta^2 J^2} \iint -\left(\tilde{Y}^{\alpha\beta}(t,t')\right)^2 dt\, dt' \right.$$

$$\left. + \sum_{i=1}^{N} \iint \left(i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') - \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \right) \tilde{Y}^{\alpha\beta}(t,t')\, dt\, dt' \right\}. \tag{3.81}$$

We now combine (3.77) and (3.81) by changing the variables to $Q_1^{\alpha\beta}(t,t')$ and $Q_2^{\alpha\beta}(t,t')$, where

$$Q_1^{\alpha\beta}(t,t') = Y^{\alpha\beta}(t,t') + \tilde{Y}^{\alpha\beta}(t,t') \tag{3.82a}$$

and

$$Q_2^{\alpha\beta}(t,t') = Y^{\alpha\beta}(t,t') - \tilde{Y}^{\alpha\beta}(t,t'). \tag{3.82b}$$

The Jacobian for this transformation is $\frac{1}{2}$.

Using the above transformation, (3.73), (3.77) and (3.81) lead to

$$\exp\left\{ \frac{\beta^2 J^2}{N} \sum_{\substack{i<j \\ \alpha,\beta}} \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \sigma_j^{\alpha}(t) \sigma_j^{\beta}(t')\, dt\, dt' \right\}$$

$$= \frac{N}{\pi\beta^2 J^2} \int \prod_{\alpha,\beta} D[Q_1^{\alpha\beta}] D[Q_2^{\alpha\beta}] \exp\left\{ \frac{-2N}{\beta^2 J^2} \int_{t_0}^{t_f}\int_{t_0}^{t_f} Q_1^{\alpha\beta}(t,t') Q_2^{\alpha\beta}(t,t') dt\, dt' \right.$$

$$+ \sum_{i=1}^{N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} \{ Q_1^{\alpha\beta}(t,t') i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') + Q_2^{\alpha\beta}(t,t') \sigma_i^{\alpha}(t) \sigma_i^{\beta}(t') \}\, dt\, dt'$$

$$\left. - \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \sigma_i^{\alpha}(t) \sigma_i^{\beta}(t')\, dt\, dt' \right\}, \qquad (3.83)$$

thereby decoupling the first four-spin interaction.

The second quartic interaction is decoupled in a similar way by introducing the auxiliary fields $Q_3^{\alpha\beta}(t,t')$ and $Q_4^{\alpha\beta}(t,t')$:

$$\exp\left\{ \frac{\beta^2 J^2}{N} \sum_{\substack{i<j \\ \alpha,\beta}} \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) \sigma_i^{\beta}(t') \sigma_j^{\alpha}(t) i\hat{\sigma}_j^{\beta}(t')\, dt\, dt' \right\} \text{ (second quartic interaction appearing in (3.70))}$$

$$= \prod_{\alpha,\beta} \exp\left\{ \frac{\beta^2 J^2}{8N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} \left\{ \left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t) \sigma_i^{\beta}(t') + \sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \right)^2 \right.\right.$$

$$\left.\left. - \left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t) \sigma_i^{\beta}(t') - \sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \right)^2 \right\} dt\, dt' \right.$$

$$\left. - \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) \sigma_i^{\beta}(t') \sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t')\, dt\, dt' \right\}$$

$$= \frac{N}{\pi\beta^2 J^2} \int \prod_{\alpha,\beta} D[Q_3^{\alpha\beta}] D[Q_4^{\alpha\beta}] \exp\left\{ \frac{-2N}{\beta^2 J^2} \int_{t_0}^{t_f}\int_{t_0}^{t_f} Q_3^{\alpha\beta}(t,t') Q_4^{\alpha\beta}(t,t') dt\, dt' \right.$$

$$+ \sum_{i=1}^{N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} \left\{ Q_3^{\alpha\beta}(t,t') i\hat{\sigma}_i^{\alpha}(t) \sigma_i^{\beta}(t') + Q_4^{\alpha\beta}(t,t') \sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \right\} dt\, dt'$$

$$\left. - \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) \sigma_i^{\beta}(t') \sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t')\, dt\, dt' \right\}. \qquad (3.84)$$

The third quartic interaction appearing in (3.70) is

$$\exp\left\{\frac{2\beta^2J^2}{N}\sum_{\substack{i<j\\ \alpha,\beta}}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\sigma_j^{\alpha}(t)\sigma_j^{\beta}(t_0)\,dt\right\}$$

$$= \prod_{\alpha,\beta}\exp\left\{\frac{\beta^2J^2}{N}\int_{t_0}^{t_f}\sum_{i\neq j} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\sigma_j^{\alpha}(t)\sigma_j^{\beta}(t_0)\,dt\right\} \qquad (3.85)$$

$$= \prod_{\alpha,\beta}\exp\left\{\frac{\beta^2J^2}{4N}\int_{t_0}^{t_f}\left\{\left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)+\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\right)^2\right.\right.$$

$$\left.\left.-\left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)-\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\right)^2\right\}dt\right.$$

$$\left.-\frac{\beta^2J^2}{N}\sum_{i=1}^{N}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\,dt\right\}. \qquad (3.86)$$

This time we write

$$X_{\pm}^{\alpha\beta} = \sum_{i=1}^{N}\int\{i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\pm\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\}\,dt \qquad (3.87a)$$

and

$$\Delta_{\pm} \equiv \pm\frac{\beta^2J^2}{2N}\frac{\partial}{\partial t}\,. \qquad (3.87b)$$

Using (3.87a) and (3.87b), the first two terms of (3.86) become

$$\exp\left\{\frac{\beta^2J^2}{4N}\int\left[\left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)+\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\right)^2-\left(\sum_{i=1}^{N} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)-\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\right)^2\right]dt\right\}$$

$$\equiv \exp\left\{\frac{1}{2}\,X_{\pm}^{\alpha\beta}\,\Delta_{\pm}\,X_{\pm}^{\alpha\beta}\right\} \qquad \text{(definition)} \qquad (3.88)$$

$$= \left(\frac{N}{\pi\beta^2 J^2} \right)^{1/2} \int D[Y_{\pm}^{\alpha\beta}] \exp \left\{ - \frac{1}{2} Y_{\pm}^{\alpha\beta} \Delta_{\pm}^{-1} Y_{\pm}^{\alpha\beta} + X_{\pm}^{\alpha\beta} Y_{\pm}^{\alpha\beta} \right\}$$

$$\equiv \left(\frac{N}{\pi\beta^2 J^2} \right)^{1/2} \int D[Y_{\pm}^{\alpha\beta}] \exp \left\{ \frac{-N}{\beta^2 J^2} \int \pm \{Y_{\pm}^{\alpha\beta}(t,t_0)\}^2 \, dt \right.$$

$$\left. + \sum_{i=1}^{N} \int \{ i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0) \pm \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0) \} Y_{\pm}^{\alpha\beta}(t,t_0) \right\} , \qquad (3.89)$$

since

$$\Delta_{\pm}^{-1} \equiv \pm \frac{2N}{\beta^2 J^2} \left(\frac{\partial}{\partial t} \right)^{-1} . \qquad (3.90)$$

Changing variables to $Q_5^{\alpha\beta}(t,t_0)$ and $Q_6^{\alpha\beta}(t,t_0)$, where

$$Q_5^{\alpha\beta}(t,t_0) = Y_+^{\alpha\beta}(t,t_0) + Y_-^{\alpha\beta}(t,t_0) \qquad (3.91a)$$

and

$$Q_6^{\alpha\beta}(t,t_0) = Y_+^{\alpha\beta}(t,t_0) - Y_-^{\alpha\beta}(t,t_0), \qquad (3.91b)$$

we have from (3.86) and (3.89) that

$$\exp\left\{ \frac{2\beta^2 J^2}{N} \sum_{\substack{i<j \\ \alpha,\beta}} \int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\sigma_j^{\alpha}(t)\sigma_j^{\beta}(t_0)dt \right\}$$

$$= \frac{N}{2\pi\beta^2 J^2} \int \prod_{\alpha,\beta} D[Q_5^{\alpha\beta}] D[Q_6^{\alpha\beta}] \exp\left\{ \frac{-N}{\beta^2 J^2} \int_{t_0}^{t_f} Q_5^{\alpha\beta}(t,t_0) Q_6^{\alpha\beta}(t,t_0) dt \right.$$

$$+ \sum_{i=1}^{N} \int_{t_0}^{t_f} \left\{ Q_5^{\alpha\beta}(t,t_0) i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0) + Q_6^{\alpha\beta}(t,t_0)\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0) \right\} dt$$

$$\left. - \frac{\beta^2 J^2}{N} \sum_{i=1}^{N} \int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0) \, dt \right\} . \qquad (3.92)$$

The final quartic interaction is given by

$$\exp\left\{\frac{\beta^2J^2}{2N}\sum_{\substack{i<j\\ \alpha,\beta}}\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\sigma_j^\alpha(t_0)\sigma_j^\beta(t_0)\right\}$$

$$=\prod_{\alpha,\beta}\exp\left\{\frac{\beta^2J^2}{4N}\sum_{i\neq j}\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\sigma_j^\alpha(t_0)\sigma_j^\beta(t_0)\right\} \tag{3.93}$$

$$=\prod_{\alpha,\beta}\exp\left\{\frac{\beta^2J^2}{4N}\left[\left(\sum_{i=1}^{N}\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\right)^2-\sum_{i=1}^{N}\{\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\}^2\right]\right\}$$

$$=\left(\frac{N}{\pi\beta^2J^2}\right)^{1/2}\int\prod_{\alpha,\beta}D[Q_7^{\alpha\beta}]\exp\left\{\frac{-N}{\beta^2J^2}\{Q_7^{\alpha\beta}(t_0,t_0)\}^2\right.$$

$$\left.+\sum_{i=1}^{N}Q_7^{\alpha\beta}(t_0,t_0)\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)-\frac{\beta^2J^2}{4N}\sum_{i=1}^{N}\{\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\}^2\right\}, \tag{3.94}$$

where we have once again made use of (3.71) and introduced $Q_7^{\alpha\beta}(t_0,t_0)$ as a seventh auxiliary field.

Thus, we can decouple the four-spin interactions by introducing seven auxiliary fields $Q_a^{\alpha\beta}(t,t')$, where a = 1,...,7, and α and β are replica indices. Combining (3.83), (3.84), (3.92) and (3.94) we can rewrite (3.70) as

$$\langle Z^n\rangle_J = C\int\prod_{\alpha,\beta}\prod_{a=1}^{7}D[Q_a^{\alpha\beta}]\exp - f\{Q_a^{\alpha\beta}\}, \tag{3.95a}$$

where

$$f\{Q_a^{\alpha\beta}\}=\frac{2N}{\beta^2J^2}\sum_{\alpha,\beta}\left[\int_{t_0}^{t_f}\int_{t_0}^{t_f}\{Q_1^{\alpha\beta}(t,t')Q_2^{\alpha\beta}(t,t')+Q_3^{\alpha\beta}(t,t')Q_4^{\alpha\beta}(t,t')\}dtdt'\right.$$

$$\left.+\frac{1}{2}\int_{t_0}^{t_f}Q_5^{\alpha\beta}(t,t_0)Q_6^{\alpha\beta}(t,t_0)dt+\frac{1}{2}\{Q_7^{\alpha\beta}(t_0,t_0)\}^2\right]$$

$$-\ln\int\exp L[\sigma_i^\alpha,i\hat{\sigma}_i^\alpha,\sigma_i^\alpha(t_0),Q_a^{\alpha\beta}]D[\sigma_i^\alpha]D[i\hat{\sigma}_i^\alpha]D[\sigma_i^\alpha(t_0)]; \tag{3.95b}$$

the effective Lagrangian is given by

$$L[\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), Q_a^{\alpha\beta}]$$

$$= L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$$

$$+ \sum_{\alpha,\beta} \sum_{i=1}^{N} \Bigg\{ \int_{t_0}^{t_f}\int_{t_0}^{t_f} [Q_1^{\alpha\beta}(t,t')i\hat{\sigma}_i^\alpha(t)i\hat{\sigma}_i^\beta(t') + Q_2^{\alpha\beta}(t,t')\sigma_i^\alpha(t)\sigma_i^\beta(t')$$

$$+ Q_3^{\alpha\beta}(t,t')i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t') + Q_4^{\alpha\beta}(t,t')\sigma_i^\alpha(t)i\hat{\sigma}_i^\beta(t')]dtdt'$$

$$+ \int_{t_0}^{t_f} [Q_5^{\alpha\beta}(t,t_0)i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t_0) + Q_6^{\alpha\beta}(t,t_0)\sigma_i^\alpha(t)\sigma_i^\beta(t_0)]dt$$

$$+ Q_7^{\alpha\beta}(t_0,t_0)\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\Bigg\}$$

$$- \frac{\beta^2 J^2}{N} \sum_{\alpha,\beta} \sum_{i=1}^{N} \Bigg\{ \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^\alpha(t)i\hat{\sigma}_i^\beta(t')\sigma_i^\alpha(t)\sigma_i^\beta(t')\, dtdt'$$

$$+ \int_{t_0}^{t_f} i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t_0)\sigma_i^\alpha(t)\sigma_i^\beta(t_0)dt + 4\{\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0)\}^2\Bigg\}, \qquad (3.96)$$

$$C = \frac{1}{2}\left(\frac{N}{\pi\beta^2 J^2}\right)^{7/2} (\Gamma\pi)^{-nN/2} \qquad (3.97)$$

and the purely local part of the Lagrangian is given by (3.63):

$$L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\} = \sum_{\alpha,i} \Bigg\{ \int_{t_0}^{t_f} \Bigg[i\hat{\sigma}_i^\alpha(t) \left(-\Gamma^{-1} \frac{\partial\sigma_i^\alpha}{\partial t} - r\sigma_i^\alpha(t) - u(\sigma_i^\alpha(t))^3 \right.$$

$$\left. + \beta h_i(t) + \Gamma^{-1} i\hat{\sigma}_i^\alpha(t) \right) + V\{\sigma_i^\alpha(t)\} + \{\ell_i^\alpha(t)\sigma_i^\alpha(t)$$

$$+ \hat{\ell}_i^\alpha(t)i\hat{\sigma}_i^\alpha(t)\}\Bigg]dt - [\tfrac{r}{2}(\sigma_i^\alpha(t_0))^2 + \tfrac{u}{4}(\sigma_i^\alpha(t_0))^4 - \beta h_i\sigma_i^\alpha(t_0)]\Bigg\}. \qquad (3.98)$$

As mentioned earlier in this chapter (Section A.3), it is the thermodynamic limit we take first. In the limit $N \to \infty$ the last term appearing in the effective Lagrangian, viz.

$$\frac{\beta^2 J^2}{N} \sum_{\alpha,\beta} \sum_{i=1}^{N} \Big\{ \int_{t_0}^{t_f}\int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t')\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t')dtdt'$$

$$+ \int_{t_0}^{t_f} i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0)\, dt + 4\{\sigma_i^{\alpha}(t_0)\sigma_i^{\beta}(t_0)\}^2 \Big\}, \qquad (3.99)$$

is of order unity and consequently of no importance; the integrations over the $Q_a^{\alpha\beta}$'s in (3.95a) can be performed by the method of steepest descent (which is exact in the limit $N \to \infty$), the functional integrals being dominated by the set $\{Q_a^{\alpha\beta}\}$ which maximises the integrand, that is minimises $f\{Q_a^{\alpha\beta}\}$. In this method one essentially replaces the $Q_a^{\alpha\beta}(t,t')$'s by their stationary point values.

At the minimum

$$\frac{\partial f\{Q_a^{\alpha\beta}\}}{\partial Q_a^{\alpha\beta}} = 0 \qquad (a = 1,\ldots,7)\,, \qquad (3.100)$$

where $f\{Q_a^{\alpha\beta}\}$ is given by (3.95b). Thus, for $Q_a^{\alpha\beta}(t,t')$ we substitute:

$$\tilde{Q}_1^{\alpha\beta}(t - t') = \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \langle\, \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \,\rangle_L\,, \qquad (3.101a)$$

$$\tilde{Q}_2^{\alpha\beta}(t - t') = \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \langle\, i\hat{\sigma}_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \,\rangle_L\,, \qquad (3.101b)$$

$$\tilde{Q}_3^{\alpha\beta}(t - t') = \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \langle\, \sigma_i^{\alpha}(t) i\hat{\sigma}_i^{\beta}(t') \,\rangle_L\,, \qquad (3.101c)$$

$$\tilde{Q}_4^{\alpha\beta}(t - t') = \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \langle\, i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t') \,\rangle_L\,, \qquad (3.101d)$$

$$\tilde{Q}_5^{\alpha\beta}(t - t_0) = \frac{\beta^2 J^2}{N} \sum_{i=1}^{N} \langle\, \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t_0) \,\rangle_L\,, \qquad (3.101e)$$

$$\tilde{Q}_6^{\alpha\beta}(t - t_0) = \frac{\beta^2 J^2}{N} \sum_{i=1}^{N} \langle\, i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0) \,\rangle_L \qquad (3.101f)$$

and

$$\tilde{Q}_7^{\alpha\beta} = \frac{\beta^2 J^2}{2N} \sum_{i=1}^{N} \langle \sigma_i^{\alpha}(t_0)\sigma_i^{\beta}(t_0) \rangle_L \quad . \tag{3.101g}$$

In equations (3.101) $\langle \ldots \rangle_L$ denotes an average with respect to the effective Lagrangian $L[\sigma_i^{\alpha}, i\hat{\sigma}_i^{\alpha}, \sigma_i^{\alpha}(t_0), \tilde{Q}_a^{\alpha\beta}]$, leading to self-consistent equations for the $\tilde{Q}_a^{\alpha\beta}$'s. Note that because the equilibrium probability distribution, $\exp(-\beta H)$, is stationary the $\tilde{Q}_a^{\alpha\beta}$'s only depend on time differences.

In the next section we present physical arguments which simplify the effective Lagrangian.

Section C: Simplification of the Effective Lagrangian

One sees from the definitions of the correlation function (3.53) and the response function (3.54) that in fact

$$\tilde{Q}_1^{\alpha\beta}(t - t') = \frac{\beta^2 J^2}{2} \; C^{\alpha\beta}(t - t') \; , \tag{3.102a}$$

$$\tilde{Q}_3^{\alpha\beta}(t - t') = \frac{\beta^2 J^2}{2} \; G^{\alpha\beta}(t - t') \; , \tag{3.102b}$$

$$\tilde{Q}_4^{\alpha\beta}(t - t') = \frac{\beta^2 J^2}{2} \; G^{\beta\alpha}(t' - t) \; , \tag{3.102c}$$

$$\tilde{Q}_5^{\alpha\beta}(t - t_0) = \beta^2 J^2 \; C^{\alpha\beta}(t - t_0) \; , \tag{3.102d}$$

$$\tilde{Q}_6^{\alpha\beta}(t - t_0) = \beta^2 J^2 \; G^{\beta\alpha}(t_0 - t) \tag{3.102e}$$

and

$$\tilde{Q}_7^{\alpha\beta} = \frac{\beta^2 J^2}{2} \; C^{\alpha\beta}(t = 0) \; . \tag{3.102f}$$

The term $\tilde{Q}_2^{\alpha\beta}$, which has no simple physical meaning, is shown below not to contribute to the Lagrangian.

Now, as Z is the partition function, differentiating $\langle T \ln Z \rangle_J$ with respect to h_k should give the magnetization, m_k, at site k, that is

$$m_k = \langle\langle \sigma_k \rangle_T \rangle_J = \left\langle \frac{\partial(T \ln Z)}{\partial h_k} \right\rangle_J \tag{3.103}$$

$$= \lim_{n\to 0} \frac{1}{n} \frac{\partial \langle Z^n \rangle_J}{\partial(\beta h_k)} \tag{3.104}$$

where we have made use of (3.7). Using (3.95a), (3.95b), (3.96) and (3.98) one gets that

$$m_k = \lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \left\langle \sigma_k^\alpha (t_0) + \int_{t_0}^{t_f} i\hat{\sigma}_k^\alpha(t)\, dt \right\rangle_L \tag{3.105}$$

$$= \lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \langle \sigma_k^\alpha(t_0) \rangle_L + \lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \left\langle \int_{t_0}^{t_f} i\hat{\sigma}_k^\alpha(t)dt \right\rangle_L . \tag{3.106}$$

Since by definition

$$m_k = \lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \langle \sigma_k^\alpha \rangle_L , \tag{3.107}$$

we have that

$$\lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \left\langle \int_{t_0}^{t_f} i\hat{\sigma}_k^\alpha(t)\, dt \right\rangle_L = 0 \tag{3.108}$$

for all t_f. Consequently

$$\lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \langle i\hat{\sigma}_k^\alpha(t) \rangle_L \equiv \langle\langle i\hat{\sigma}_k \rangle_T \rangle_J$$

$$= \langle i\hat{\sigma}_k \rangle_T$$

$$= 0. \tag{3.109}$$

We first consider the off-diagonal elements of $\tilde{Q}_2^{\alpha\beta}$. Now,

$$\lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} \langle i\hat{\sigma}_k^{\alpha}(t) i\hat{\sigma}_k^{\beta}(t') \rangle_L \equiv \langle \langle i\hat{\sigma}_k(t) \rangle_T \langle i\hat{\sigma}_k(t') \rangle_T \rangle_J \qquad (3.110)$$

$$= 0, \qquad (3.111)$$

where we have used (3.109). It then follows from the definition (3.101b) of $\tilde{Q}_2^{\alpha\beta}$ that

$$\sum_{\alpha\neq\beta} \tilde{Q}_2^{\alpha\beta}(t - t') = 0. \qquad (3.112)$$

One now makes the ansatz that (3.112) holds for each pair ($\alpha \neq \beta$) separately [de Dominicis & Young, 1983a]:

$$\tilde{Q}_2^{\alpha\neq\beta}(t - t') = 0. \qquad (3.113)$$

A similar argument implies that

$$\tilde{Q}_6^{\alpha\neq\beta}(t - t_0) = 0. \qquad (3.114)$$

Further, as $\langle i\hat{\sigma}_k^{\alpha}(t) \rangle_L$ is zero for all fields, one has from (3.109) that

$$\lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \frac{\partial \langle i\hat{\sigma}_k^{\alpha}(t) \rangle_L}{\partial h_k} = 0 \qquad (3.115)$$

$$\Rightarrow \lim_{n\to 0} \frac{1}{n} \sum_{\alpha,\beta} \langle i\hat{\sigma}_k^{\alpha}(t) \{\sigma_k^{\beta}(t_0) + \int_{t_0}^{t_f} i\hat{\sigma}_k^{\beta}(t')\, dt'\} \rangle_L = 0, \qquad (3.116)$$

where we have used the definition of $\langle \ldots \rangle_L$ to derive (3.116).

Once again, because of (3.111), the $\alpha \neq \beta$ terms in (3.116) vanish and one is left with just the diagonal contribution:

$$\lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \langle i\hat{\sigma}_k^{\alpha}(t)\{\sigma_k^{\alpha}(t_0) + \int_{t_0}^{t_f} i\hat{\sigma}_k^{\alpha}(t')dt'\}\rangle_L = 0. \tag{3.117}$$

By definition

$$\lim_{n\to 0} \frac{1}{n} \sum_{\alpha=1}^{n} \langle i\hat{\sigma}_k^{\alpha}(t)\sigma_k^{\alpha}(t_0)\rangle_L = \langle\langle i\hat{\sigma}_k(t)\sigma_k(t_0)\rangle_T\rangle_J \tag{3.118}$$

describes the response in σ_k at time t_0 due to an applied field at time t [(3.54)] and consequently vanishes for $t > t_0$ because of causality, that is

$$\langle i\hat{\sigma}_k^{\alpha}(t)\sigma_k^{\alpha}(t_0)\rangle_L = 0 \qquad \text{for } t > t_0 . \tag{3.119}$$

Hence, by the definition of $\tilde{Q}_6^{\alpha\beta}$, (3.101f), we have that

$$\tilde{Q}_6^{\alpha\alpha}(t - t_0) = 0 \qquad \text{for } t > t_0. \tag{3.120}$$

Substituting (3.119) into (3.117) yields

$$\langle i\hat{\sigma}_k^{\alpha}(t) \int_{t_0}^{t_f} i\hat{\sigma}_k^{\alpha}(t')dt'\rangle_L = 0 \quad (t > t_0) \tag{3.121}$$

for all t_f; so

$$\langle i\hat{\sigma}_k^{\alpha}(t) i\hat{\sigma}_k^{\alpha}(t')\rangle_L = 0 \tag{3.122}$$

$$\Rightarrow \quad \tilde{Q}_2^{\alpha\alpha}(t - t') = 0 \qquad t > t_0,\ t' \geqslant t_0, \tag{3.123}$$

on using definition (3.101b).

We now look at (3.117) with $t = t_0$:

$$\langle i\hat{\sigma}_k^{\alpha}(t_0)\sigma_k^{\alpha}(t_0)\rangle_L + \langle i\hat{\sigma}_k^{\alpha}(t_0)\int_{t_0}^{t_f} i\hat{\sigma}_k^{\alpha}(t')dt'\rangle_L = 0 \tag{3.124}$$

$$\Rightarrow \quad \langle i\hat{\sigma}_k^{\alpha}(t_0)\sigma_k^{\alpha}(t_0)\rangle_L + \{1 - \tfrac{1}{2}[\delta(t-t_0)+\delta(t-t_f)]\}\langle i\hat{\sigma}_k^{\alpha}(t_0)i\hat{\sigma}_k^{\alpha}(t)\rangle_L = 0,$$

$$(t \geqslant t_0) \tag{3.125}$$

the endpoints of the integration giving a factor of $\frac{1}{2}$ [see Appendix I for details]. Since (3.122) holds for $t' = t_0$, the only non-zero contribution to the second term in (3.125) occurs when $t = t_0$, that is,

$$\langle i\hat{\sigma}_k^{\alpha}(t_0)\sigma_k^{\alpha}(t_0)\rangle_L + \tfrac{1}{2}\langle i\hat{\sigma}_k^{\alpha}(t_0)i\hat{\sigma}_k^{\alpha}(t_0)\rangle_L = 0. \tag{3.126}$$

Thus, one sees from definition (3.101) that when $Q_2^{\alpha\beta}(t - t')$ and $Q_6^{\alpha\beta}(t - t_0)$ do not vanish individually they are related by the relation

$$\tilde{Q}_6^{\alpha\alpha}(t = 0) + \tilde{Q}_2^{\alpha\alpha}(t = 0) = 0. \tag{3.127}$$

We now return to the effective Lagrangian, $L[\sigma_i^{\alpha}, i\hat{\sigma}_i^{\alpha}, \sigma_i^{\alpha}(t_0), \tilde{Q}_a^{\alpha\beta}]$, and substitute for $\tilde{Q}_a^{\alpha\beta}$ from equations (3.102):

$$L[\sigma_i^{\alpha}, i\hat{\sigma}_i^{\alpha}, \sigma_i^{\alpha}(t_0), \tilde{Q}_a^{\alpha\beta}] = L_0\{\sigma_i^{\alpha}, i\hat{\sigma}_i^{\alpha}, \sigma_i^{\alpha}(t_0)\}$$

$$+ \frac{\beta^2 J^2}{2} \sum_{\alpha,\beta} \sum_{i=1}^{N} \int_{t_0}^{t_f}\int_{t_0}^{t_f} \Big[C^{\alpha\beta}(t-t')i\hat{\sigma}_i^{\alpha}(t)i\hat{\sigma}_i^{\beta}(t')$$

$$+ G^{\alpha\beta}(t-t')i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t') + G^{\beta\alpha}(t'-t)\sigma_i^{\alpha}(t)i\hat{\sigma}_i^{\beta}(t')\Big]dtdt'$$

$$+ 2\int_{t_0}^{t_f} C^{\alpha\beta}(t-t_0)i\hat{\sigma}_i^{\alpha}(t)\sigma_i^{\beta}(t_0)dt$$

$$+ C^{\alpha\beta}(t=0)\sigma_i^{\alpha}(t_0)\sigma_i^{\beta}(t_0)\Big\}$$

$$+ \sum_{\alpha,i}\Big\{\int_{t_0}^{t_f}\int_{t_0}^{t_f} \tilde{Q}_2^{\alpha\alpha}(t-t')\sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t')dtdt'$$

$$+ \int_{t_0}^{t_f} \tilde{Q}_6^{\alpha\alpha}(t-t_0)\sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t_0)dt\Big\}, \tag{3.128}$$

where $L_0\{\sigma_i^{\alpha}, i\hat{\sigma}_i^{\alpha}, \sigma_i^{\alpha}(t_0)\}$ is given by (3.98). Since by definition (3.101)

$$\int_{t_0}^{t_f}\int_{t_0}^{t_f} \tilde{Q}_2^{\alpha\alpha}(t-t')\sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t')dtdt' + \int_{t_0}^{t_f} \tilde{Q}_6^{\alpha\alpha}(t-t_0)\sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t_0)dt$$

$$= \frac{\beta^2 J^2}{N}\sum_{k=1}^{N}\Big\{\frac{1}{2}\int_{t_0}^{t_f}\int_{t_0}^{t_f} \langle i\hat{\sigma}_k^{\alpha}(t)i\hat{\sigma}_k^{\alpha}(t')\rangle_L \sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t')dtdt'$$

$$+ \int_{t_0}^{t_f} \langle i\hat{\sigma}_k^{\alpha}(t)\sigma_k^{\alpha}(t_0)\rangle_L \sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t_0)dt\Big\} \tag{3.129}$$

$$= \frac{\beta^2 J^2}{N}\sum_{k=1}^{N}\int_{t_0}^{t_f}\Big\{\frac{1}{2}\langle i\hat{\sigma}_k^{\alpha}(t)i\hat{\sigma}_k^{\alpha}(t)\rangle_L \sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t)$$

$$+ \langle i\hat{\sigma}_k^{\alpha}(t)\sigma_k^{\alpha}(t_0)\rangle_L \sigma_i^{\alpha}(t)\sigma_i^{\alpha}(t_0)\Big\}dt \tag{3.130}$$

$$= \frac{\beta^2 J^2}{2N}\sum_{k=1}^{N}\Big\{\frac{1}{2}\langle i\hat{\sigma}_k^{\alpha}(t_0)i\hat{\sigma}_k^{\alpha}(t_0)\rangle_L + \langle i\hat{\sigma}_k^{\alpha}(t_0)\sigma_k^{\alpha}(t_0)\rangle_L\Big\}\sigma_i^{\alpha}(t_0)\sigma_i^{\alpha}(t_0) \tag{3.131}$$

$$= 0, \tag{3.132}$$

where we have used (3.126). Consequently, neither $Q_2^{\alpha\beta}$ nor $Q_6^{\alpha\beta}$ contribute to the Lagrangian and one can rewrite it as

$$L[\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), \tilde{Q}_a^{\alpha\beta}] = L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$$

$$+ \frac{\beta^2 J^2}{2} \sum_{\alpha,\beta} \sum_{i=1} \Bigg\{ \int_{t_0}^{t_f}\int_{t_0}^{t_f} \Big[C^{\alpha\beta}(t-t') i\hat{\sigma}_i^\alpha(t) i\hat{\sigma}_i^\beta(t')$$

$$+ 2G^{\alpha\beta}(t-t') i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t') \Big] dtdt'$$

$$+ 2\int_{t_0}^{t_f} C^{\alpha\beta}(t-t_0) i\hat{\sigma}_i^\alpha(t)\sigma_i^\beta(t_0)dt$$

$$+ C^{\alpha\beta}(t=0)\sigma_i^\alpha(t_0)\sigma_i^\beta(t_0) \Bigg\}. \qquad (3.133)$$

The Lagrangian can be simplified further by once again using (3.109). From $\langle i\hat{\sigma}_k \rangle_T = 0$ we deduced that $\sum_{\alpha\neq\beta} \tilde{Q}_2^{\alpha\beta}(t-t') = \sum_{\alpha\neq\beta} \tilde{Q}_6^{\alpha\beta}(t-t_0) = 0$ and consequently that $\tilde{Q}_2^{\alpha\neq\beta}(t-t') = \tilde{Q}_6^{\alpha\neq\beta}(t-t_0) = 0$. Since by definition (3.55)

$$G^{\alpha\beta}(t - t') = \frac{1}{N} \sum_{i=1}^{N} \langle i\hat{\sigma}_i^\beta(t')\sigma_i^\alpha(t) \rangle_L \qquad t > t', \qquad (3.134)$$

the same argument as above applies and we have that

$$\sum_{\alpha\neq\beta} G^{\alpha\beta}(t - t') = 0, \qquad (3.135)$$

which implies, on making the de Dominicis-Young ansatz [de Dominicis & Young 1983a], that

$$G^{\alpha\neq\beta}(t - t') = 0. \qquad (3.136)$$

Since [de Dominicis & Young, 1983a]

$$\lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} \langle \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \rangle_L = \langle \langle \sigma_i(t) \rangle_T \langle \sigma_i(t') \rangle_T \rangle_J \qquad (3.137)$$

and

$$C^{\alpha\beta}(t - t') = N^{-1} \sum_{i=1}^{N} \langle \sigma_i^{\alpha}(t)\sigma_i^{\beta}(t') \rangle_L \qquad (3.138)$$

by definition (3.53), we have that

$$\lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} C^{\alpha\beta}(t - t') = \frac{1}{N} \sum_{i=1}^{N} \langle \langle \sigma_i(t) \rangle_T \langle \sigma_i(t') \rangle_T \rangle_J . \qquad (3.139)$$

As $\exp(-\beta H)$ is a stationary distribution, (3.35), $\langle \sigma_i(t) \rangle_T$ is independent of time and consequently $\sum_{\alpha\neq\beta} C^{\alpha\beta}(t-t')$ contains only a time-persistent part. Once again we assume that $C^{\alpha\neq\beta}(t-t')$ does not depend on time for each pair $(\alpha \neq \beta)$ separately. Recalling the definition, (3.56), of order parameters $q^{\alpha\beta}$ we see that for $\alpha \neq \beta$ the limit $t \to \infty$ is superfluous as the right-hand side is independent of t; for $\alpha = \beta$ we have

$$q^{\alpha\alpha} = \lim_{\substack{N\to\infty \\ n\to 0 \\ t\to\infty}} C^{\alpha\alpha}(t), \qquad (3.139)$$

that is, the order parameter $q^{\alpha\alpha}$ is the long-time limit of the corresponding correlation function. So defining [(3.56)]

$$C^{\alpha\alpha}(t) = \tilde{C}^{\alpha\alpha}(t) + q^{\alpha\alpha}, \qquad (3.140)$$

where

$$\lim_{t\to\infty} \tilde{C}^{\alpha\alpha}(t) = 0 \qquad (3.141)$$

is the finite-time contribution, we see from (3.136), (3.139) and (3.140) that the Lagrangian (3.133) can be written as the sum of a finite-time part, arising solely from the diagonal ($\alpha = \beta$) terms, and a time-persistent part:

$$
\begin{aligned}
L[\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_o), q^{\alpha\beta}] = {} & L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\} \\
& + \frac{\beta^2 J^2}{2} \sum_{i=1}^{N} \Bigg\{ \sum_{\alpha=1}^{n} \Bigg[\int_{t_0}^{t_f}\int_{t_0}^{t_f} \Big(\tilde{C}^{\alpha\alpha}(t-t') i\hat{\sigma}_i^\alpha(t) i\hat{\sigma}_i^\alpha(t') \\
& + 2G^{\alpha\alpha}(t-t') i\hat{\sigma}_i^\alpha(t)\sigma_i^\alpha(t') \Big) dt dt' \\
& + 2\int_{t_0}^{t_f} \tilde{C}^{\alpha\alpha}(t-t_0) i\hat{\sigma}_i^\alpha(t)\sigma_i^\alpha(t_0) dt \\
& + [C^{\alpha\alpha}(0) - q^{\alpha\alpha}]\{\sigma_i^\alpha(t_0)\}^2 \Bigg] \\
& + \sum_{\alpha,\beta} \Big(\sigma_i^\alpha(t_0) + \int_{t_0}^{t_f} i\hat{\sigma}_i^\alpha(t) dt \Big) q^{\alpha\beta} \Big(\sigma_i^\beta(t_0) + \int_{t_0}^{t_f} i\hat{\sigma}_i^\beta(t) dt \Big) \Bigg\},
\end{aligned}
\tag{3.142}
$$

where $L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$ is given by (3.98) and $G^{\alpha\alpha}(t)$ is defined by (3.55).

In the next section we take the Ising limit (3.27a,b).

Section D: The Ising Limit

By comparing the structures of $L[\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), q^{\alpha\beta}]$, (3.142), and $L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$, (3.98), we can write down an effective equation of motion for $\sigma_i^\alpha(t)$:

$$
\begin{aligned}
\Gamma^{-1} \frac{\partial \sigma_i^\alpha}{\partial t} = {} & -r\sigma_i^\alpha(t) - u(\sigma_i^\alpha(t))^3 + \beta h_i(t) + \beta^2 J^2 \int_{t_0}^{t_f} G^{\alpha\alpha}(t-t')\sigma_i^\alpha(t') dt' \\
& + \varphi_i(t),
\end{aligned}
\tag{3.143}
$$

where we have also made use of (3.29) and (3.45), and $\varphi_i(t)$ is the effective random noise with

$$\langle \varphi_i(t)\varphi_j(t') \rangle = 2\Gamma^{-1}\delta_{ij}\delta(t-t') + \beta^2 J^2 \delta_{ij} \tilde{C}^{\alpha\alpha}(t-t')$$

$$= 2\delta_{ij}[\Gamma^{-1}\delta(t-t') + \frac{\beta^2 J^2}{2} \tilde{C}^{\alpha\alpha}(t-t')]. \qquad (3.144)$$

We now let $t_0 \to -\infty$ and $t_f \to +\infty$, thereby enabling conventional Fourier transforms, (3.20), to be defined.

Multiplying (3.143) by $e^{i\omega t}$ and integrating with respect to t from $-\infty$ to $+\infty$ we get

$$-i\omega\Gamma^{-1}\sigma_i^\alpha(\omega) = -r\sigma_i^\alpha(\omega)+\varphi_i(\omega)+\beta h_i(\omega)- \frac{u}{(2\pi)^2}\int_{-\infty}^{+\infty}\int \sigma_i^\alpha(\omega_1)\sigma_i^\alpha(\omega_2)\sigma_i^\alpha(\omega-\omega_1-\omega_2)d\omega_1 d\omega_2$$

$$+ \beta^2 J^2 G^{\alpha\alpha}(\omega)\sigma_i^\alpha(\omega). \qquad (3.145)$$

$$\Rightarrow \{r-i\omega\Gamma^{-1}-\beta^2 J^2 G^{\alpha\alpha}(\omega)\}\sigma_i^\alpha(\omega) = \varphi_i(\omega)+\beta h_i(\omega)$$

$$- \frac{u}{(2\pi)^2}\int_{-\infty}^{+\infty}\int \sigma_i^\alpha(\omega_1)\sigma_i^\alpha(\omega_2)\sigma_i^\alpha(\omega-\omega_1-\omega_2)d\omega_1 d\omega_2, \qquad (3.146)$$

where we have made use of the convolution theorem for Fourier transforms in deriving (3.145).

Defining

$$[G_0^{\alpha\alpha}(\omega)]^{-1} = r - i\omega\Gamma^{-1} - \beta^2 J^2 G^{\alpha\alpha}(\omega), \qquad (3.147)$$

we have from (3.146) that

$$\sigma_i^{\alpha}(\omega) = G_0^{\alpha\alpha}(\omega)[\varphi_i(\omega)+\beta h_i(\omega)] - \frac{uG_0^{\alpha\alpha}(\omega)}{(2\pi)^2}\int_{-\infty}^{+\infty}\sigma_i^{\alpha}(\omega_1)\sigma_i^{\alpha}(\omega_2)\sigma_i^{\alpha}(\omega-\omega_1-\omega_2)\,d\omega_1 d\omega_2 . \tag{3.148}$$

Hence, we see that the inverse bare (that is, u = 0) propagator is modified from

$$[G_0^{\alpha\alpha}(\omega)]^{-1} = r - i\omega\Gamma^{-1} \tag{3.149}$$

to (3.147). Fourier transforming equation (3.144) gives

$$\langle\varphi_i(\omega)\varphi_i(\omega')\rangle = [2\Gamma^{-1} + \beta^2J^2\tilde{C}^{\alpha\alpha}(\omega)]\delta(\omega+\omega'). \tag{3.150}$$

So, as Sompolinsky and Zippelius (1981, 1982) pointed out, the spin-glass interaction alters both the inverse bare propagator and the width of the Gaussian noise.

The term in the Lagrangian proportional to $(\sigma_i^{\alpha}(t_0))^2$ modifies the strength of the quadratic term in the initial Hamiltonian (3.61):

$$r \to r' = r - \beta^2J^2[C^{\alpha\alpha}(t=0) - q^{\alpha\alpha}] \tag{3.151a}$$

$$= r - \beta^2J^2\tilde{C}^{\alpha\alpha}(t=0) \qquad \text{(definition (3.140))} \tag{3.151b}$$

$$= r - \beta^2J^2G^{\alpha\alpha}(\omega=0), \qquad \text{(from (3.57))} \tag{3.151c}$$

which is just the $\omega = 0$ limit of (3.147); the term in (3.142) involving $\tilde{C}^{\alpha\alpha}(t-t_0)$ is of no significance as it vanishes for $t \gg t_0$.

A final simplification of the Lagrangian results from decoupling the time-persistent part by a Gaussian transformation. From (3.44a) we have the identity

$$e^{\frac{\beta^2 J^2}{2}\sum_{\alpha,\beta,i}\{\sigma_i^\alpha(t_0)+\int_{-\infty}^{+\infty} i\hat{\sigma}_i^\alpha(t)dt\}q^{\alpha\beta}\{\sigma_i^\beta(t_0)+\int_{-\infty}^{+\infty} i\hat{\sigma}_i^\beta(t)dt\}}$$

$$= (2\pi)^{-n/2}(\det q^{-1})^{1/2}\int\prod_{\alpha,i} dz^\alpha e^{-\frac{1}{2}\sum_{\alpha,\beta} z^\alpha (q^{-1})^{\alpha\beta} z^\beta + \beta J\sum_\alpha z^\alpha\{\sigma_i^\alpha(t_0)+\int_{-\infty}^{+\infty} i\hat{\sigma}_i^\alpha(t)dt\}}, \tag{3.152}$$

where $(q^{-1})^{\alpha\beta}$ is defined by

$$\sum_\beta q^{\alpha\beta}(q^{-1})^{\beta\gamma} = \delta_{\alpha\gamma} \quad \text{(Kronecker-delta)} . \tag{3.153}$$

As the exponent on the left-hand side of (3.152) is just the time-persistent part of the Lagrangian, (3.142), we see by comparing the exponent of the integrand on the right-hand side of (3.152) with $L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$, (3.98), that the time-persistent contribution adds a term Jz^α to the field acting on the spins at both the initial time ($t = t_0$) and later times.

The above modifications can now be absorbed into $L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$, thereby further simplifying the effective Lagrangian.

So, using (3.152) we write (3.142) as

$$L[\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), q^{\alpha\beta}, z^\alpha] = \tilde{L}_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), z^\alpha\} - \frac{1}{2}\sum_{\alpha,\beta} z^\alpha (q^{-1})^{\alpha\beta} z^\beta , \tag{3.154}$$

where

$$\tilde{L}_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), z^\alpha\} = L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$$

$$+ \frac{\beta^2 J^2}{2} \sum_{\alpha,i} \Bigg[\int_{-\infty}^{+\infty}\int \Big(\tilde{C}^{\alpha\alpha}(t-t') i\hat{\sigma}_i^\alpha(t) i\hat{\sigma}_i^\alpha(t')$$

$$+ 2G^{\alpha\alpha}(t-t') i\hat{\sigma}_i^\alpha(t)\sigma_i^\alpha(t')\Big) dt dt'$$

$$+ [C^{\alpha\alpha}(0) - q^{\alpha\alpha}](\sigma_i^\alpha(t_0))^2\Bigg]$$

$$+ \beta J \sum_{\alpha,i} z^\alpha \Big(\sigma_i^\alpha(t_0) + \int_{-\infty}^{+\infty} i\hat{\sigma}_i^\alpha(t) dt \Big) \; . \qquad (3.155)$$

Note that the negligible term discussed above has been omitted from (3.155). Since $L_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0)\}$ is given by (3.98) we have from (3.155) that

$$\tilde{L}_0\{\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), z^\alpha\} = \sum_{\alpha,i} \Bigg\{ \int_{-\infty}^{+\infty} \Big(i\hat{\sigma}_i^\alpha(t) \Big[-\Gamma^{-1} \frac{\partial \sigma_i^\alpha}{\partial t} - r\sigma_i^\alpha(t) - u(\sigma_i^\alpha(t))^3$$

$$+ \beta^2 J^2 \int_{-\infty}^{+\infty} G^{\alpha\alpha}(t-t')\sigma_i^\alpha(t') dt' + \beta[h_i(t) + Jz^\alpha]$$

$$+ \int_{-\infty}^{+\infty} [\Gamma^{-1}\delta(t-t') + \frac{\beta^2 J^2}{2} \tilde{C}^{\alpha\alpha}(t-t')] i\hat{\sigma}_i^\alpha(t') dt' \Big]$$

$$+ V\{\sigma_i^\alpha(t)\} + \{\ell_i^\alpha(t)\sigma_i^\alpha(t) + \hat{\ell}_i^\alpha(t)\hat{\sigma}_i^\alpha(t)\}\Big) dt$$

$$- \{\frac{r'}{2}(\sigma_i^\alpha(t_0))^2 + \frac{u}{4}(\sigma_i^\alpha(t_0))^4 - \beta(h_i + Jz^\alpha)\sigma_i^\alpha(t_0)\}\Bigg\} \; , \qquad (3.156)$$

where $V\{\sigma_i^\alpha(t)\}$ is given by (3.62) and r' by (3.151).

So far we have shown that averages have to be calculated with respect to the Lagrangian $L[\sigma_i^\alpha, i\hat{\sigma}_i^\alpha, \sigma_i^\alpha(t_0), q^{\alpha\beta}, z^\alpha]$, that is if we write

$$F = (2\pi)^{-n/2}(\det q^{-1})^{1/2}\int\prod_{\alpha} dz^{\alpha}\, D[\sigma_i^{\alpha}]\, D[i\hat{\sigma}_i^{\alpha}]\, D[\sigma_i^{\alpha}(t_0)]e^{L[\sigma_i^{\alpha},i\hat{\sigma}_i^{\alpha},\sigma_i^{\alpha}(t_0),q^{\alpha\beta},z^{\alpha}]} \tag{3.157}$$

then averages are evaluated over the integrand in (3.157) divided by F. However, as we want to extract information concerning the equilibrium behaviour of the system, we now reformulate the problem in terms of an equivalent static Hamiltonian. So, regarding both z^{α} and $\sigma_i^{\alpha}(t_0)$ to be held fixed, we see by comparing the structure of $\tilde{L}_0\{\sigma_i^{\alpha},i\hat{\sigma}_i^{\alpha},\sigma_i^{\alpha}(t_0),z^{\alpha}\}$, (3.156), with (3.45) that an equivalent static Hamiltonian, H_s, which describes the finite-time part of the problem is given by

$$\beta H_s = \sum_{\alpha,i}\left\{\frac{r'}{2}(\sigma_i^{\alpha})^2 + \frac{u}{4}(\sigma_i^{\alpha})^4 - \beta[h_i+Jz^{\alpha}]\sigma_i^{\alpha}\right\} \tag{3.158}$$

where

$$r' = [G_0^{\alpha\alpha}(\omega=0)]^{-1}. \qquad \text{(from (3.147) and (3.151))} \tag{3.159}$$

So the conditional probability density of σ_i^{α} given $\sigma_i^{\alpha}(t_0)$ and z^{α} is given by

$$e^{-\beta H_s}\Big/\sum_{\{\sigma_i^{\alpha}\}} e^{-\beta H_s}, \tag{3.160}$$

which is the analogue of (3.41). If we now allow both $\sigma_i^{\alpha}(t_0)$ and z^{α} to vary, we see from (3.154), (3.156), (3.157) and (3.160) that averages are now to be evaluated with a (normalised) weight

$$D^{-1}\times\left(e^{-\beta H_s}\Big/\sum_{\{\sigma_i^{\alpha}\}} e^{-\beta H_s}\right)\times\left(e^{-\beta H_0}\right)\times\left((2\pi)^{-n/2}(\det q^{-1})^{1/2}e^{-\frac{1}{2}\sum_{\alpha,\beta} z^{\alpha}(q^{-1})^{\alpha\beta}z^{\beta}}\right) \tag{3.161}$$

where, from (3.59) and (3.156), H_0 is given by

$$\beta H_0 = \sum_{\alpha,i} \left\{ \frac{r'}{2}(\sigma_i^\alpha(t_0))^2 + \frac{u}{4}(\sigma_i^\alpha(t_0))^4 - \beta[h_i+JZ^\alpha]\sigma_i^\alpha(t_0) \right\} \tag{3.162}$$

and D is the normalization constant; (3.161) should be compared with equation (3.31) in Section A.2.

One now retrieves the Ising (± 1) system by allowing $r \sim r' \to -\infty$ and $u \to \infty$, (3.27). This means that (3.158) and (3.162) become

$$H_s = -\sum_{\alpha,i} (h_i + JZ^\alpha)S_i^\alpha \qquad (S_i^\alpha \equiv \sigma_i^\alpha = \pm 1) \tag{3.163a}$$

and

$$H_0 = -\sum_{\alpha,i} (h_i + JZ^\alpha)s_i^\alpha \qquad (s_i^\alpha \equiv \sigma_i^\alpha(t_0) = \pm 1) \tag{3.163b}$$

respectively. Now, using (3.163a), we have that

$$\sum_{\{S_i^\alpha=\pm1\}} e^{-\beta H_s} = \sum_{\{S_i^\alpha=\pm1\}} e^{\beta_{\alpha,i}\Sigma (h_i+JZ^\alpha)S_i^\alpha} \tag{3.164}$$

$$= \prod_{\alpha,i} \left\{ \sum_{\{S_i^\alpha=\pm1\}} e^{\beta(h_i+JZ^\alpha)S_i^\alpha} \right\} \tag{3.165}$$

$$= \prod_{\alpha,i} 2\cosh[\beta(h_i + JZ^\alpha)]. \tag{3.166}$$

Hence, by substituting (3.163) and (3.166) into (3.161) we see that the weighting factor becomes

$$\frac{(2\pi)^{-n/2}(\det q^{-1})^{1/2} e^{-\frac{1}{2}\alpha,\beta\Sigma\, z^\alpha(q^{-1})^{\alpha\beta}z^\beta + \beta_{\alpha,i}\Sigma (h_i+JZ^\alpha)(S_i^\alpha+s_i^\alpha)}}{D \times \prod_{\alpha,i} 2\cosh[\beta(h_i+JZ^\alpha)]} . \tag{3.167}$$

So the order-parameters $q^{\alpha\beta}$, given by (3.56), are now evaluated by considering

$$q^{\alpha\beta} = \lim_{\substack{N\to\infty \\ t\to\infty \\ n\to 0}} C^{\alpha\beta}(t) \qquad \text{(definition (3.56))} \tag{3.168}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty \\ n\to 0}} N^{-1} \sum_{i=1}^{N} \langle\, \sigma_i^{\alpha}(t+t_0)\sigma_i^{\beta}(t_0)\,\rangle_L \qquad \text{(definition (3.53))} \tag{3.169}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty \\ n\to 0}} \langle\, \sigma_i^{\alpha}(t+t_0)\sigma_i^{\beta}(t_0)\,\rangle_L \tag{3.170}$$

$$= \lim_{n\to 0} \langle\, s_i^{\alpha} s_i^{\beta}\,\rangle, \qquad \text{(notation as in (3.163))} \tag{3.171}$$

where $\langle \ldots \rangle$ denotes an average with weight (3.167). We now define

$$\langle \ldots \rangle \equiv [\langle \ldots \rangle_H]_Z \tag{3.172}$$

where $\langle \ldots \rangle_H$ denotes an average over

$$e^{\beta \sum_{\alpha,i} (h_i + JZ^{\alpha})(S_i^{\alpha} + s_i^{\alpha})} \Big/ \prod_{\alpha,i} 2\cosh[\beta(h_i + JZ^{\alpha})], \tag{3.173}$$

keeping Z^{α} held fixed, and $[\ldots]_Z$ denotes an average over

$$D^{-1} \times (2\pi)^{-n/2} (\det q^{-1})^{1/2}\, e^{-\frac{1}{2} \sum_{\alpha,\beta} Z^{\alpha} (q^{-1})^{\alpha\beta} Z^{\beta}} \tag{3.174}$$

where

$$D = (2\pi)^{-n/2}(\det q^{-1})^{1/2}\int\prod_{\alpha} dz^{\alpha}\left(\left[\sum_{\substack{\{S_k^{\alpha}=\pm 1;\\ s_k^{\alpha}=\pm 1\}}} \exp\left\{-\frac{1}{2}\sum_{\alpha,\beta} z^{\alpha}(q^{-1})^{\alpha\beta}z^{\beta}\right.\right.\right.$$

$$\left.\left.\left. + \beta\sum_{\alpha,k}\left(h_k + Jz^{\alpha}\right)\left(S_k^{\alpha} + s_k^{\alpha}\right)\right\}\right]\Big/\prod_{\alpha,\ell} 2\cosh[\beta(h_{\ell}+Jz^{\alpha})]\right) \tag{3.175}$$

$$= (2\pi)^{-n/2}(\det q^{-1})^{1/2}\int\prod_{\alpha} dz^{\alpha}\left(\exp\left\{-\frac{1}{2}\sum_{\alpha,\beta} z^{\alpha}(q^{-1})^{\alpha\beta}z^{\beta}\right\}\right.$$

$$\left.\times\prod_{\alpha,\ell} 2\cosh\left[\beta(h_{\ell} + Jz^{\alpha})\right]\right) . \tag{3.176}$$

Thus, combining (3.171) and (3.172) we have that

$$q^{\alpha\beta} = \lim_{n\to 0}\left[\left\langle S_i^{\alpha}s_i^{\beta}\right\rangle_H\right]_Z. \tag{3.177}$$

In the next section we derive expressions for the order parameters $q^{\alpha\beta}$.

Section E: Order Parameters

We are now in a position to evaluate the order parameters, $q^{\alpha\beta}$, defined by (3.177). Now, using (3.173), we have that

$$\left\langle S_i^{\alpha_0}s_i^{\beta_0}\right\rangle_H = \sum_{\substack{\{S_k^{\alpha}=\pm 1;\\ s_k^{\alpha}=\pm 1\}}} S_i^{\alpha_0}s_i^{\beta_0}\,\frac{e^{\beta\sum_{\alpha,k}(h_k+Jz^{\alpha})(S_k^{\alpha}+s_k^{\alpha})}}{\prod_{\alpha,\ell} 2\cosh[\beta(h_{\ell}+Jz^{\alpha})]} \tag{3.178}$$

$$= \left(\prod_{\alpha,\ell} 2\cosh[\beta(h_{\ell}+Jz^{\alpha})]\right)^{-1}\times\left[\sum_{\{S_k^{\alpha}=\pm 1\}} S_i^{\alpha_0}\, e^{\beta\sum_{\alpha,k}(h_k+Jz^{\alpha})S_k^{\alpha}}\right]$$

$$\times\left[\sum_{\{s_k^{\alpha}=\pm 1\}} s^{\beta_0}\, e^{\beta\sum_{\alpha,k}(h_k+Jz^{\alpha})s_k^{\alpha}}\right] \tag{3.179}$$

$$= \Big(\prod_{\alpha,\ell} 2\cosh[\beta(h_\ell + Jz^\alpha)] \Big)^{-1} \times \big(2\sinh[\beta(h_i + Jz^{\alpha_0})]\big)$$

$$\times \Big(\prod_{\substack{\alpha\neq\alpha_0 \\ k\neq i_0}} 2\cosh[\beta(h_k + Jz^\alpha)] \Big) \times \big(2\sinh[\beta(h_i + Jz^{\beta_0})]\big)$$

$$\times \Big(\prod_{\substack{\alpha\neq\beta \\ k\neq i_0}} 2\cosh[\beta(h_k + Jz^\alpha)] \Big) \qquad (3.180)$$

$$= \tanh[\beta(h_i + Jz^{\alpha_0})]\tanh[\beta(h_i + Jz^{\beta_0})] \prod_{\mu,k} 2\cosh[\beta(h_k + Jz^\mu)] \,. \qquad (3.181)$$

Thus, substituting (3.174) and (3.181) into (3.177) we get

$$q^{\alpha_0\beta_0} = \lim_{n\to 0} D^{-1}(2\pi)^{-n/2}(\det q^{-1})^{1/2} \int \prod_\alpha dz^\alpha \exp\Big\{-\frac{1}{2}\sum_{\alpha,\beta} z^\alpha (q^{-1})^{\alpha\beta} z^\beta\Big\}$$

$$\times \tanh[\beta(h_i + Jz^{\alpha_0})]\tanh[\beta(h_i + Jz^{\beta_0})] \prod_{\mu,k} 2\cosh[\beta(h_k + Jz^\mu)], \qquad (3.182)$$

which becomes for $\alpha_0 = \beta_0$

$$q^{\alpha_0\alpha_0} = \lim_{n\to 0} D^{-1}(2\pi)^{-n/2}(\det q^{-1})^{1/2} \int \prod_\alpha dz^\alpha \exp\Big\{-\frac{1}{2}\sum_{\alpha,\beta} z^\alpha (q^{-1})^{\alpha\beta} z^\beta\Big\}$$

$$\times \tanh^2[\beta(h_i + Jz^{\alpha_0})] \prod_{\mu,k} 2\cosh[\beta(h_k + Jz^\mu)] \qquad (3.183)$$

- a result also derived by de Dominicis and Young (1983a) from the TAP equations (1977). (3.183) is an extremely complicated self-consistent equation for $q^{\alpha_0\alpha_0}$ in terms of the off-diagonal elements $q^{\alpha\beta}$. De Dominicis and Young (1983a) have shown that, if one makes Parisi's ansatz (1979) for $q^{\alpha\neq\beta}$, the right-hand side of (3.183) is equal to q(x=1), where q(x) is Parisi's order-parameter function. [Parisi's ansatz and

the interpretation of the dummy variable x are both discussed in Chapter I.] But we also have from (3.21) that

$$q_{EA} = \lim_{\substack{N\to\infty \\ t\to\infty}} C(t) \tag{3.184}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty}} N^{-1} \sum_{i=1}^{N} \langle\langle S_i(t+t_0)S_i(t_0)\rangle_T\rangle_J \qquad \text{(from (3.20))} \tag{3.185}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty}} \langle\langle S_i(t+t_0)S_i(t_0)\rangle_T\rangle_J \tag{3.186}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty \\ n\to 0}} \frac{1}{n} \sum_{\alpha=1}^{n} \langle\sigma_i^{\alpha}(t+t_0)\sigma_i^{\alpha}(t_0)\rangle_L \qquad \text{(from (3.53))} \tag{3.187}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t+t_0)\sigma_i^{\alpha_0}(t_0)\rangle_L \tag{3.188}$$

$$= q^{\alpha_0\alpha_0} \qquad \text{(from (3.170))}; \tag{3.189}$$

it then follows from (3.183) and (3.189) that

$$q^{\alpha\alpha} = q_{EA} = q(x = 1). \tag{3.190}$$

As was mentioned in Section A.1, Sompolinsky's theory (1981) also gives this result for the Edwards-Anderson (1975) order parameter.

For $\alpha_0 \neq \beta_0$ we go back to (3.181) and re-write it as

$$\langle S_i^{\alpha_0} s_i^{\beta_0}\rangle_H = 2\sinh[\beta(h_i+Jz^{\alpha_0})]2\sinh[\beta(h_i+Jz^{\beta_0})] \prod_{\substack{k \\ \mu\neq\alpha_0,\beta_0}} 2\cosh[\beta(h_k+Jz^{\mu})] \tag{3.191}$$

$$= \left(\sum_{\{S_i^{\alpha_0}=\pm 1\}} S_i^{\alpha_0} \, e^{\beta(h_i + JZ^{\alpha_0})S_i^{\alpha_0}} \right) \times \left(\sum_{\{S_i^{\beta_0}=\pm 1\}} S_i^{\beta_0} \, e^{\beta(h_i + JZ^{\beta_0})S_i^{\beta_0}} \right)$$

$$\times \left(\sum_{\{S_k^{\mu \neq \alpha_0, \beta_0}=\pm 1\}} e^{\sum_k \beta(h_k + JZ^{\mu})S_k^{\mu}} \right) \tag{3.192}$$

$$= \sum_{\{S_k^{\mu}=\pm 1\}} S_i^{\alpha_0} S_i^{\beta_0} \, e^{\mu, \sum_k \beta(h_k + JZ^{\mu})S_k^{\mu}} . \tag{3.193}$$

Hence, from (3.174), (3.175) and (3.193) we have

$$q^{\alpha_0 \neq \beta_0} = \lim_{n \to 0} D^{-1} (2\pi)^{-n/2} (\det q^{-1})^{1/2} \int \prod_{\alpha} dz^{\alpha} \exp \left\{ -\frac{1}{2} \sum_{\alpha, \beta} z^{\alpha} (q^{-1})^{\alpha\beta} z^{\beta} \right\}$$

$$\times \sum_{\{S_k^{\mu}=\pm 1\}} S_i^{\alpha_0} S_i^{\beta_0} \, e^{\mu, \sum_k \beta(h_k + JZ^{\mu})S_k^{\mu}} \tag{3.194}$$

$$= \lim_{n \to 0} D^{-1} \times \sum_{\{S_k^{\mu}=\pm 1\}} S_i^{\alpha_0} S_i^{\beta_0} \, e^{\mu, \sum_k \beta h_k S_k^{\mu}} \left[(2\pi)^{-n/2} (\det q^{-1})^{1/2} \right.$$

$$\left. \times \int \prod_{\alpha} dz^{\alpha} \exp \left\{ -\frac{1}{2} \sum_{\alpha, \beta} z^{\alpha} (q^{-1})^{\alpha\beta} z^{\beta} + \sum_{\mu, k} \beta J S_k^{\mu} z^{\mu} \right\} \right] . \tag{3.195}$$

The integrals over z^{α} can now be evaluated using equation (3.44a).

With the aid of this identity, (3.195) now becomes

$$q^{\alpha_0 \neq \beta_0} = \lim_{n \to 0} D^{-1} \times \sum_{\{S_k^\mu = \pm 1\}} S_i^{\alpha_0} S_i^{\beta_0} \exp\left\{ \frac{\beta^2 J^2}{2} \sum_{\substack{\alpha,\beta \\ k}} S_k^\alpha q^{\alpha\beta} S_k^\beta + \beta \sum_{\alpha,k} h_k S_k^\alpha \right\} \tag{3.196}$$

$$= \lim_{n \to 0} D^{-1} \times \sum_{\{S_k^\mu = \pm 1\}} S_i^{\alpha_0} S_i^{\beta_0} \exp\left\{ \frac{\beta^2 J^2}{2} \sum_{\substack{\alpha \neq \beta \\ k}} S_k^\alpha q^{\alpha\beta} S_k^\beta + \beta \sum_{\alpha,k} h_k S_k^\alpha \right\}, \tag{3.197}$$

where

$$D = \sum_{\{S_k^\mu = \pm 1\}} \exp\left\{ \frac{\beta^2 J^2}{2} \sum_{\substack{\alpha \neq \beta \\ k}} S_k^\alpha q^{\alpha\beta} S_k^\beta + \beta \sum_{\alpha,k} h_k S_k^\alpha \right\}. \tag{3.198}$$

The $q^{\alpha\alpha}$ term has dropped out of (3.197) because of the constraint $(S_k^\alpha)^2 = 1$ and the limit $n \to 0$. Notice that (3.197) is just the result derived directly from statistical mechanics by Sherrington and Kirkpatrick (1975). If $T > T_c$, one has symmetry among the replicas and the statistical mechanics order parameter, q, is given by (3.14), that is

$$q = q^{\alpha_0 \neq \beta_0}. \tag{3.199}$$

However, when $T < T_c$ the replica symmetry is broken and q is obtained by averaging over all distinct replicas [de Dominicis & Young 1983a]

$$q = \lim_{n \to 0} \frac{1}{n(n-1)} \sum_{\alpha \neq \beta} q^{\alpha\beta} \tag{3.200}$$

$$= \int_0^1 q(x)\, dx, \tag{3.201}$$

where the final equality has been obtained by making Parisi's ansatz

for $q^{\alpha\neq\beta}$. As was mentioned in the introductory section, equation (3.201) implies that Parisi's theory is consistent with the FDT.

In deriving (3.142) [see Section C] we made the implicit assumption that

$$q^{\alpha_0\neq\beta_0} = \lim_{\substack{N\to\infty \\ t,t'\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t)\sigma_i^{\beta_0}(t') \rangle_L \tag{3.202a}$$

$$= \lim_{\substack{N\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t_0)\sigma_i^{\beta_0}(t_0) \rangle_L \tag{3.202b}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t)\sigma_i^{\beta_0}(t_0) \rangle_L \ . \tag{3.202c}$$

As we actually took (3.202c) as our definition for the order parameters, $q^{\alpha\beta}$, we need to check only (3.202a) and (3.202b). Now,

$$\lim_{\substack{N\to\infty \\ t,t'\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t)\sigma_i^{\beta_0}(t') \rangle_L = \lim_{n\to 0} \langle S_i^{\alpha_0} S_i^{\beta_0} \rangle \qquad (\alpha_0\neq\beta_0\text{; notation as in (3.163))} \tag{3.203}$$

$$= \lim_{n\to 0} \left[\langle S_i^{\alpha_0} S_i^{\beta_0} \rangle_H \right]_Z \tag{3.204}$$

and

$$\lim_{\substack{N\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t_0)\sigma_i^{\beta_0}(t_0) \rangle_L = \lim_{n\to 0} \left[\langle s_i^{\alpha_0} s_i^{\beta_0} \rangle_H \right]_Z \ . \tag{3.205}$$

Using the definition, (3.173), of $\langle \ldots \rangle_H$ we have that

$$\langle S_i^{\alpha_0} S_i^{\beta_0} \rangle_H = \tanh[\beta(h_i + JZ^{\alpha_0})]\tanh[\beta(h_i + JZ^{\beta_0})] \prod_{\mu,k} 2\cosh[\beta(h_k + JZ^{\mu})] \tag{3.206}$$

$$= \langle s_i^{\alpha_0} s_i^{\beta_0} \rangle_H \tag{3.207}$$

$$= \langle S_i^{\alpha_0} s_i^{\beta_0} \rangle_H \qquad \text{(from (3.181))} \tag{3.208}$$

and since from (3.170), (3.171) and (3.175) we have

$$\lim_{\substack{N\to\infty \\ t\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t)\sigma_i^{\beta_0}(t_0) \rangle_L = \lim_{n\to 0} [\langle S_i^{\alpha_0} s_i^{\beta_0} \rangle_H]_Z \ , \tag{3.209}$$

it follows that equations (3.202) hold.

In the next section we investigate in greater detail the role played by the initial conditions.

Section F: The Initial Conditions

It was emphasised in Section A.3 that, as the SK spin-glass is non-ergodic, in order to generate quilibrium correlation functions in the thermodynamic limit one needs to impose a Boltzmann distribution at the initial time. As a consequence, we were able to retrieve in the previous section the conventional result for the statistical-mechanics order parameter, q. If one ignores the initial conditions, replicas are unnecessary and one obtains the SK solution [Sompolinsky 1981; Sompolinsky & Zippelius 1981, 1982]. We can easily check the outcome of neglecting the initial Boltzmann factor in our formalism.

From an examination of (3.51), (3.59) and (3.156) it is clear that if the initial conditions are not taken into account the factor

$e^{-\beta H_0}$ does not appear in the normalised weight (3.161). Consequently, in this case the weighting factor, (3.167), becomes

$$\frac{(2\pi)^{-n/2}(\det q^{-1})^{1/2}\, e^{-\frac{1}{2}\sum_{\alpha,\beta} z^{\alpha}(q^{-1})^{\alpha\beta} z^{\beta} + \beta\sum_{\alpha,i}(h_i + Jz^{\alpha})S_i^{\alpha}}}{\prod_{\alpha,i} 2\cosh[\beta(h_i + Jz^{\alpha})]}, \tag{3.210}$$

which is normalised to unity.

We now define

$$\langle \ldots \rangle \equiv [\langle \ldots \rangle_{H'}]_Z \tag{3.211}$$

where $\langle \ldots \rangle_{H'}$ denotes an average over

$$e^{\beta\sum_{\alpha,i}(h_i + Jz^{\alpha})S_i^{\alpha}} \Big/ \prod_{\alpha,i} 2\cosh[\beta(h_i + Jz^{\alpha})], \tag{3.212}$$

keeping z^{α} held fixed, and $[\ldots]_Z$ denotes an average over

$$(2\pi)^{-n/2}(\det q^{-1})^{1/2}\, e^{-\frac{1}{2}\sum_{\alpha,\beta} z^{\alpha}(q^{-1})^{\alpha\beta} z^{\beta}}. \tag{3.213}$$

We now re-evaluate the order parameters, $q^{\alpha\beta}$, using

$$q^{\alpha_0\beta_0} = \lim_{n\to 0} \langle S_i^{\alpha_0} s_i^{\beta_0} \rangle \qquad \text{(from (3.171))} \tag{3.214}$$

$$= \lim_{n\to 0} [\langle S_i^{\alpha_0} s_i^{\beta_0} \rangle_{H'}]_Z \qquad \text{(from (3.211))}. \tag{3.215}$$

From (3.212) we have

$$\langle S_i^{\alpha_0} S_i^{\beta_0} \rangle_{H'} = \sum_{\{S_k^\alpha = \pm 1\}} S_i^{\alpha_0} S_i^{\beta_0} \left(\frac{e^{\beta \sum_{\alpha,k} (h_k + JZ^\alpha) S_k^\alpha}}{\prod_{\alpha,\ell} 2 \cosh[\beta(h_i + JZ^\alpha)]} \right) \tag{3.216}$$

$$= \tanh[\beta(h_i + JZ^{\alpha_0})] \tanh[\beta(h_i + JZ^{\beta_0})]. \tag{3.217}$$

So, ignoring the initial conditions has removed the "cosh factors" appearing in (3.181). Combining (3.217) with (3.213) and (3.215) yields

$$q^{\alpha_0 \beta_0} = \lim_{n \to 0} (2\pi)^{-n/2} (\det q^{-1})^{1/2} \int \prod_\alpha dZ^\alpha \tanh[\beta(h_i + JZ^{\alpha_0})] \tanh[\beta(h_i + JZ^{\beta_0})]$$

$$\times e^{-\frac{1}{2} \sum_{\alpha,\beta} Z^\alpha (q^{-1})^{\alpha\beta} Z^\beta} \tag{3.218}$$

$$= \lim_{n \to 0} (2\pi)^{-n} \int \prod_\alpha dZ^\alpha d\nu^\alpha \tanh[\beta(h_i + JZ^{\alpha_0})] \tanh[\beta(h_i + JZ^{\beta_0})]$$

$$\times \exp\left\{ \frac{1}{2} \sum_{\alpha,\beta} (i\nu^\alpha) q^{\alpha\beta} (i\nu^\beta) + \sum_\alpha (i\nu^\alpha) Z^\alpha \right\}, \tag{3.219}$$

where we have used (3.44a) to introduce the Gaussian variable ν^α. Since

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{iZ^\alpha \nu^\alpha} dZ^\alpha = \delta(\nu^\alpha), \tag{3.220}$$

it follows that for $\alpha_0 = \beta_0$ (3.219) becomes

$$q^{\alpha_0 \alpha_0} = q_{EA}$$

$$= \lim_{n \to 0} (2\pi)^{-n} \int dZ^{\alpha_0} d\nu^{\alpha_0} \tanh^2[\beta(h_i + JZ^{\alpha_0})] \left[\prod_{\alpha \neq \alpha_0} 2\pi\delta(\nu^\alpha) \right]$$

$$\times e^{\frac{1}{2} \sum_{\alpha,\beta} (i\nu^\alpha) q^{\alpha\beta} (i\nu^\beta) + i\nu^{\alpha_0} Z^{\alpha_0}} \tag{3.221}$$

$$= (2\pi)^{-1} \int dz^{\alpha_0} d\nu^{\alpha_0} \tanh^2[\beta(h_i + Jz^{\alpha_0})]\, e^{-\frac{q_{EA}(\nu^{\alpha_0})^2}{2} + i\nu^{\alpha_0} z^{\alpha_0}} \tag{3.222}$$

$$= \frac{1}{\sqrt{2\pi q_{EA}}} \int dz^{\alpha_0} \tanh^2[\beta(h_i + Jz^{\alpha_0})]\, e^{-(z^{\alpha_0})^2/2q_{EA}}, \tag{3.223}$$

where we have once again used (3.44a) to go from (3.222) to (3.223). Defining

$$z = z^{\alpha_0}/q_{EA}^{1/2}, \tag{3.224}$$

(3.223) becomes

$$q^{\alpha_0\alpha_0} = q_{EA} = \frac{1}{\sqrt{2\pi}} \int dz\, \tanh^2[\beta(h_i + Jzq_{EA}^{1/2})]\, e^{-z^2/2} \tag{3.225}$$

$$= q^{SK}, \tag{3.226}$$

the order parameter obtained by Sherrington and Kirkpatrick (1975) assuming replica symmetry. Thus, ignoring the initial conditions leads to the replica symmetric solution.

Conversely, if one makes a replica symmetric ansatz for $q^{\alpha\beta}$ then one can easily show that the memory of the initial configuration is lost at large times. So we now assume that

$$q^{\alpha\beta} = q \quad \text{for all } \alpha,\beta. \tag{3.227}$$

Consider first

$$q = q^{\alpha_0\alpha_0} \qquad \text{(from (3.227))} \tag{3.228}$$

$$= q_{EA} \qquad \text{(from (3.190))} \tag{3.229}$$

$$= \lim_{t\to\infty} \lim_{N\to\infty} C(t) \qquad \text{(from (3.21))} \tag{3.230}$$

$$= \lim_{t\to\infty} \lim_{N\to\infty} N^{-1} \sum_{i=1}^{N} \langle\langle S_i(t+t_0)S_i(t_0)\rangle_T\rangle_J \tag{3.231}$$

on using definition (3.20a). But we also have from (3.16) that

$$q = \lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} q^{\alpha\beta} \tag{3.232}$$

$$= \lim_{\substack{N\to\infty \\ n\to 0 \\ t\to\infty}} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} C^{\alpha\beta}(t) \qquad \text{(from (3.56a))} \tag{3.233}$$

$$= \lim_{\substack{N\to\infty \\ n\to 0 \\ t\to\infty}} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} \left\{ N^{-1} \sum_{i=1}^{N} \langle \sigma_i^{\alpha}(t+t_0)\sigma_i^{\beta}(t_0)\rangle_L \right\} \text{(from (3.53))} \tag{3.234}$$

$$= \lim_{\substack{N\to\infty \\ t\to\infty}} N^{-1} \sum_{i=1}^{N} \langle\langle \sigma_i(t+t_0)\rangle_T \langle \sigma_i(t_0)\rangle_T\rangle_J \quad \text{(from (3.137))} \tag{3.235}$$

$$\equiv \lim_{\substack{N\to\infty \\ t\to\infty}} N^{-1} \sum_{i=1}^{N} \langle\langle S_i(t+t_0)\rangle_T \langle S_i(t_0)\rangle_T\rangle_J \tag{3.236}$$

on taking the Ising limit. So, we see from (3.231) and (3.236) that, in fact,

$$\langle\langle S_i(t+t_0)S_i(t_0)\rangle_T\rangle_J = \langle\langle S_i(t+t_0)\rangle_T \langle S_i(t_0)\rangle_T\rangle_J \ . \tag{3.237}$$

So, if one assumes replica symmetry, the system loses memory of the initial spin configuration, that is, there is no correlation between the spins at an initial time t_0 and at much later times t.

In the next section we briefly indicate as to why the finite-

time dynamics in our formalism are identical to that of Sompolinsky and Zippelius (1981, 1982).

Section G: Finite-time Dynamics

We now consider dynamics on time scales which, although finite in the thermodynamic ($N \to \infty$) limit, are much longer than the microscopic time scale.

We see from (3.142) that the finite-time part of the Lagrangian is a sum over n independent replicas. It is only in the time-persistent part that the replicas interact.

Now, we can re-write the response function $G^{\alpha\alpha}(\omega)$ - defined by (3.20d) and (3.54a) - as

$$G^{\alpha\alpha}(\omega) = [G^{\alpha\alpha}(\omega,Z)]_Z \tag{3.238}$$

where (3.174) defines the average over Z. We follow Sompolinsky and Zippelius (1982) by defining a self-energy $\Sigma^{\alpha\alpha}(\omega,Z)$ by a Dyson equation:

$$\{G^{\alpha\alpha}(\omega,Z)\}^{-1} = \{G_0^{\alpha\alpha}(\omega,Z)\}^{-1} + \Sigma^{\alpha\alpha}(\omega,Z), \tag{3.239}$$

where $G_0^{\alpha\alpha}(\omega,Z)$ is obtained from (3.147). One now performs perturbation theory in the coupling constant u. [Further details can be found in Sompolinsky and Zippelius (1982).] In particular, one examines the renormalised expansion for $\partial\Sigma^{\alpha\alpha}(\omega,Z)/\partial\omega$. For $T > T_c$, as there is no coupling between the replicas, our approach trivially gives the same results as Sompolinsky and Zippelius (1981, 1982). Below T_c the perturbation expansion contains vertices depending on fully renormalised spin expectations. In the dynamical approach the expectation values are given by

$$\lim_{\substack{N\to\infty \\ t_{\nu+1}-t_\nu\to\infty}} N^{-1} \sum_{i=1}^{N} \langle\langle S_i(t_1)S_i(t_2)\ldots S_i(t_k)\rangle_T\rangle_J \quad (\nu = 1,2,\ldots,k-1) \tag{3.240}$$

$$= \lim_{\substack{N\to\infty \\ t_{\nu+1}-t_\nu\to\infty \\ n\to 0}} \langle \sigma_i^{\alpha_0}(t_1)\sigma_i^{\alpha_0}(t_2)\ldots\sigma_i^{\alpha_0}(t_k)\rangle_L \tag{3.241}$$

$$= \lim_{n\to 0} [\langle (S^1)_i^{\alpha_0}(S^2)_i^{\alpha_0}\ldots(S^k)_i^{\alpha_0}\rangle_H]_Z \tag{3.242}$$

where we have taken the Ising limit in (3.242) [we define $(S^\nu)_i = \pm 1$ for $\nu = 1,\ldots,k$] - see Section D for further details. We evaluate (3.242) in much the same way as we evaluated the Edwards-Anderson order parameter, $q^{\alpha\alpha}$, in Section E. From an inspection of equations (3.178) - (3.183) we see that (3.242) is given by

$$\lim_{n\to 0} [\langle (S^1)_i^{\alpha_0}(S^2)_i^{\alpha_0} \ldots (S^k)_i^{\alpha_0}\rangle_H]_Z$$

$$= \lim_{n\to 0} D^{-1}(2\pi)^{-n/2}(\det q^{-1})^{1/2}\int \prod_\alpha dz^\alpha \left(\exp\left\{-\frac{1}{2}\sum_{\alpha,\beta} z^\alpha (q^{-1})^{\alpha\beta} z^\beta\right\}\right.$$

$$\left. \times \tanh^k[\beta(h_i + Jz^{\alpha_0})] \prod_{\mu,\ell} 2\cosh[\beta(h_\ell + Jz^\mu)]\right), \tag{3.243}$$

where $k = 1,2,\ldots$. In the "no-replica" approach of Sompolinsky and Zippelius (1981, 1982) the spin expectation values are also given by (3.243); the technical details can be found in the Appendix to de Dominicis and Young (1983a), where the Parisi ansatz for $q^{\alpha\beta}$ ($\alpha \neq \beta$) is made. Hence, the results for finite-time dynamics are the same in the two approaches.

Section H: Conclusions

In this chapter we discussed the dynamics of the Sherrington-Kirkpatrick spin-glass. As the latter is non-ergodic below T_c, in order to extract information concerning the equilibrium behaviour of the model, one needs to impose a Boltzmann distribution at an initial time, t_0. Unfortunately, this necessitates the use of replicas.

The diagonal order parameter, which is equivalent to the Edwards-Anderson order parameter, is given by

$$q^{\alpha\alpha} = q_{EA} = q(x = 1) \tag{3.244}$$

on making the Parisi ansatz for $q^{\alpha\beta}$ [de Dominicis & Young 1984a]; Sompolinsky (1981) also gives this result. As couplings between replicas only occur at long times, all finite-time dynamics are the same as in Sompolinsky and Zippelius (1981, 1982).

We find that the statistical-mechanics order parameter, q, is given by

$$q = \int_0^1 q(x)dx, \tag{3.245}$$

which means that the FDT holds once an average over samples is performed; Sompolinsky and Zippelius (1981, 1982), on the other hand, find that $q = q(0)$.

On ignoring the initial conditions we retrieve the replica symmetric solution of Sherrington and Kirkpatrick (1975). Conversely, if we make a replica symmetric ansatz for $q^{\alpha\beta}$, the system "loses" the memory of the initial states after a sufficiently long time.

CHAPTER IV

MONTE CARLO SIMULATIONS OF X-Y SPIN-GLASSES

Section A: Introduction

1. The ferromagnet

The classical ferromagnet is one of the simplest non-trivial models which we can consider. Its Hamiltonian is given by

$$H = - \sum_{\langle ij \rangle} J_{ij} \, \underline{S}_i . \underline{S}_j \qquad (4.1)$$

where the classical spins $\underline{S}_i$ are situated on every site of a regular lattice and the interactions $\{J_{ij}\}$ act between nearest neighbours only, that is

$$\begin{aligned} J_{ij} &= J > 0 \qquad \text{if } i,j \text{ are nearest neighbours} \\ &= 0 \qquad\quad \text{otherwise.} \end{aligned} \qquad (4.2)$$

Theoretically, one can consider n-component spins and d-dimensional lattices, where n is an integer and $d \geqslant 1$; the spins are conventionally normalized to unity: $\underline{S}_i^2 = 1$.

When $n = 1$ one obtains the Ising ($S_i = \pm 1$) system; $n = 2$ corresponds to the X-Y (or classical planar) model; and $n = 3$ gives the Heisenberg case.

For arbitrary n and d the above model Hamiltonian, (4.1), is extremely difficult to solve. However, by neglecting all 'short-range order', that is if each spin sees only the average effect of its neighbours - fluctuations about the average being ignored - one can obtain a mean field theory (MFT). It can be shown that, provided one scales the strength of the interaction by the number of spins, MFT follows from an infinite-range model which assumes

that each spin interacts with all other spins [Stanley 1971].

For clarity, the rest of this sub-section will be restricted to Ising spins (n = 1), although the concepts discussed apply equally to all values of n. Now, for suitable choices of the spatial dimensionality, d, the Ising ferromagnet has a second-order phase transition in the thermodynamic limit; at a critical temperature, T_c, the system goes from a disordered high temperature phase to an ordered low temperature phase with a non-zero order parameter. For the ferromagnet the order parameter is the magnetization per spin, m:

$$m = N^{-1} \sum_{i=1}^{N} \langle S_i \rangle_T \tag{4.3}$$

where $\langle ... \rangle_T$ denotes a thermal average and N is the number of spins. One then has

$$\begin{aligned} m &= 0 \quad \text{for } T > T_c \\ &\neq 0 \quad \text{for } T < T_c. \end{aligned} \tag{4.4}$$

Further, for $|T_c - T| \ll 1$ the order parameter obeys [Stanley 1971]

$$m \sim |T_c - T|^{\beta}, \tag{4.5}$$

thereby defining a critical exponent β. Above T_c the susceptibility conjugate to the order parameter, that is

$$\chi = \lim_{h \to 0} \frac{\partial m}{\partial h} , \tag{4.6}$$

diverges as $T \to T_c$; in fact, one defines a critical exponent γ by

$$\chi \sim (T-T_c)^{-\gamma} \quad . \tag{4.7}$$

We also define the correlation function, $\Gamma(r)$, by

$$\Gamma(r) = \langle S(r)S(0) \rangle_T \tag{4.8}$$

where r is the spatial distance. In the disordered state ($T > T_c$) correlations decay exponentially:

$$\lim_{r\to\infty} \Gamma(r) \sim e^{-r/\xi} \quad ; \tag{4.9}$$

here ξ is a correlation length.

As $T \to T_c$ the variation of ξ yields yet another exponent ν:

$$\xi \sim (T-T_c)^{-\nu} \quad . \tag{4.10}$$

Exactly at T_c correlations decay with a power law as

$$\lim_{r\to\infty} \Gamma(r)_{T=T_c} \sim r^{-(d-2+\eta)} \quad , \tag{4.11}$$

where η is another critical exponent,

whereas in the ordered phase ($T < T_c$) one has

$$\lim_{r\to\infty} \Gamma(r) = \text{const} \neq 0. \tag{4.12}$$

In MFT, which predicts $T_c = zJ$, the exponents mentioned above assume

their mean field values [Stanley 1971]: (See later for z_c)

$$\beta = \frac{1}{2} , \gamma = 1, \nu = \frac{1}{2} , \eta = 0. \tag{4.13}$$

However, by introducing the renormalization group technique, Wilson and Kogut (1974) have shown that for a given spin dimensionality, n, MFT is qualitatively valid only for space dimensionalities greater than four; that is, although fluctuations reduce T_c from its mean field value for $d > 4$, the critical exponents take on their mean field values. We call $d = 4$ the 'Upper Critical Dimensionality' (UCD). At or below four dimensions one has non-mean field exponents. As mentioned above, the fluctuations reduce T_c; the dimension (d) at which the ordering is completely destroyed is known as the 'Lower Critical Dimensionality' (LCD).

The Ising ferromagnet in one dimension ($n = d = 1$) does not order at any finite T_c (that is, $T_c = 0$) [Ising 1925]. The two-dimensional case was solved by Onsager (1944) and has a transition at $T_c = 2J[\ln(1 + \sqrt{2})]^{-1}$. Thus, for the Ising ferromagnet LCD = 1.

For the one-dimensional model with vector spins, which was solved by Fisher (1964) for the Heisenberg case ($n = 3$) and by Stanley (1969) for arbitrary n, $T_c = 0$. The two-dimensional planar model ($n = d = 2$) is a special case because it has a Kosterlitz-Thouless transition [Kosterlitz & Thouless 1973]: although there is a transition at a finite T_c, the system does not order. That is, the susceptibility is infinite below T_c but the order parameter vanishes. For $d = 2$, $n > 2$ it is known that there is no transition at any finite temperature, while there is a finite temperature transition for $n \geq 2$, $d \geq 3$. So, for the vector ferromagnet ($n \geq 2$) the LCD = 2.

From the above discussion it is apparent that MFT is qualitatively invalid at or below the LCD.

We note that although the LCD of the Heisenberg ferromagnet (n = 3) is two, it nevertheless has a 'zero-temperature phase transition' ($T_c = 0$) in one-dimension.

2. The Edwards-Anderson model

The SK spin-glass investigated in the previous two chapters is physically unacceptable as any given spin interacts with all other spins of the system. Its solution provides a mean field theory of spin-glasses.

As discussed in Chapter I, the Edwards-Anderson (EA) model (1975) is widely accepted to be a realistic theoretical model of spin-glasses; it contains the two ingredients thought to be essential for a system to exhibit spin-glass behaviour, namely both disorder and frustration. [See Chapter I for further details.] The Hamiltonian of the EA model is given by (4.1):

$$H = - \sum_{\langle ij \rangle} J_{ij} \underline{S}_i \cdot \underline{S}_j \qquad (4.14)$$

where the n-component classical spins, $\underline{S}_i$, are once again situated on the sites of a d-dimensional hypercubic lattice and the quenched interactions $\{J_{ij}\}$ act between nearest neighbours only. The models considered usually have either a Gaussian distribution, that is the bonds $\{J_{ij}\}$ are drawn from

$$P(J_{ij}) = \frac{1}{J\sqrt{2\pi}} \exp \{-J_{ij}^2/2J^2\} , \qquad (4.15)$$

or a binary distribution, that is

$$P(J_{ij}) = \frac{1}{2}\,\delta(J_{ij} - J) + \frac{1}{2}\,\delta(J_{ij} + J). \tag{4.16}$$

Once again without loss of generality, we shall restrict the present discussion to Ising spins; the case of planar spins is dealt with in Section B.

Defining the magnetization per spin, m, by

$$m = N^{-1} \sum_{i=1}^{N} \langle\langle S_i \rangle_T \rangle_J \tag{4.17}$$

and an order parameter ('statistical mechanics'), q, by

$$q = N^{-1} \sum_{i=1}^{N} \langle\langle S_i \rangle_T^2 \rangle_J \quad , \tag{4.18}$$

where $\langle \ldots \rangle_J$ denotes an average over the bond distribution, Edwards and Anderson (1975) suggested that in the thermodynamic limit one could obtain a phase transition from a disordered ($m = q = 0$) high temperature phase to a low temperature spin-glass phase with a non-zero order parameter: $m = 0$, $q \neq 0$ ($T < T_c$).

As with the ferromagnet, one can define critical exponents for the Edwards-Anderson spin-glass. The order parameter is expected to obey

$$q \sim |T_c - T|^{\beta_{SG}} \quad \text{for } |T_c - T| \ll 1. \tag{4.19}$$

As the magnetization is also given by [Stanley 1971]

$$m = - \left\langle \frac{\partial F}{\partial h} \right\rangle_J \quad , \tag{4.20}$$

where F is the free energy per spin and h is a uniform external

field, we can use the method described in Chapter II to expand the right-hand side of (4.20) as a power series in h. Thus, using (2.28) in (4.20) we have that

$$m = \chi_0 h - \chi_{n\ell} h^3 + \ldots \tag{4.21}$$

where χ_0, the zero-field susceptibility, is given by

$$T\chi_0 = N^{-1} \sum_{i,j} \langle\langle S_i S_j \rangle_{c_0} \rangle_J \quad , \tag{4.22}$$

and $\chi_{n\ell}$, the non-linear susceptibility, by

$$T^3 \chi_{n\ell} = \frac{-1}{6N} \sum_{i,j,k,\ell} \langle\langle S_i S_j S_k S_\ell \rangle_{c_0} \rangle_J \quad . \tag{4.23}$$

[Here $\langle \ldots \rangle_{c_0}$ denotes a cumulant average in zero field - see Chapter II for further details.] For systems with a symmetric bond distribution the non-linear susceptibility becomes [Suzuki & Miyashita 1981; Kinzel & Binder 1983]

$$T^3 \chi_{n\ell} = N^{-1} \sum_{i,j} \langle\langle S_i S_j \rangle_T^2 \rangle_J - \frac{2}{3} \, . \tag{4.24}$$

The first term on the right-hand side of (4.24) is defined to be the 'spin-glass susceptibility', χ_{SG}:

$$\chi_{SG} = N^{-1} \sum_{i,j} \langle\langle S_i S_j \rangle_T^2 \rangle_J \tag{4.25}$$

$$= T^3 \chi_{n\ell} + \frac{2}{3} \, . \tag{4.26}$$

One now identifies the spin-glass correlation function, $\Gamma_{SG}(r)$, as

$$\Gamma_{SG}(r) = \langle\langle\, S(r)S(0)\,\rangle_T^2\,\rangle_J \quad , \tag{4.27}$$

which is assumed to behave as

$$\Gamma_{SG}(r) \sim r^{-(d-2+\eta_{SG})}\; e^{-r/\xi_{SG}} \; ; \tag{4.28}$$

here ξ_{SG} is the spin-glass correlation length and η_{SG} is a critical exponent. Further, from (4.25), (4.27) and (4.28) one gets on approximating the sum by an integral

$$\chi_{SG} \sim \int_0^{\xi_{SG}} \Gamma_{SG}(r) \times r^{d-1}\, dr \tag{4.29}$$

$$\sim \int_0^{\xi_{SG}} r^{1-\eta_{SG}} \times e^{-r/\xi_{SG}}\, dr \tag{4.30}$$

$$\sim \int_0^{\xi_{SG}} r^{1-\eta_{SG}} \times \left(\sum_{n=0}^{\infty} \frac{1}{n!} (-r/\xi_{SG})^n \right) dr \tag{4.31}$$

$$\sim \xi_{SG}^{2-\eta_{SG}} \quad . \tag{4.32}$$

As $T \to T_c$ the behaviour of χ_{SG} and ξ_{SG} is assumed to be given by

$$\chi_{SG} \sim (T - T_c)^{-\gamma_{SG}} \tag{4.33}$$

and

$$\xi_{SG} \sim (T - T_c)^{-\nu_{SG}} \quad . \tag{4.34}$$

From (4.32), (4.33) and (4.34) one obtains the scaling relation

$$\gamma_{SG} = \nu_{SG}(2 - \eta_{SG}). \tag{4.35}$$

One also has from (4.18) and (4.27) that

$$\lim_{r\to\infty} \Gamma_{SG}(r) = q^{(2)} \geq q^2, \tag{4.36}$$

where $q^{(2)}$ is given by (2.20) and the inequality holds in the 'replica symmetry broken' situation [Young et al. 1984]. Combining (4.29) and (4.36), one gets that

$$\chi_{SG} \sim \int_0^{\xi_{SG}} q^2 \times r^{d-1}\, dr \tag{4.37}$$

$$\sim q^2\, \xi^d, \tag{4.38}$$

which yields on using (4.19), (4.33) and (4.34) the hyperscaling relation

$$\beta_{SG} = \frac{1}{2}\,(d\nu_{SG} - \gamma_{SG}) \tag{4.39}$$

$$= \frac{\nu_{SG}}{2}\,[d - 2 + \eta_{SG}], \tag{4.40}$$

where we have used (4.35).

As with the ferromagnet one can evaluate a mean field theory of spin-glasses [SK 1975]. The mean field values of the exponents defined above are [Harris et al. 1976]

$$\beta_{SG} = 1,\ \gamma_{SG} = 1,\ \nu_{SG} = \frac{1}{2},\ \eta_{SG} = 0. \tag{4.41}$$

We are also interested in the dynamical behaviour of the model. At a finite temperature transition one expects the relaxation

time, τ, to exhibit "ordinary" critical slowing down [Hohenberg & Halperin 1977]:

$$\tau \sim \xi_{SG}^{z_{SG}} , \tag{4.42}$$

where z_{SG} is a dynamic exponent. Combining equations (4.34) and (4.42) gives that as $T \to T_c$

$$\tau \sim (T - T_c)^{-\nu_{SG} z_{SG}} . \tag{4.43}$$

Near a zero-temperature phase transition, however, one expects the system to go between ordered states via thermal activation over energy barriers, ΔE [Bruce & Wallace 1981, 1983]. So, if we assume that the heights of the energy barriers depend on the correlation length, we have that [Binder & Young 1984]

$$\tau \sim e^{\Delta E(\xi_{SG})/T} . \tag{4.44}$$

Therefore

$$\ln \tau \sim \Delta E(\xi_{SG})/T \tag{4.45}$$

$$\sim T^{-1} \times \xi_{SG}^{z_{SG} - 1/\nu_{SG}} \tag{4.46}$$

$$\sim T^{-\nu_{SG} z_{SG}} . \tag{4.47}$$

Van Hove theory predicts that $z_{SG} = 2(2 - \eta_{SG})$ [Zippelius 1984].

In the next sub-section we discuss the role of critical dimensions in spin-glasses.

3. Critical dimensions

A naive value for the UCD for spin-glasses can be obtained by determining the critical dimension, d_c, for which the hyper-scaling relation, (4.40), holds exactly with mean field exponents, (4.41) [Wilson & Kogut 1974]. This approach clearly gives six as the UCD for the spin-glass problem. However, Green et al. (1983), using a field-theory formulation for the Ising spin-glass, have suggested that the SK solution is invalid for $d < 8$.

In order to determine the LCD Fisch and Harris (1977) performed a high-temperature series expansion for the spin-glass susceptibility for the random (±J) Ising spin-glass. Although this series has been re-analysed recently for $d = 3$ by Palmer and Bantilan (1984), it is highly irregular and as a consequence it is not possible to give a definitive answer for the LCD. Fisch and Harris (1977), however, did find that the critical exponent, γ_{SG}, diverged in four dimensions. Further, Bray and Moore (1979) used the replica method to perform perturbation theory for the order parameter. As their solution became unstable for $d \leqslant 4$, four was suggested as the LCD for the Ising spin-glass.

Reed (1978) repeated the analysis of Fisch and Harris (1977) for the n-component spin-glass with Gaussian couplings, (4.15). Once again, the LCD was interpreted to be four.

As the above analytic results are somewhat tentative, one has to resort to numerical techniques to pursue the problem further.

It should be noted that precisely at the LCD the correlation length, ξ_{SG}, is expected to behave as [McMillan 1984a]

$$\xi_{SG} \sim e^{A/T^{\rho_{SG}}} \tag{4.48}$$

where ρ_{SG} is now the critical exponent. We see from (4.32), (4.42) that one then expects both χ_{SG} and τ to have the same critical exponent as ξ_{SG}, that is

$$\chi_{SG} \sim e^{B/T^{\rho_{SG}}} \tag{4.49}$$

and

$$\tau \sim e^{C/T^{\rho_{SG}}} . \tag{4.50}$$

In the next sub-section the various numerical approaches used to study the Ising spin-glass are discussed.

4. The Ising spin-glass

The one-dimensional (d = 1) case has no frustration [see Chapter I] and consequently is uninteresting.

As mentioned in Section A.2 of this chapter, one normally works with either Gaussian or random couplings. These models are probably in different universality classes [Morgenstern & Binder 1980a; Cheung & McMillan 1983a,b].

The two-dimensional Ising spin-glass was studied by Morgenstern and Binder (1979, 1980a) by a transfer-matrix method. They found that both the Gaussian and the random ($\eta_{SG} = 0.4 \pm 0.1$) models have a zero-temperature phase transition. However, whereas there is no order at T = 0 in the ±J spin-glass, for a continuous bond distribution there is a discontinuity at zero temperature in the order-parameter; one goes from a disordered state to a state with non-zero order parameter. Thus, from (4.19)

one has that $\beta_{SG} = 0$, and consequently from (4.40) that $\eta_{SG} = 0$ for Gaussian bonds in two-dimensions.

The static behaviour of the d = 2, ±J model has also been studied by Monte Carlo simulations [Young 1983, 1984; McMillan 1983] and by a method combining the ideas of transfer-matrix with those of finite size scaling [Cheung & McMillan 1983a]. These studies confirm that $T_c = 0$ for this model.

The two-dimensional model with Gaussian bonds has been considered by Bray and Moore (1984a), and by McMillan (1984b,c). Whereas Bray and Moore (1984a) considered the scaling of the effective couplings at zero temperature with the sample size, McMillan (1984b,c) presented a domain-wall renormalization-group argument; Cheung and McMillan (1983b) have also investigated a two-dimensional model with the bonds drawn from a rectangular distribution. Once again, a zero-temperature phase transition is predicted. The various critical exponents that were obtained by the above authors are tabulated in Chapter I (Section D).

Young (1983, 1984) and McMillan (1983) have also studied the dynamical behaviour of the d = 2, ±J model. Whereas Young (1983, 1984) found that

$$\Delta E \propto T^{-1} \text{ as } T \to 0 \qquad (4.51)$$

(here ΔE is a characteristic energy barrier), McMillan (1983) suggested that at low temperatures $\Delta E \to 14.16J$. The Monte Carlo simulation of the 2D Gaussian Ising spin-glass by Nemoto and Takayama (1983) is not inconsistent with (4.51). So, although one can interpret the data available for the 2D Ising spin-glass in terms

of a zero-temperature phase transition [Binder & Young 1984], there is some controversy concerning its dynamics.

Recent numerical work would appear to suggest that the 3D Ising spin-glass has a transition at a finite temperature. Monte Carlo simulations of the d = 3, ±J model by Bhatt and Young (1984) suggest a transition at T_c = (1.15 ± 0.15)J, while Ogielski and Morgenstern (1984) find evidence for T_c = (1.22 ± 0.04)J. Further, Bray and Moore (1984b) and McMillan (1984d) - by extending their work on the Gaussian Ising spin-glass to three-dimensions - propose that T_c = 0.85 and T_c = 1.0 ± 0.2, respectively [see Chapter I (Section D.2)].

If the above prediction of a finite-temperature transition is correct, it would mean that the LCD for the Ising spin-glass lies between 2 and 3, which disagrees with the value of 4 (see Section A.3, this chapter). It would, however, be consistent with the real-space renormalization group calculation [Young & Stinchcombe 1976; Southern and Young 1977].

Clearly, as the LCD of vector spin-glasses is also predicted to be 4, one would like to investigate the outcome of increasing the spin components. Although the random Ising model has been given considerable attention, the same cannot be said of n-component models. The rest of this chapter is concerned with 2-component ('planar' or 'X-Y') spins.

The pure X-Y model undergoes a Kosterlitz-Thouless transition in 2D [Kosterlitz & Thouless 1973]: although the susceptibility diverges at a critical temperature, T_c, the order parameter vanishes for all non-zero temperatures.

By introducing the concept of 'chirality' Villain (1977a,b) has shown that the disordered (random-bond) 2D, X-Y model is

equivalent at low temperatures to an Ising model with Coulombic interactions. [The 'chirality' indicates the direction in which the spins rotate as one moves clockwise around a frustrated (see Chapter I) plaquette (square).] From a consideration of the spin-spin correlation functions, Jose (1978) has suggested that the 2D, random X-Y model does not have a phase transition at any finite temperature. On the other hand, Shastry (1979) claims that there should be a transition à la Kosterlitz-Thouless (1973).

The only Monte Carlo simulations of the X-Y spin-glass performed to date [Binder & Kinzel 1981; Stauffer & Binder 1981] suggest that the Edwards-Anderson order-parameter vanishes in two- and three-dimensions for all non-zero temperatures.

The rest of this chapter is concerned with the results of extensive Monte Carlo simulations of X-Y spin-glasses in two and three spatial dimensions.

Section B: The Model

1. The X-Y spin-glass

The results discussed in this section were obtained on the DAP (Distributed Array Processor) by performing Monte Carlo simulations using the conventional Metropolis [Metropolis et al. 1953] method of updating each spin. [The Monte Carlo method is discussed in Appendix III and the DAP in Appendix V.]

The Hamiltonian of the X-Y spin-glass in zero magnetic field is given by

$$H = - \sum_{\langle ij \rangle} J_{ij} \underline{S}_i . \underline{S}_j \quad , \quad |\underline{S}_i| = 1, \; k_B = 1; \tag{4.52}$$

here $\langle \ldots \rangle$ indicates a summation over nearest neighbours only and the planar spins, $\underline{S}_i$, occupy the sites of a regular lattice; we shall consider both a square and a cubic lattice. The interactions $\{J_{ij}\}$ are selected from a binary distribution, (4.16), with J set to unity, that is

$$P(J_{ij}) = \frac{1}{2}\,\delta(J_{ij} - 1) + \frac{1}{2}\,\delta(J_{ij} + 1). \tag{4.53}$$

This choice for the bond distribution is extremely convenient when we come to perform the sum in (4.52) on the DAP [see Appendix V for further details].

As we shall only consider a continuous model, each spin is categorised by just one polar angle θ_i [see Figure 4.1a]:

$$\underline{S}_i = (\cos\theta_i, \sin\theta_i) \equiv (S_i^1, S_i^2). \tag{4.54}$$

From (4.52) and (4.54) we see that the Hamiltonian can be written as

$$H = -\sum_{\langle ij \rangle} J_{ij} \cos(\theta_i - \theta_j). \tag{4.55}$$

An alternative approach would be to consider a discrete vector model (the 'clock-model'). Although such a modification would probably speed up the simulation [Suzuki et al. 1977] at fairly high temperatures, it is, nevertheless, dangerous at low temperatures and also near a possible phase transition [Miyashita et al. 1978].

We shall only consider lattices with a linear dimension L = 16, and employ periodic boundary conditions in all directions.

As we are working with nn interactions only, we can regard the lattice as being composed of two sub-lattices [see Figure 4.1b] and perform the Monte Carlo process [see Appendix III] simultaneously on all of the sites of one sub-lattice. An iteration throughout the whole lattice - that is, both sub-lattices - is defined to be a MCS/spin (Monte Carlo Step/spin) and is identified as time in the simulation; in the subsequent discussion time, t, and MCS/spin are used interchangeably.

For any given temperature, T, we start the simulation with all of the spins parallel, that is $\theta_i = 0$ for all i. The number of MCS/spin it takes for the system to equilibrate is discarded and the equilibrium configuration is taken as the initial state of the system.

In the next sub-section we discuss how one decides whether the system is in equilibrium or not and also the various quantities one measures.

2. Statics and dynamics

The quantities we are interested in were mentioned in the introductory section of this chapter (Section A.2).

In order to investigate the equilibrium behaviour of the system we first look at the autocorrelation function, q(t), which is defined by

$$q(t) = N^{-1} \sum_{i=1}^{N} \underline{S}_i(t_0) . \underline{S}_i(t + t_0) \tag{4.56}$$

$$= N^{-1} \sum_{i=1}^{N} \sum_{\alpha=1}^{2} S_i^{\alpha}(t_0) S_i^{\alpha}(t + t_0), \tag{4.57}$$

where N is the number of spins (N = 256 for 2D and N = 4096 for the 3D case), t_0 is an initial equilibration time as discussed in the previous section, t is a later time and we have also made use of definition (4.54). At any given temperature, T, we perform a preliminary simulation in order to determine the time, τ_0, it takes for q(t) to reach its equilibrium value and then we choose $t_0 \geq \tau_0$, à posteriori.

Now, for $t \to \infty$ (in practice for $t > \tau_0$) (4.56) becomes

$$\lim_{t\to\infty} q(t) = N^{-1} \sum_{i=1}^{N} \langle\langle \underline{S}_i \rangle_T \cdot \langle \underline{S}_i \rangle_T \rangle_J \tag{4.58}$$

$$= q_{EA} \quad , \tag{4.59}$$

the Edwards-Anderson order parameter (1.8). Note that the Monte Carlo method simulates thermal averages by time averages and configurational averages by spatial integration [see Appendix III].

As we are working with a finite system in zero field, the Edwards-Anderson order parameter vanishes in equilibrium [see Chapter II]. So

$$\lim_{t\to\infty} q(t) = 0. \tag{4.60}$$

Thus, q(t), which is initially one, decreases with t and eventually reaches zero after a time τ_0; only when q(t) is consistently zero can we be sure that equilibrium has been achieved [see Figure 4.2]. As our initial (t = 0) and final ($t \geq \tau_0$) states are equilibrium states, τ_0 gives us an indication of the longest relaxation times of the system.

Information concerning the spatial range of correlations can be extracted from the spin-glass susceptibility, χ_{SG}, which is a four-spin correlation function. For our model the time-dependent version, $\chi_{SG}(t)$, is defined by

$$\chi_{SG}(t) = \frac{1}{N} \sum_{i,j} \underline{S}_i(t_0).\underline{S}_j(t_0)\underline{S}_i(t+t_0).\underline{S}_j(t+t_0) \tag{4.61}$$

$$= N^{-1} \sum_{\substack{i,j \\ \alpha,\beta}} S_i^{\alpha}(t_0)S_j^{\alpha}(t_0)S_i^{\beta}(t+t_0)S_j^{\beta}(t+t_0) \tag{4.62}$$

$$= N^{-1} \sum_{\alpha,\beta=1}^{2} \left(\sum_{i=1}^{N} S_i^{\alpha}(t_0)S_i^{\beta}(t+t_0) \right)^2 . \tag{4.63}$$

We evaluate $\chi_{SG}(t)$ in the form given by (4.63). After a sufficiently long time (once again, in practice for $t > \tau_0$) the spins lose the memory of their states at t_0 and $\chi_{SG}(t)$ becomes independent of time, that is

$$\chi_{SG}(t) \xrightarrow{t\to\infty} \chi_{SG} = N^{-1} \sum_{i,j} \langle\langle \underline{S}_i.\underline{S}_j \rangle_T^2 \rangle_J . \tag{4.64}$$

We also obtain the correlation length, ξ_{SG}, from a suitable correlation function. As we are working with a random system, one expects the correlations to be independent of the spatial direction. So, we calculate the correlations, $\Gamma_{SG}(n)$, between single spins, where

$$\Gamma_{SG}(n) = N^{-1} \sum_{i=1}^{N} \langle\langle \underline{S}_i.\underline{S}_{i+n} \rangle_T^2 \rangle_J \tag{4.65}$$

and here n indicates the displacement in the chosen direction; for the 2D model we examine correlations between spins in the

y-direction, whereas for the 3D case we investigate spins in the z-direction.

As we are also interested in the dynamical behaviour of the system, we also measure an 'average relaxation time', τ. This is conveniently extracted from the autocorrelation function (4.56) [Nemoto & Takayama 1983; Young 1983]. Now, (4.56) can be written as

$$q(t) = N^{-1} \sum_{i=1}^{N} C_i(t) \tag{4.66}$$

where

$$C_i(t) = \underline{S}_i(t_0).\underline{S}_i(t + t_0). \tag{4.67}$$

So, if one makes the ansatz that $C_i(t)$ decays as

$$C_i(t) = P_i e^{-t/\tau_i}, \tag{4.68}$$

where τ_i is the relaxation time and P_i is a constant, then (4.66) becomes

$$q(t) = N^{-1} \sum_{i=1}^{N} P_i e^{-t/\tau_i} \tag{4.69}$$

$$= \int_0^\infty P(\tilde{\tau}) e^{-t/\tilde{\tau}} \, d\tilde{\tau} \tag{4.70}$$

and here

$$P(\tilde{\tau}) = N^{-1} \sum_{i=1}^{N} P_i \delta(\tilde{\tau} - \tau_i) \tag{4.71}$$

is a spectrum of relaxation times. It then follows that one can define an average relaxation time, τ, by

$$\tau = \int_0^\infty q(t)\, dt \tag{4.72}$$

$$= \int_0^\infty P(\tilde{\tau})d\tilde{\tau} \int_0^\infty e^{-t/\tilde{\tau}}\, dt \tag{4.73}$$

$$= \int_0^\infty \tilde{\tau}P(\tilde{\tau})\, d\tilde{\tau}. \tag{4.74}$$

Note that although the upper limit of integration in (4.72) is infinity, in practice, as mentioned above,

$$q(t) = 0 \quad \text{for } t > \tau_0. \tag{4.75}$$

So, the quantity we actually measure is

$$\tau = \int_0^{\tau_0} q(t)\, dt \tag{4.76}$$

$$\simeq \sum_{t_i=0}^{\tau_0} q(t_i)\ , \tag{4.77}$$

where we replace the integral by a sum.

It should be mentioned at this stage that whereas the Ising model does not have any intrinsic dynamics and, consequently, one can interpret the time arising in the Monte Carlo method [see Appendix III] as the sole dynamics of the system, the X-Y spin-glass <u>does</u> have a relaxational dynamics which could be described by, say, a Langevin equation. In our algorithm we do <u>not</u> incorporate

this relaxational dynamics explicitly but expect the time in the Monte Carlo process to describe qualitatively the dynamical behaviour of the model.

So, we investigate four quantities: $q(t)$, χ_{SG}, $\Gamma_{SG}(n)$ and τ. These are measured for a given sample, that is, a particular choice of interactions $\{J_{ij}\}$ and then re-measured for a different sample; the values quoted in the subsequent sections of this chapter are averages over the stated number of samples. Further, from the sample-to-sample variation we are able to evaluate statistical error-bars by using [Meyer 1969]

$$\text{Error-bars} = \pm \sqrt{\left\{ \frac{\langle X^2 \rangle_{NS} - \langle X \rangle_{NS}^2}{NS - 1} \right\}}, \qquad NS > 1 \qquad (4.78)$$

where NS is the number of samples and $\langle X \rangle_{NS}$ denotes an average over samples of the quantity 'X'.

Next, we briefly discuss some of the ways in which we check the computer program.

3. Checks on the program

In order to check the program we also measure the energy per spin, U/N, the specific heat per spin, C/N, the magnetization per spin, $\underset{\sim}{M}$/N, and the susceptibility per spin, χ/N.

The energy is given by [Stanley 1971]

$$U = \langle \langle H \rangle_T \rangle_J \qquad (4.79)$$

where the Hamiltonian is given by (4.52); one then obtains the specific heat from the fluctuations in the energy:

$$T^2C = \langle\langle H^2 \rangle_T - \langle H \rangle_T^2 \rangle_J \quad . \tag{4.80}$$

As we are working with a vector model, the magnetization has two components:

$$\underset{\sim}{M} = \sum_{i=1}^{N} \langle\langle \underline{S}_i \rangle_T \rangle_J \ , \qquad \underline{S}_i = (S_i^1, S_i^2). \tag{4.81}$$

From the fluctuations in the magnetization one obtains the susceptibility:

$$T\chi = \langle\langle \left(\sum_{i=1}^{N} \underline{S}_i\right) \cdot \left(\sum_{j=1}^{N} \underline{S}_j\right) \rangle_T - \langle \sum_{i=1}^{N} \underline{S}_i \rangle_T \cdot \langle \sum_{j=1}^{N} \underline{S}_j \rangle_T \rangle_J \ . \tag{4.82}$$

Now, substituting (4.52) into (4.79) gives

$$U = - \langle\langle \sum_{\langle ij \rangle} J_{ij} \underline{S}_i \cdot \underline{S}_j \rangle_T \rangle_J \tag{4.83}$$

$$\Rightarrow \quad U/N = - \frac{Z_c}{2} \langle\langle J_{ij} \underline{S}_i \cdot \underline{S}_j \rangle_T \rangle_J \tag{4.84}$$

where i,j are nearest neighbours, Z_c is the co-ordination number ($Z_c = 4$ in 2D and $Z_c = 6$ in 3D) and we have to divide by 2 because each bond connects 2 sites. Using the definition

$$\langle J_{ij} \underline{S}_i \cdot \underline{S}_j \rangle_T = \frac{\mathrm{Tr}(J_{ij} \underline{S}_i \cdot \underline{S}_j e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} \quad , \quad \beta = 1/T, \tag{4.85}$$

we perform a high temperature expansion for the energy; this involves expanding the exponentials in (4.85) and explicitly performing both the trace and the average over the $\{J_{ij}\}$ [Stanley 1971]. One finds that

$$U/N = -\frac{z_c}{2}\left(\frac{\beta}{2} - \frac{\beta^3}{16}\right) + \ldots \quad . \tag{4.86}$$

Further, we also have that [Stanley 1971]

$$T^2C/N = -\frac{dU}{d\beta} \tag{4.87}$$

$$= \frac{z_c}{4} - \frac{3z_c\beta^2}{32} + \ldots \quad . \tag{4.88}$$

As we are working in zero field, we expect the magnetization to vanish, that is

$$\underset{\sim}{M} = \underset{\sim}{0} \; . \tag{4.89}$$

Since

$$\langle \underline{S}_i \cdot \underline{S}_j \rangle_T = \frac{\mathrm{Tr}(\underline{S}_i \cdot \underline{S}_j e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} \qquad \text{(all i,j)}, \tag{4.90}$$

we can repeat the above calculation to obtain a high temperature expansion for the spin-glass susceptibility (4.64):

$$\chi_{SG} = 1 + z_c\left(\frac{\beta}{2}\right)^2 + z_c(z_c-1)\left(\frac{\beta}{2}\right)^4 + \ldots \; ; \tag{4.91}$$

and for the susceptibility (4.82):

$$T\chi/N = 1 + \ldots \quad . \tag{4.92}$$

Note that by setting the second term in (4.91) to one we obtain the mean field critical temperature, $M_F(T_c)$, viz.

$$M_F(T_c) = \sqrt{\frac{Z_c}{4}} \qquad \text{(in units of J)} \tag{4.93}$$

$$= \begin{cases} 1 & \text{(2D)} \\ \sqrt{3/2} & \text{(3D)} \ . \end{cases} \tag{4.94}$$

Using (4.86), (4.88), (4.89), (4.91) and (4.92) we first verify that the simulation gives the expected results - within the statistical error-bars - at relatively high temperatures and only then do we go down to lower temperatures.

In two-dimensions we are interested in whether there is a transition à la Kosterlitz-Thouless [Kosterlitz & Thouless 1973], that is, we would like to know if χ_{SG}, (4.64), diverges at a finite T_c. Further, as the two-dimensional Ising spin-glass relaxes by activation over energy barriers [Young 1983, 1984; McMillan 1983; Nemoto & Takayama 1983], we are also interested in the analogous behaviour for X-Y spin-glasses; in general, we want to compare X-Y spin-glasses with their Ising counterparts.

In the next section we discuss the results for the square lattice.

Section C: Results for the Square Lattice

1. The data

In this section we discuss the two-dimensional case, working with a 16 × 16 lattice.

The program was checked (see the previous section) by performing simulations at temperatures T = 5.0, 4.0, 3.0 and 2.0; the results that were obtained for χ_{SG} for $0.25 \leqslant T \leqslant 1.4$ and for τ for $0.35 \leqslant T \leqslant 1.4$ are tabulated below in Table 4.1.[ξ_{SG} is dealt with separately.] For low temperatures, namely T = 0.25 and 0.30,

Table 4.1

DATA FOR χ_{SG} AND τ (2D)

T/J	Total number of MCS/spin	Number of MCS/spin needed to equilibrate	Samples	χ_{SG} ± error	τ ± error
1.4	300	100	240	1.64 ± 0.01	3.60 ± 0.10
1.2	300	100	240	1.96 ± 0.02	4.90 ± 0.15
1.0	300	100	448	2.58 ± 0.02	8.49 ± 0.15
0.9	600	200	240	3.19 ± 0.05	12.35 ± 0.30
0.8	1200	400	352	3.82 ± 0.05	21.28 ± 0.65
0.7	1290	440	240	4.85 ± 0.09	38.80 ± 1.35
0.6	4500	1500	288	6.69 ± 0.12	87.25 ± 5.00
0.5	6000	2000	144	9.14 ± 0.26	221.41 ± 15.30
0.45	9000	3000	64	11.59 ± 0.46	340.00 ± 50.00
0.40	10500	3500	128	13.86 ± 0.45	624.89 ± 49.70
0.35	22500	7500	80	19.05 ± 0.96	1300.61 ± 127.10
0.30	33000	14000	32	21.67 ± 1.32	
0.25	45000	20000	64	29.78 ± 1.59	

the statistical errors in q(t) do not allow us to evaluate a meaningful value for τ. For temperatures lower than 0.25 the system does not achieve equilibrium within the available computer time [see Appendix V].

At the lowest temperature we are able to simulate we discard

the first 20,000 MCS/spin in order to equilibrate the system and then perform a further 25,000 MCS/spin; information concerning the statics is extracted by averaging over the final 5,000 MCS/spin. It took approximately 5 mS to perform 1 MCS/spin and at the lowest temperature simulated, on average, $17\frac{1}{2}\%$ of the lattice was updated on each occasion.

The results quoted in Table 4.1 were obtained with an unrestricted 'acceptance angle' [see Appendix III], that is, during the Monte Carlo simulation the updated angle for any given spin was allowed to lie anywhere within the circle. Restricting the acceptance angle at low temperatures, namely for $T \leqslant 0.35$, did not speed up the simulation appreciably. For example, for $T = 0.35$ the acceptance angle was restricted to 10%, 25%, 50% and 75% of the circle and the number of MCS/spin that were required for the system to equilibrate ranged from 6,000 to 8,000.

We analyse the data for $T \leqslant 1.0$ [note that this is the mean field critical temperature for this model (4.94)] by using the chi-squared (χ^2) test [see Appendix IV]. Throughout the next two sections we shall frequently refer to a "good" fit and, whenever appropriate, also quote error-bars; both of these quantities are defined by values of χ^2 less than $2\chi^2_{min}$, where χ^2_{min} is the absolute minimum in χ^2, or by the 75% confidence level in question, whichever is smaller [see Appendix IV for further details].

We now discuss the results of the analysis.

2. Statistical analysis

a. The spin-glass susceptibility, χ_{SG}

We first investigate whether the data is consistent with (4.33) or not. As we are working at relatively high temperatures,

we allow for a possible background, χ_0. This means that we actually try and fit the data to

$$\chi_{SG} = \chi_0 + \frac{A}{(T - T_0)^{\gamma_{SG}}} \tag{4.95}$$

where χ_0, A, T_0 and γ_{SG} are all unknowns. We are primarily interested in the values of T_0 for which there is a good fit and also in the corresponding values for the critical exponent γ_{SG}.

We first fix the background χ_0 (= χ_0') and treat A, T_0 and γ_{SG} as adjustable parameters. These are allowed to vary until a minimum in χ^2 is located [see Appendix IV]. This procedure is repeated for different backgrounds χ_0 (= χ_0'',χ_0''',...). In this way we obtain χ^2 as a function of the background χ_0. Figure 4.3a shows the variation of χ^2 with χ_0.

By considering χ_0, A and γ_{SG} as adjustable parameters for a fixed T_0, we also obtain $\chi^2(T_0)$. Figure 4.3b shows a plot of χ^2 versus T_0.

So we see from Figures 4.3a,b that we obtain a good fit for a whole range of values of T_0 and χ_0, viz. for

$$\begin{aligned} &- 2.25 \leqslant T_0 \leqslant 0.02 \quad , \\ &- 0.25 \leqslant \chi_0 \leqslant 1.68 \end{aligned} \tag{4.96}$$

and the best fit for $T_0 = - 0.30$, $\chi_0 = 0.92$. On the basis of (4.96) we rule out a finite T_c.

In Table 4.2 we tabulate some of the acceptable values for the four parameters appearing in (4.95) together with the "goodness-of-fit" (the value of χ^2) at those values, as well as the consequent χ_{SG} at T = 0.

Table 4.2

THE QUALITY OF FIT FOR VARIOUS VALUES OF T_0

T_0	χ_0	ln A	γ_{SG}	$\chi_{SG}(T=0)$	χ^2
0.0	- 0.07	0.98	1.80 ± 0.05	-	12.98
- 0.2	0.71	1.14	2.82	293.25	8.36
- 0.3	0.92	1.26	3.32	192.86	8.07
- 0.4	1.04	1.72	3.80	182.66	8.20
- 0.45	1.09	1.91	4.03	169.77	8.34

Hence, we have two possibilities: either $T_c = 0$ or χ_{SG} remains finite at $T = 0$. One way in which the latter situation could arise would be for the spin-glass susceptibility to behave as

$$\chi_{SG} = A_1 + A_2 T + A_3 T^2. \tag{4.97}$$

We note in passing that (4.97) gives an extremely poor fit to the data ($\chi^2 \simeq 6{,}000$).

We also tried fitting the data to (4.49), that is assuming that the system is at its LCD:

$$\chi_{SG} = B_1 \, e^{B_2/T^{\rho_{SG}}} \tag{4.98}$$

As the best fit to (4.98) gives $\chi^2 \simeq 17.5$ we reject this possibility too; note that in this case the quality of the fit improves as $B_1, \rho_{SG} \to 0$, which suggests that one should actually try fitting the data to (4.95).

However, the data is consistent with a zero temperature transition, in which case

$$T_c = 0.0,\ \chi_0 = -0.07,\ \ln A = 0.98 \text{ and } \gamma_{SG} = 1.80 \pm 0.05. \qquad (4.99)$$

Figure 4.4 shows a plot of the data assuming $T_c = 0$. As the linear dimension of our system is much larger than the correlation length (see sub-section 2.c of this section), one does not expect finite size effects to be relevant. However, we note that a consequence of working with a finite system is that we underestimate χ_{SG} and that any such underestimation should be most pronounced at the lowest temperatures simulated - where ξ_{SG} is biggest. This could explain the fractional deviation of the last two data points in Figure 4.4.

b. The average relaxation time, τ

As this time we have only 9 data points ($0.35 \leqslant T \leqslant 1.0$) the 75% confidence level for the χ^2-test is 11.45 [see Appendix IV]. We shall test three different hypotheses.

If the system relaxes by ordinary critical slowing down [Hohenberg & Halperin 1977] one would expect that (4.43):

$$\tau = \tau_0 + \frac{B}{(T - T_0)^{\nu_{SG} z_{SG}}} , \qquad (4.100)$$

where τ_0 (a background correction term), B, T_0 and $\nu_{SG} z_{SG}$ are unknown constants. As the values of T_0, if any, for which (4.100) gives a good fit to the data have to be consistent with the range of values, (4.96), obtained in the previous sub-section, we restrict our quest for a possible critical temperature to the range $-2.25 \leqslant T_0 \leqslant 0.05$.

Figures 4.5a,b show the variation of χ^2 with T_0 and τ_0

respectively. As the minimum in χ^2 is 2.08, a good fit is determined by those values of χ^2 less than 4.16. Thus, we obtain a good fit for a range of values of T_0 and τ_0:

$$\begin{aligned} -0.43 \leqslant T_0 \leqslant 0.05 \\ 2.05 \leqslant \tau_0 \leqslant 4.70 \quad , \end{aligned} \tag{4.101}$$

and the best fit is obtained for $\tau_0 = 3.50$, $T_0 = -0.12$.

Below, in Table 4.3, we give some of the acceptable values of the parameters in question.

Table 4.3

ACCEPTABLE FITS FOR τ

T_0	τ_0 (MCS/spin)	ln B	$\nu_{SG} Z_{SG}$	$\tau(T=0)$ ($\times 10^6$ MCS/spin)	χ^2
0.0	2.64	1.76	5.16 ± 0.18	-	2.98
- 0.12	3.50	2.32	6.35	7.16	2.08
- 0.2	3.90	2.82	7.14	1.64	2.31
- 0.3	4.27	3.57	8.11	0.62	3.00
- 0.4	4.55	4.43	9.08	0.35	3.84
- 0.45	4.66	4.90	9.56	0.28	4.29

Once again we can rule out a finite T_c. From Table 4.3 it is clear that a negative T_0, which would be the case if there were no transition at zero temperature, would result in an extremely large value for τ at $T = 0$. Further,

$$\tau = B_1 + B_2\tau + B_3\tau^2 \tag{4.102}$$

gives an extremely bad fit to the data ($\chi^2 \simeq 780{,}000$).

We also try and fit the data to (4.47), that is we assume that the system relaxes via activation over energy barriers:

$$\tau = \tau_0 \exp(E/T^{\nu_{SG} z_{SG}}) \ , \tag{4.103}$$

where τ_0, E and $\nu_{SG} z_{SG}$ are unknown constants. This time, however, the minimum in χ^2 is 9.22, which means that (4.100) gives a better fit.

Finally, we also examine the quality of the fit to the Vogel-Fulcher law [Fulcher 1925]:

$$\tau = \tau_0 \exp(E'/(T - T_0)) \tag{4.104}$$

and here τ_0, E' and T_0 are unknowns. Once again this gives a worse fit than (4.100), the minimum in χ^2 being 6.71.

Thus, we conclude that the most likely explanation of the data is in terms of a zero-temperature transition, with the system relaxing via ordinary critical slowing down. Figure 4.6 shows a plot of the data assuming that (4.100) holds with

$$T_c = 0.0, \ \tau_0 = 2.64, \ \ln B = 1.76 \text{ and } \nu_{SG} z_{SG} = 5.16 \pm 0.18. \tag{4.105}$$

We now analyse the correlation length, ξ_{SG}.

c. The correlation length, ξ_{SG}

The correlation length, $\xi_{SG}(T)$, is extracted from the correlation function $\Gamma_{SG}(n)$, (4.65).

For a given temperature T, $0.25 \leqslant T \leqslant 1.0$, we evaluate $\Gamma_{SG}(n)$, where n (n = 0,1,...,5) is the displacement in the y-direction. We then fit the data to (4.28), that is

$$\Gamma_{SG}(n) = K \frac{e^{-n/\xi_{SG}}}{n^{\eta_{SG}}} \tag{4.106}$$

where K is a constant, and η_{SG} and ξ_{SG} are critical exponents. For a given value of η_{SG} we treat K and ξ_{SG} as adjustable parameters and perform a weighted least-squares fit of the data to (4.106). The quality of the fit is then examined by using the chi-squared test on $\chi^2(\eta_{SG})$ at the 75% confidence level [see Appendix IV]. This procedure is repeated for all the temperatures. As a consequence we find that

$$\eta_{SG} = 0.3 \pm 0.3 \ , \tag{4.107}$$

where the lower value ($\eta_{SG} \simeq 0.0$) is favoured at the higher temperatures ($T \simeq 1.0$) and the middle value ($\eta_{SG} \simeq 0.3$) at the lower temperatures ($T \simeq 0.25$). In the following analysis we shall take

$$\eta_{SG} = 0.3 \ . \tag{4.108}$$

Assuming (4.108), we now extract the correlation length, $\xi_{SG}(T)$, at each of the temperatures concerned. For a given $\xi_{SG}(T)$, we now treat just K as an adjustable parameter. Once again a weighted least-squares fit of the data to (4.106) (with $\eta_{SG} = 0.3$) is performed and the fit examined via the χ^2-test on $\chi^2(\xi_{SG})$ at the 75% confidence level. The resulting values of ξ_{SG} are tabulated in Table 4.4.

Table 4.4

DATA FOR ξ_{SG} (η_{SG} = 0.3)

T/J	Samples	ξ_{SG} ± error
1.0	208	0.73 ± 0.03
0.8	112	0.94 ± 0.04
0.6	64	1.38 ± 0.07
0.5	48	1.60 ± 0.10
0.4	64	2.13 ± 0.14
0.35	48	2.58 ± 0.24
0.30	16	2.98 ± 0.47
0.25	32	3.50 ± 0.57

Once again we examine the fit of the data to a power law variation with temperature (4.34):

$$\xi_{SG} = \xi_0 + \frac{D}{(T - T_0)^{\nu_{SG}}} , \qquad (4.109)$$

with ξ_0, D, T_0 and ν_{SG} unknown. To be consistent with (4.96) and (4.101) we restrict our attention to $-0.45 \leqslant T_0 \leqslant 0.05$. Figures 4.7a,b indicate the variation of χ^2 with ξ_0 and T_0, respectively. The minimum in χ^2 is 0.845, which implies that a good fit is obtained for all values of χ^2 less than 1.69. As we can see from Figure 4.7b, the curve of $\chi^2(T_0)$ versus T_0 is extremely shallow and we are unable to improve on the range, (4.101), obtained from the analysis of the relaxation time, τ. So, one gets an acceptable fit for

$$-0.84 \leq \xi_0 \leq 0.44,$$
$$-0.43 \leq T_0 \leq 0.05; \tag{4.110}$$

the best fit is obtained for $\xi_0 = 0.00$, $T_0 = -0.06$. Clearly, (4.110) is consistent with the analysis carried out above, that is, with a zero-temperature transition. Assuming that (4.109) holds with $T_0 \equiv T_c = 0$, we get that

$$T_c = 0.0,\ \xi_0 = -0.11,\ \ln D = -0.18 \text{ and } \nu_{SG} = 1.08 \pm 0.27. \tag{4.111}$$

We plot the data in Figure 4.8 with the parameters taking on the above values.

3. Summary

In this section we presented the data for the two-dimensional X-Y spin-glass.

From a statistical analysis we have shown that there is no finite temperature transition; further, we have argued that the results are consistent with a zero-temperature transition. However, unlike the two-dimensional Ising spin-glass, we found that the system relaxes by long wavelength fluctuations, that is ordinary critical slowing down.

Assuming that $T_c = 0$, we estimate the critical exponents to be

$$\gamma_{SG} = 1.80 \pm 0.05, \quad \eta_{SG} = 0.3 \pm 0.3$$
$$\nu_{SG} = 1.08 \pm 0.27 \text{ and } \nu_{SG} z_{SG} = 5.16 \pm 0.18. \tag{4.112}$$

Section D: Results for the Cubic Lattice

1. The data

For the three-dimensional case we work with a 16^3 lattice.

Preliminary "runs" at T = 5.0, 4.0, 3.0 and 2.0 were performed to check the program [see Section B.3 of this chapter]. The results for χ_{SG} and τ for $0.65 \leqslant T \leqslant 1.75$ are tabulated in Table 4.5. [Once again we look at ξ_{SG} separately.]

Table 4.5

DATA FOR 3D (χ_{SG} and τ)

T/J	Total number of MCS/spin	Number of of MCS/spin needed to equilibrate	Samples	χ_{SG} ± error	τ ± error
1.75	300	100	115	1.75 ± 0.02	3.52 ± 0.05
1.50	300	100	135	2.09 ± 0.02	5.20 ± 0.05
1.30	620	200	125	2.74 ± 0.05	8.80 ± 0.15
1.20	620	200	125	3.43 ± 0.07	12.27 ± 0.20
1.10	640	220	95	4.36 ± 0.12	18.60 ± 0.30
1.00	2000	500	67	6.04 ± 0.17	34.62 ± 0.75
0.95	3000	1000	35	7.25 ± 0.39	48.18 ± 1.65
0.90	4000	1500	43	8.47 ± 0.34	68.26 ± 2.60
0.85	6000	2000	33	10.78 ± 0.48	104.02 ± 4.50
0.80	15000	5000	14	12.49 ± 0.75	194.60 ± 15.10
0.75	20000	7500	35	18.18 ± 0.87	308.62 ± 14.24
0.70	25000	10000	24	25.62 ± 2.12	639.82 ± 36.40
0.65	42000	18000	6	35.61 ± 7.00	1571.43 ± 376.14

At T = 0.65 a run of 42,000 MCS/spin was required, the system equilibrating after 18,000 MCS/spin. It took approximately 43 mS to perform 1 MCS/spin and, on average, 25% of the sites were updated each time at T = 0.7.

For T = 0.7 the acceptance angle was restricted to 10%, 25%, 50% and 75% of the circle and the number of MCS/spin it took the system to achieve equilibrium ranged from approximately 7,500 to 10,000. Note that the data in Table 4.5 was obtained with an unrestricted acceptance angle.

We now analyse the data for $T \leqslant 1.2$ [note that the mean field critical temperature for this model is $\sqrt{3/2}$, (4.94)] with the aid of the χ^2-test [see Appendix IV].

2. Statistical analysis

a. The spin-glass susceptibility

We first try and fit the data to (4.33), or rather to

$$\chi_{SG} = \chi_0' + \frac{A'}{(T - T_0')^{\gamma_{SG}}} \qquad (4.113)$$

where χ_0', A', T_0' and γ_{SG} are unknowns. Figures 4.9a,b exhibit the variation of χ^2 with the background, χ_0', and T_0' respectively. We see from the plots that the acceptable values of the two parameters in question are

$$\begin{aligned} -4.20 &\leqslant \chi_0' \leqslant 1.80 \\ -1.30 &\leqslant T_0' \leqslant 0.60 \quad , \end{aligned} \qquad (4.114)$$

and that one obtains the best fit for $\chi_0' = -0.05$, $T_0' = 0.475$. So, the data can be explained either in terms of a finite T_c or a zero-temperature transition. Below, in Table 4.6, we tabulate χ^2 for a few of the acceptable values of T_0'.

Table 4.6

BEST FITS FOR SOME VALUES OF T_0'(3D)

T_0'	χ_0'	A'	γ_{SG}	χ^2
0.00	1.55	4.37	4.57 ± 0.69	4.50
0.20	1.20	2.24	3.37 ± 0.49	3.91
0.40	0.45	1.85	2.14 ± 0.31	3.17
0.45	0.08	1.97	1.82 ± 0.25	3.03
0.475	- 0.20	2.13	1.66 ± 0.25	3.01
0.50	- 0.49	2.29	1.50 ± 0.22	3.05
0.55	- 1.51	3.00	1.15 ± 0.20	3.54

In Figures 4.10a,b we plot the data assuming that T_c (= T_0') = 0.0 and $T_c = 0.45$, respectively.

We now try fitting the data to (4.49):

$$\chi_{SG} = B_1' \, e^{B_2'/T^{\rho_{SG}}} \qquad (4.115)$$

that is, we assume that three is the LCD for the X-Y spin-glass. [Note that in (4.115) we have three adjustable parameters, namely B_1', B_2' and ρ_{SG}].

This time $\chi^2_{minimum} = 3.37$, which compares favourably with

the values shown in Table 4.6; at the minimum one has that

$$\ln B_1' = -1.42,\ \ln B_2' = 1.17 \text{ and } \rho_{SG} = 1.03 \pm 0.48. \qquad (4.116)$$

Figure 4.11 shows the data assuming that (4.115) and (4.116) hold.

b. The average relaxation time

We test the quality of the fit of the data for τ to the three different laws mentioned above, (4.47), (4.104) and (4.43):

$$\tau = \tau_0 \exp[E/(T-T_0')^{\nu_{SG}z_{SG}}] , \qquad (4.117a)$$

$$\tau = \tau_0 \exp[E'/(T-T_0')] \qquad (4.117b)$$

and

$$\tau = \tau_0 + \frac{B'}{(T - T_0')^{\nu_{SG}z_{SG}}} . \qquad (4.117c)$$

To be consistent with (4.114) we restrict ourselves to the range $-1.30 \leq T_0' \leq 0.6$. As we have 10 data points the appropriate 75% confidence level for the χ^2-test is 12.61.

In Figures 4.12a,b,c we plot $\chi^2(T_0')$ for the three cases mentioned above. We find that when we try and fit the data to (4.117a) $\tau_0 \to 0$ and $\nu_{SG}z_{SG} \ll 1$ for $T_0' \gtrsim 0.2$. This suggests that for this region of T_0' we should get a good fit with (4.117c), which is confirmed by Figure 4.12c. It is apparent from Figures 4.12a,b,c that, depending on our choice of T_0', the data can be explained by any of the three possibilities considered.

If one assumes that T_0' is small, then one gets a good fit with (4.117a) for

$$-1.3 \leqslant T_0' \leqslant 0.2,$$
$$0.11 \leqslant \tau_0 \leqslant 1.54 \qquad (4.118)$$

where the best fit results for $T_0' = -0.40$ with $\tau_0 = 0.88$, $E = 8.33$, $\nu_{SG}z_{SG} = 2.45 \pm 0.34$; whereas, if we assume that T_0' is fairly large, (4.117c) gives a good fit for

$$0.17 \leqslant T_0' \leqslant 0.54,$$
$$-0.30 \leqslant \tau_0 \leqslant 5.95 \qquad (4.119)$$

with the best fit for $T_0' = 0.44$, $\tau_0 = 2.98$, $B' = 3.13$, $\nu_{SG}z_{SG} = 3.94 \pm 0.18$.

There is also a region, $0.075 \leqslant T_0' \leqslant 0.218$, where we cannot exclude the Vogel-Fulcher law (4.117b); this time the best fit is obtained for $T_0' = 0.155$, $\tau_0 = 0.16$ and $E' = 4.52$.

In Figure 4.13a we plot the data assuming that (4.117a) holds with $T_c = T_0' = 0.0$; in this case we have that $\tau_0 = 0.38$, (the energy barriers) $E = 4.48$ and $\nu_{SG}z_{SG} = 1.41 \pm 0.24$. In Figure 4.13b we plot the best fit possible with the Vogel-Fulcher law, and in Figure 4.13c we assume that $T_c = 0.45$ ($\tau_0 = 2.77$, $B' = 3.13$, $\nu_{SG}z_{SG} = 3.83 \pm 0.19$).

We now look at the correlation length, ξ_{SG}.

c. The correlation length

We fit the data for $\Gamma_{SG}(n)$, (4.65), where n (n = 0,1,...,5) is the displacement in the z-direction, to (4.28):

$$\Gamma_{SG}(n) = K \frac{e^{-n/\xi_{SG}}}{n^{1+\eta_{SG}}} \quad , \tag{4.120}$$

here K is a constant. The procedure we use was outlined above in Section C.2.c. We find that

$$\eta_{SG} = - 0.5 \pm 0.5, \tag{4.121}$$

the lower values ($\eta_{SG} \simeq - 0.75$) being favoured at high temperatures ($T \simeq 1.2$) and the higher values ($\eta_{SG} \simeq - 0.30$) at low temperatures ($T \simeq 0.65$). The values of ξ_{SG} that we obtain on assuming $\eta_{SG} = - 0.50$ are tabulated in Table 4.7.

Table 4.7

DATA FOR ξ_{SG} (3D : $\eta_{SG} = - 0.5$)

T/J	Samples	ξ_{SG} ± error
1.20	55	0.67 ± 0.01
1.10	25	0.74 ± 0.02
1.00	32	0.87 ± 0.03
0.95	10	0.91 ± 0.05
0.90	25	0.99 ± 0.03
0.85	21	1.08 ± 0.04
0.80	14	1.17 ± 0.03
0.75	9	1.25 ± 0.06
0.70	6	1.41 ± 0.08
0.65	6	1.65 ± 0.06

We first examine the fit of the data to (4.34):

$$\xi_{SG} = \xi'_0 + \frac{D'}{(T - T'_0)^{\nu_{SG}}} \quad , \tag{4.122}$$

where ξ_0', D', T_0' and ν_{SG} are adjustable parameters. From the above analysis of χ_{SG} and τ [see (4.114) and (4.119)] we see that we need only look at the range $-1.3 \leqslant T_0' \leqslant 0.55$. We find that we can obtain a good fit for any given T_0', with χ^2 : $1.19 \leqslant \chi^2 \leqslant 1.76$.

Below, in Table 4.8, we tabulate the fits for some selected values of T_0':

Table 4.8

BEST FITS FOR ξ_{SG} FOR SELECTED VALUES OF T_0' (3D)

T_0'	ξ_0'	D'	ν_{SG}	χ^2
0.00	0.27	0.58	1.98 ± 0.54	1.53
0.20	0.15	0.52	1.30 ± 0.37	1.43
0.40	- 0.28	0.84	0.60 ± 0.25	1.29
0.45	- 0.62	1.14	0.42 ± 0.21	1.25
0.475	- 0.95	1.46	0.33 ± 0.20	1.23
0.50	- 1.54	2.03	0.24 ± 0.17	1.21

In Figures 4.14a,b we plot the data assuming that T_c (= T_0') = 0.0 and T_c = 0.45, respectively.

We can also fit the data to (4.48):

$$\xi_{SG} = \tilde{\xi}_0 \, e^{\tilde{D}/T^{\rho_{SG}}} , \tag{4.123}$$

where $\tilde{\xi}_0$, $\tilde{D}$ and ρ_{SG} are unknowns. One obtains a minimum in χ^2 of 1.45 for

$$\tilde{\xi}_0 = 0.08, \; \tilde{D} = 2.41, \; \rho_{SG} = 0.56 \pm 0.48. \tag{4.124}$$

Although ρ_{SG} as given in (4.124) agrees - within the error-bars - with the value, (4.116), obtained from the analogous fit to χ_{SG}, it does not tally with the exponent ($\rho_{SG} = 1.41 \pm 0.24$) resulting from a 3-parameter fit of the average relaxation time τ [see Section D.2.b of this chapter]. If we constrain the exponent in (4.123) to agree with the previous values, that is if we set $\rho_{SG} = 1.2$, say, then

$$\rho_{SG} = 1.2, \quad \tilde{\xi}_0 = 0.30, \quad \tilde{D} = 1.03; \tag{4.125}$$

we find that although the consequent fit of the data has a χ^2 value typically 3 times larger than its minimum value [$\chi^2(\rho_{SG} = 1.2) = 4.10$], it is, nevertheless, acceptable within the 75% confidence level for the χ^2-test [this is 12.61 in this case - see Appendix IV]. Both fits - (4.124) and (4.125) - are shown in Figures 4.15a,b.

3. Summary

The data for the cubic lattice is consistent with any of the three possibilities considered:

i) a zero-temperature transition,

ii) a finite temperature transition or

iii) an LCD of 3.

The statistical analysis marginally favours a transition at a finite temperature. One could probably improve on this situation by working with a lattice of a smaller size; for example, one should be able to perform simulations down to $T = 0.55$ on an 8^3 lattice.

i) If one assumes that $T_c = 0.0$, one finds that the system has to overcome energy barriers (E = 4.48J) and the critical exponents take on the values

$$\gamma_{SG} = 4.57 \pm 0.69, \quad \eta_{SG} = -0.5 \pm 0.5$$

$$\nu_{SG} = 1.98 \pm 0.54, \quad \nu_{SG} z_{SG} = 1.41 \pm 0.24. \qquad (4.126)$$

ii) On the other hand, if one assumes a finite T_c, one may also have $T_c = 0.45$, in which case the system slows down critically with exponents

$$\gamma_{SG} = 1.82 \pm 0.25, \quad \nu_{SG} = 0.42 \pm 0.21,$$

$$\nu_{SG} z_{SG} = 3.83 \pm 0.19. \qquad (4.127)$$

[We choose $T_c = 0.45$ because this is the best value favoured by both χ_{SG} and τ.] Note that the scaling relation (4.35) is only just satisfied by the exponents (4.127), that is, as we assume $\eta_{SG} = -0.5$, it is satisfied within the error-bars if $\nu_{SG} = 0.63$. This suggests that, if there is a finite T_c, ν_{SG} probably lies at the upper-end of the values mentioned in (4.127).

iii) Finally, if we assume that we are working exactly at the LCD, we can also obtain a value for the exponent ρ_{SG}. Now, such a fit for χ_{SG} gives [see (4.116)]

$$\rho_{SG} = 1.03 \pm 0.48 \qquad (4.128)$$

and for the average relaxation time, τ, gives [see (4.126)]

$$\rho_{SG} = 1.41 \pm 0.24 . \tag{4.129}$$

Consequently, a value consistent with both (4.128) and (4.129) is

$$\rho_{SG} = 1.34 \pm 0.17. \tag{4.130}$$

As mentioned above, (4.125), the correlation length data, gives an acceptable fit with values of ρ_{SG} at the lower end of the range quoted in (4.130).

APPENDIX I

THE FUNCTIONAL JACOBIAN

In Chapter III we made use of a functional integral formalism [Martin et al. 1973; Janssen 1976; Bausch et al. 1976; de Dominicis 1978; de Dominicis and Peliti 1978]. In this appendix we elaborate on this technique, in particular we give a formal derivation of the functional Jacobian, $J[\sigma_i]$.

First consider a general system whose macroscopic state is determined by a set of fluctuating time-dependent variables $\{\eta_i(t)\}$, where $i = 1,\ldots,N$. Consequently, $\{\eta_i(t)\}$ forms a random process which can be characterized by a set of probability densities:

$$P^1(\{\eta_i^{(t_1)}\},t_1)$$

$$P^2(\{\eta_i^{(t_2)}\},t_2;\{\eta_i^{(t_1)}\},t_1)$$

$$\vdots$$

$$P^\mu(\{\eta_i^{(t_\mu)}\},t_\mu;\{\eta_i^{(t_{\mu-1})}\},t_{\mu-1};\ldots;\{\eta_i^{(t_1)}\},t_1); \qquad \text{(A1.1)}$$

one interprets P^μ as a μ-fold probability density for finding $\{\eta_i(t)\}$ near $\{\eta_i^{(t_1)}\}$ at $t = t_1$, near $\{\eta_i^{(t_2)}\}$ at $t = t_2$,... and near $\{\eta_i^{(t_\mu)}\}$ at $t = t_\mu$.

One now evaluates a probability density functional, $P(\{\eta_i\} : t_0 \leqslant t \leqslant t_f)$, for an entire path in some given time interval $[t_0,t_f]$, say. This is obtained by first discretizing $[t_0,t_f]$ by a method which introduces an error of order $(\Delta t)^2$ and then taking the limit $\Delta t \to 0$ at the end. In such a limit, the path probability density may be regarded as a function of an infinite number of variables taken at all times in the interval $[t_0,t_f]$.

One makes two basic postulates [Graham 1973]:

1) $\{\eta_i(t)\}$ is assumed to be a stationary Markov process.

2) The probability density functional, $P(\{\eta_i\} : t_0 \leqslant t \leqslant t_f)$, is characterized by the Onsager-Machlup function, $O(\{\eta_i(t)\},\{\dot{\eta}_i(t)\})$, that is

$$P(\{\eta_i\} : t_0 \leqslant t \leqslant t_f) = H(O_{t_f,t_0}) \tag{A1.2}$$

where

$$O_{t_f,t_0} = \int O(\{\eta_i(t)\},\{\dot{\eta}_i(t)\})dt; \tag{A1.3}$$

the only restriction on H is that it assumes non-negative values.

To gain an insight into the function H we look at the interval $[t_0,t_{\mu-1},t_\mu]$. Now, from (A1.1) and (A1.2) one has that

$$P(\{\eta_i^{(t_\mu)}\}|\{\eta_i^{(t_0)}\} : t_\mu - t_0) = \int_{(\{\eta_i^{(t_0)}\},t_0)}^{(\{\eta_i^{(t_\mu)}\},t_\mu)} H(O_{t_\mu,t_0})D[\eta_i] \tag{A1.4}$$

where $D[\eta_i] \equiv \prod_{i,t} d\eta_i(t)$ and one integrates over all paths between the boundaries. Notice that the first postulate means that the conditional probability density appearing in (A1.4) depends on the difference of the two times concerned, that is $t_\mu - t_0$. Further, the probability densities satisfy the Smoluchowski equation [Wang & Uhlenbeck 1945]:

$$P(\{\eta_i^{(t_\mu)}\}|\{\eta_i^{(t_0)}\} : t_\mu - t_0) = \int P(\{\eta_i^{(t_\mu)}\}|\{\eta_i^{(t_{\mu-1})}\} : t_\mu - t_{\mu-1}) \times P(\{\eta_i^{(t_{\mu-1})}\}|\{\eta_i^{(t_0)}\} : t_{\mu-1}-t_0)D[\eta_i^{(t_{\mu-1})}]. \tag{A1.5}$$

From (A1.4) and (A1.5) one has that

$$\int_{(\{\eta_i^{(t_0)}\},t_0)}^{(\{\eta_i^{(t_\mu)}\},t_\mu)} \left\{ H(O_{t_\mu,t_0}) - H(O_{t_\mu,t_{\mu-1}})H(O_{t_{\mu-1},t_0}) \right\} D[\eta_i] = 0. \quad \text{(A1.6)}$$

So, an arbitrary function, f(x), has the same structure as H if

$$f(x_1 + x_2) = f(x_1)f(x_2). \quad \text{(A1.7)}$$

Now, from (A1.7) we get that

$$\ln f(x_1+x_2) = \ln f(x_1) + \ln f(x_2) \quad \text{(A1.8)}$$

$$\Rightarrow \frac{f'(x_1+x_2)}{f(x_1+x_2)} = \frac{f'(x_1)}{f(x_1)} = A, \text{ a constant.} \quad \text{(A1.9)}$$

Thus,

$$\frac{df}{dx} = Af \quad \text{(A1.10)}$$

$$\Rightarrow f(x) \sim e^{Ax}. \quad \text{(A1.11)}$$

Consequently, from (A1.2), (A1.3) and (A1.11) we have that

$$P(\{\eta_i\} : t_0 \leqslant t \leqslant t_f) \sim \exp\left\{ - \int_{t_0}^{t_f} O(\{\eta_i(t)\},\{\dot{\eta}_i(t)\})dt \right\}, \quad \text{(A1.12)}$$

where we have conveniently chosen units in which A = - 1. (A1.12) determines the path probability density up to a normalization constant which is independent of both $\{\eta_i(t)\}$ and $\{\dot{\eta}_i(t)\}$. [See Graham 1973 for a detailed discussion of the functional integral method.]

In Chapter III we introduced the path probability density, $\omega\{\xi_i\}$, for the Gaussian random noise, $\xi_i(t)$:

$$\omega(\{\xi_i\}:t_0\leqslant t\leqslant t_f) \sim \exp\left[-\frac{\Gamma}{4} \sum_{i=1}^{N} \int_{t_0}^{t_f} \xi_i^2(t)dt \right] \tag{A1.13}$$

and used the transformation

$$\omega(\{\xi_i\}:t_0\leqslant t\leqslant t_f)D[\xi_i] = W(\{\sigma_i\}:t_0\leqslant t\leqslant t_f)D[\sigma_i] \tag{A1.14}$$

to derive a path probability density for σ_i. The rest of this appendix is concerned with a formal derivation of the functional Jacobian, $J[\sigma_i]$, involved in the above transformation.

The transformation in question is given by Equation (3.29):

$$\xi_i(t) = \Gamma^{-1} \frac{\partial\sigma_i}{\partial t} + \frac{\delta(\beta H)}{\delta\sigma_i} \qquad i = 1,\ldots,N \tag{A1.15}$$

$$\equiv \Gamma^{-1} \frac{\partial\sigma_i}{\partial t} + V\{\sigma_i(t)\} \tag{A1.16}$$

and the functional Jacobian is defined by

$$J[\sigma_i] = \mathrm{Det}\left(\frac{D[\xi_i]}{D[\sigma_i]} \right) \tag{A1.17}$$

$$= \prod_{i=1}^{N} \mathrm{Det}\left(\frac{\partial\xi_i(t)}{\partial\sigma_i(t')} \right). \tag{A1.18}$$

We first integrate (A1.16) from t_0 to t_r:

$$\int_{t_0}^{t_r} \xi_i(t)dt = \int_{t_0}^{t_r} \left\{ \Gamma^{-1} \frac{\partial\sigma_i}{\partial t} + V\{\sigma_i(t)\} \right\} dt \tag{A1.19}$$

$$= \Gamma^{-1}\{\sigma_i(t_r)-\sigma_i(t_0)\} + \int_{t_0}^{t_r} V\{\sigma_i(t)\}dt. \tag{A1.20}$$

The time interval $[t_0,t_f]$ is discretized as follows:

$$t_0 < t_1 < \ldots < t_r < \ldots < t_M = t_f \tag{A1.21}$$

where

$$t_r = t_0 + r\Delta t, \quad \Delta t = \frac{t_f - t_0}{M} ; \tag{A1.22}$$

so we obtain the continuum limit when $M \to \infty$, that is $\Delta t \to 0$.

The integral is discretized via the trapezoidal rule which introduces errors of order $(\Delta t)^2$:

$$\int_{t_0}^{t_r} v\{\sigma_i(t)\}dt \simeq \left\{\frac{1}{2}\left[v\{\sigma_i(t_0)\} + v\{\sigma_i(t_r)\}\right] + \left[v\{\sigma_i(t_1)\} + v\{\sigma_i(t_2)\} + \ldots + v\{\sigma_i(t_{r-1})\}\right]\right\}\Delta t \tag{A1.23}$$

$$\equiv \sum_{j=0}^{r} v\{\sigma_i(t_j)\}\,\Theta(r-j)\Delta t, \tag{A1.24}$$

where $\Theta(x)$ is the step-function which is defined for $0 \leqslant x \leqslant r$ by

$$\Theta(x) = \begin{cases} \frac{1}{2} & x = 0 \\ 1 & x > 0 \\ \frac{1}{2} & x = r \end{cases} . \tag{A1.25}$$

Using (A1.24) in (A1.20) we get that

$$\sum_{j=0}^{r} \xi_i(t_j)\Theta(r-j)\Delta t = \Gamma^{-1}\{\sigma_i(t_r) - \sigma_i(t_0)\} + \sum_{j=0}^{r} v\{\sigma_i(t_j)\}\,\Theta(r-j)\Delta t. \tag{A1.26}$$

Thus,

$$\sum_{j=0}^{r} \frac{\partial \xi_i(t_j)}{\partial(\Gamma^{-1}\sigma_i(t_k))}\,\Theta(r-j)\Delta t = \delta_{rk} + \sum_{j=0}^{r} \frac{\partial v\{\sigma_i(t_j)\}}{\partial\{\Gamma^{-1}\sigma_i(t_k)\}}\,\Theta(r-j)\Delta t, \qquad \text{(A1.27)}$$

where $k = 0,1,\ldots,r$. Taking $r = 0,1,2,\ldots,M$, we can rewrite the right-hand side of (A1.27) in matrix form, viz.:

$$\begin{pmatrix} 1 + \frac{\Delta t}{2}\frac{\partial v\{\sigma_i(t_0)\}}{\partial\{\Gamma^{-1}\sigma_i(t_0)\}} & \frac{\Delta t}{2}\frac{\partial v\{\sigma_i(t_0)\}}{\partial\{\Gamma^{-1}\sigma_i(t_1)\}} & \cdots & \frac{\Delta t}{2}\frac{\partial v\{\sigma_i(t_0)\}}{\partial\{\Gamma^{-1}\sigma_i(t_M)\}} \\ 0 & 1 + \frac{\Delta t}{2}\frac{\partial v\{\sigma_i(t_1)\}}{\partial\{\Gamma^{-1}\sigma_i(t_1)\}} & \cdots & \Delta t\frac{\partial v\{\sigma_i(t_1)\}}{\partial\{\Gamma^{-1}\sigma_i(t_M)\}} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & 1 + \frac{\Delta t}{2}\frac{\partial v\{\sigma_i(t_M)\}}{\partial\{\Gamma^{-1}\sigma_i(t_M)\}} \end{pmatrix}$$

$$(M+1) \times (M+1)$$

$$\equiv \underline{1} + \Delta t\underline{P} \qquad \text{(A1.28)}$$

where $\underline{1}$ is the $(M+1)\times(M+1)$ identity matrix and $\underline{P}$ is the appropriate upper triangular matrix. We now set

$$D_N(\Delta t) = \det(\underline{1} + \Delta t\underline{P}). \qquad \text{(A1.29)}$$

One expands $D_N(\Delta t)$ in powers of Δt to obtain

$$D_N(\Delta t) = 1 + \frac{\Delta t}{2} \sum_{j_1=0}^{M} \frac{\partial v\{\sigma_i(t_{j_1})\}}{\partial\{\Gamma^{-1}\sigma_i(t_{j_1})\}} + \left(\frac{\Delta t}{2}\right)^2 \frac{1}{2!} \sum_{j_1 \neq j_2}^{M} \frac{\partial v\{\sigma_i(t_{j_1})\}}{\partial\{\Gamma^{-1}\sigma_i(t_{j_1})\}} \frac{\partial v\{\sigma_i(t_{j_2})\}}{\partial\{\Gamma^{-1}\sigma_i(t_{j_2})\}}$$

$$+ \ldots + \left(\frac{\Delta t}{2}\right)^{M+1} \frac{1}{(M+1)!} \sum_{\substack{j_1 \neq j_2 \neq \cdot \\ \cdot\cdot \neq j_{M+1}}}^{M+1} \frac{\partial v\{\sigma_i(t_{j_1})\}}{\partial\{\Gamma^{-1}\sigma_i(t_{j_1})\}} \cdots \frac{\partial v\{\sigma_i(t_{j_{M+1}})\}}{\partial\{\Gamma^{-1}\sigma_i(t_{j_{M+1}})\}} . \tag{A1.30}$$

Taking the limit $M \to \infty$ we obtain the continuum limit, that is $\Delta t \to 0$ (see A1.22), in which case $D_N(\Delta t) \to D$, where

$$D = 1 + \frac{1}{2} \int_{t_0}^{t_f} \frac{\partial v\{\sigma_i(t)\}}{\partial\{\Gamma^{-1}\sigma_i(t)\}} dt + \frac{1}{2!} \left(\frac{1}{2} \int_{t_0}^{t_f} \frac{\partial v\{\sigma_i(t)\}}{\partial\{\Gamma^{-1}\sigma_i(t)\}} dt\right)^2$$

$$+ \ldots + \frac{1}{r!} \left(\frac{1}{2} \int_{t_0}^{t_f} \frac{\partial v\{\sigma_i(t)\}}{\partial\{\Gamma^{-1}\sigma_i(t)\}} dt\right)^r + \ldots \tag{A1.31}$$

$$= \exp\left\{\frac{1}{2} \int_{t_0}^{t_f} \frac{\partial v\{\sigma_i(t)\}}{\partial\{\Gamma^{-1}\sigma_i(t)\}} dt\right\} . \tag{A1.32}$$

So we see from (A1.27)-(A.32) that

$$\mathrm{Det}\left(\frac{\partial \xi_i(t)}{\partial\{\Gamma^{-1}\sigma_i(t')\}}\right) = \exp\left\{\frac{1}{2} \int_{t_0}^{t_f} \frac{\partial v\{\sigma_i(t)\}}{\partial\{\Gamma^{-1}\sigma_i(t)\}} dt\right\} . \tag{A1.33}$$

Now, the functional Jacobian is given by

$$J[\sigma_i] = \prod_{i=1}^{N} \mathrm{Det}\left(\frac{\partial \xi_i(t)}{\partial \sigma_i(t')}\right) \tag{A1.34}$$

$$= \prod_{i=1}^{N} \mathrm{Det} \left(\Gamma^{-1} \frac{\partial \xi_i(t)}{\partial\{\Gamma^{-1}\sigma_i(t')\}} \right) \tag{A1.35}$$

$$\sim \prod_{i=1}^{N} \mathrm{Det} \left(\frac{\partial \xi_i(t)}{\partial\{\Gamma^{-1}\sigma_i(t')\}} \right) , \tag{A1.36}$$

up to a constant which we absorb into the normalization constant [see Chapter III]. Thus, we get, finally, from (A1.15), (A1.16), (A1.33) and (A1.36) that

$$J[\sigma_i] = \exp\left\{ \frac{\Gamma}{2} \sum_{i=1}^{N} \int_{t_0}^{t_f} \frac{\delta^2(\beta H)}{\delta\sigma_i^2} \, dt \right\} . \tag{A1.37}$$

APPENDIX II

THE FLUCTUATION-DISSIPATION THEOREM

In this appendix we discuss the various versions of the Fluctuation-Dissipation Theorem (FDT) mentioned in Chapter III. [Note that in this appendix we shall assume that an average over samples has been performed so that we expect the FDT to hold - see Chapter I for further details.]

The linear-response function (3.55b) describes the behaviour of the system under the influence of a very weak perturbation (the external magnetic field, h_i). In equilibrium the response function is related to the correlation function (3.55a) by the FDT. For conventional systems the FDT states [Ma 1976] that

$$C(\omega) = \frac{2}{\omega} \text{ Im } G(\omega) \tag{A2.1}$$

and

$$C(t = 0) = G(\omega = 0), \tag{A2.2}$$

where C(t) and G(t) are given by (3.20a) and (3.20b) respectively, and the Fourier transforms are defined by (3.20c) and (3.20d).

As discussed in Chapter III, for spin-glasses the time-dependent correlation function, C(t), is given by

$$C(t) = \tilde{C}(t) + q_{EA} , \tag{A2.3}$$

where

$$\lim_{t\to\infty} \tilde{C}(t) = 0 \qquad \text{(A2.4)}$$

is the finite-time contribution and

$$q_{EA} = \lim_{t\to\infty} C(t) \qquad \text{(A2.5)}$$

is the time-persistent part of C(t). Fourier transforming (A2.3) we get

$$C(\omega) = \tilde{C}(\omega) + 2\pi\delta(\omega)q_{EA} \qquad \text{(A2.6)}$$

where we have used (3.20c) and (3.220). Since $\omega\delta(\omega) = 0$, the δ-function contribution to $C(\omega)$ does not affect the response function, that is the <u>full</u> response function is related to the finite-time part of the correlation function. So the FDT now becomes

$$\tilde{C}(\omega) = \frac{2}{\omega} \text{Im } G(\omega). \qquad \text{(A2.7)}$$

In the $\omega = 0$ limit we refer to the response function as the uniform susceptibility, $\chi(T)$ - see (2.10). The static, that is $\omega = 0$, limit of (A2.7) is the Fischer (1976) relation (3.19). [See Chapter II for further details.]

As mentioned by Sompolinsky and Zippelius (1982), the FDT is satisfied self-consistently in our case. To see this one first assumes that (A2.7) holds. Now, the bare ($u = 0$) correlation function is given by

$$\langle \sigma_i(\omega)\sigma_i(\omega') \rangle = G_0(\omega)\ G_0(\omega')\ \langle \varphi_i(\omega)\varphi_i(\omega') \rangle\ , \qquad \text{(A2.8)}$$

where we have used (3.148) and $\langle \ldots \rangle$ denotes an average over the effective random noise φ_i - see Section D of Chapter III for further details. [Note that, without loss of generality, we have omitted the replica indices.] In (A2.8) $G_0(\omega)$ is the bare propagator, defined by (3.149), and $\langle \varphi_i(\omega)\varphi_i(\omega') \rangle$ is given by (3.150). So, on substituting from (3.150), (A2.8) becomes

$$\langle \sigma_i(\omega)\sigma_i(\omega') \rangle = G_0(\omega)G_0(\omega')[2\Gamma^{-1} + \beta^2 J^2 \tilde{C}(\omega)]\delta(\omega + \omega') \qquad \text{(A2.9)}$$

$$= G_0(\omega)G_0(\omega')[2\Gamma^{-1} + \beta^2 J^2 \frac{2}{\omega} \text{Im } G(\omega)]\delta(\omega + \omega') \qquad \text{(A2.10)}$$

where we have also used (A2.7). As from (3.147) we have that

$$\text{Im } G(\omega) = \left\{ \frac{\text{Im } G_0(\omega)}{|G_0(\omega)|^2} - \omega\Gamma^{-1} \right\} / \beta^2 J^2 \ , \qquad \text{(A2.11)}$$

it follows that the bare correlation function is given by

$$\langle \sigma_i(\omega)\sigma_i(\omega') \rangle = \frac{2}{\omega} \text{Im } G_0(\omega) \ , \qquad \text{(A2.12)}$$

which means that (A2.7) is obeyed for $u = 0$. The usual diagrammatic expansion [Ma 1976; Sompolinsky and Zippelius 1982] is then used to show that the FDT remains valid in the non-linear case ($u \neq 0$).

APPENDIX III

THE MONTE CARLO METHOD

The results discussed in Chapter IV were obtained by Monte Carlo simulations. In this appendix we outline the method used. We shall first discuss the Monte Carlo method in general and then consider its most suitable form for our particular problem.

The Monte Carlo method was introduced by Metropolis et al. (1953) in order to perform high-dimensional integrals [Binder 1979; Creutz et al. 1979; Mackenzie 1982]. Now, by definition, the thermodynamic average, $\langle O \rangle_T$, of an observable $O(\underline{x})$, where $\underline{x}$ denotes a point in phase space, is given by

$$\langle O \rangle_T = \int_V O(\underline{x}) e^{-\beta H(\underline{x})} \, d\underline{x} \; / \int_V e^{-\beta H(\underline{x})} \, d\underline{x}, \tag{A3.1}$$

here V denotes the volume of phase space over which the integration is to be performed and $\beta = 1/T$. (Once again, we set Boltzmann's constant to unity.) Conventional numerical techniques approximate integrals by a sum containing only a finite number of terms:

$$\int_V g(\underline{x}) d\underline{x} \simeq \sum_\alpha g(\underline{x}_\alpha) \Delta \underline{x}_\alpha, \tag{A3.2}$$

where the set of points $\{\underline{x}_\alpha\}$ is obtained by subdividing the phase space in some ordered fashion. Clearly, such an approach is out of the question if the phase space is high-dimensional.

A crude form of the Monte Carlo method involves selecting $\{\underline{x}_\alpha\}$ at random in the phase space. However, this random sampling of points is not very appropriate if, as in (A3.1), the integrand varies over many orders of magnitude since one will probably never

sample the points with the most weight.

Metropolis et al. (1953) overcame the problems discussed above by using an algorithm based on "importance sampling", that is, the phase space points are chosen according to some probability $f(\underline{x}_\alpha)$, in which case (A3.1) becomes

$$\langle O \rangle_T \simeq \frac{\sum_{\alpha=1}^{M} O(\underline{x}_\alpha) f^{-1}(\underline{x}_\alpha) e^{-\beta H(\underline{x}_\alpha)}}{\sum_{\alpha=1}^{M} f^{-1}(\underline{x}_\alpha) e^{-\beta H(\underline{x}_\alpha)}} \tag{A3.3}$$

where $f^{-1}(\underline{x}_\alpha)$ is the inverse of $f(\underline{x}_\alpha)$ and M is the number of points selected in the phase space. Obviously, one would like to choose

$$f(\underline{x}_\alpha) \propto e^{-\beta H(\underline{x}_\alpha)}, \tag{A3.4}$$

the equilibrium distribution, as in this case the thermodynamic averages reduce to just arithmetic averages:

$$\langle O \rangle_T \simeq \frac{1}{M} \sum_{\alpha=1}^{M} O(\underline{x}_\alpha). \tag{A3.5}$$

Although the equilibrium distribution is not known explicitly, one achieves the desired result by means of a Markov process: a random walk is constructed in phase space such that, regardless of the initial distribution, $f(\underline{x}_\alpha)$ converges towards the equilibrium distribution as $M \to \infty$. The Markov process is defined by a transition probability from one point in the phase space to another and convergence towards equilibrium is ensured by satisfying the detailed balance condition (see below) [Binder 1979].

The rest of the discussion is concerned with continuous planar spins. As is indicated in Figure 4.1a, each spin is specified by just one polar angle. The phase space in our problem is the set of all possible values for the polar angle. At any given temperature, T, one starts with all of the spins parallel: $\vartheta_j = 0$ for all spins j. One then uses the following Monte Carlo algorithm:

1) Consider a given spin $\underline{S}_i = (\cos \vartheta_i, \sin \vartheta_i)$.

2) Calculate the local energy, E_i, for the spin from

$$E_i = - \sum_{\langle ij \rangle}{}' J_{ij} \underline{S}_i . \underline{S}_j \qquad \text{(A3.6)}$$

where $\sum_{\langle ij \rangle}{}'$ denotes a summation over the nearest neighbours of i.

3) Choose a random number x: $0 < x < 1$; this gives us a new possible value, ϑ_i', for the polar angle where

$$\vartheta_i' = 2\pi x. \qquad \text{(A3.7)}$$

We call ϑ_i' the acceptance angle and when, as in (A3.7), $0 < \vartheta_i' < 2\pi$ it is said to be unrestricted.

4) Calculate the new local energy E_i':

$$E_i' = - \sum_{\langle ij \rangle}{}' J_{ij} \underline{S}_i' . \underline{S}_j \qquad \text{(A3.8)}$$

where $\underline{S}_i' = (\cos \vartheta_i', \sin \vartheta_i')$.

5) Evaluate the transition probability, $W(\underline{S}_i \rightarrow \underline{S}_i')$, given by

$$W(\underline{S}_i \rightarrow \underline{S}_i') = e^{-\Delta E_i / T} \qquad \text{(A3.9)}$$

where $\Delta E_i = E_i' - E_i$.

6) Choose a new random number y: $0 < y < 1$.

7) If $W > y$ accept the new spin orientation, otherwise keep the old version; this procedure is equivalent to

$$W(\underline{S}_i \rightarrow \underline{S}_i') = \begin{cases} e^{-\Delta E_i/T} & \Delta E_i > 0 \\ 1 & \Delta E_i \leq 0 \end{cases} \qquad \text{(A3.10)}$$

8) Repeat steps 1-7 for a different spin.

As our choice for the transition probability satisfies the detailed balance condition, which is given by

$$e^{-\beta H(\underline{S}_i)} W(\underline{S}_i \rightarrow \underline{S}_i') = e^{-\beta H(\underline{S}_i')} W(\underline{S}_i' \rightarrow \underline{S}_i), \qquad \text{(A3.11)}$$

convergence towards equilibrium is guaranteed. [We follow the customary practice of setting to unity the arbitrary coefficient which should appear in (A3.10).]

The above algorithm is repeated throughout the lattice and such an iteration is referred to as a Monte Carlo Step/Spin (MCS/Spin). One gives a dynamical interpretation to the Monte Carlo process by identifying the MCS/Spin with time in the simulation.

Although the stochastic dynamics introduced above will eventually equilibrate the system in question, the number of MCS/Spins required to achieve equilibrium is not known a priori. In practice, one starts the simulation with $\vartheta_i \equiv 0$ for all spins $\underline{S}_i$ and then allows the system to evolve until equilibrium is attained. Whereas the evolution to equilibrium allows us to investigate the dynamical aspects of the problem, information regarding the static behaviour of the system is only extracted once equilibrium has been achieved. [See Chapter IV for further details.]

APPENDIX IV

THE CHI-SQUARED TEST

The results in Chapter IV were obtained by a statistical analysis of the data. In this appendix we give further details about the method used, in particular we discuss weighted linear regressions and the chi-squared test (χ^2-test) [Meyer 1975; Spiegel 1961].

Suppose that we measure the quantity Y for i (i = 1,...,N) given values of X and that the statistical error, that is the sample error, in the measurement is σ; to be specific, we have a set of values $Y_i(X_i,\sigma_i)$, i = 1,...,N. Assuming Y to be linearly dependent on X, that is

$$Y = aX + b \ , \tag{A4.1}$$

we wish to determine the line of best fit through the data. In order to do this, we first weight each Y_i by $\omega_i = 1/\sigma_i^2$ and define

$$\bar{\omega} = \frac{1}{N} \sum_{i=1}^{N} \omega_i \tag{A4.2}$$

and

$$c_i = \omega_i/\bar{\omega} \ . \tag{A4.3}$$

It then follows [Meyer 1975] that the weighted line of best fit through the data is specified by taking a = α and b = β where

$$\alpha = \frac{\sum_{i=1}^{N} C_i X_i Y_i - \left(\sum_{i=1}^{N} C_i X_i\right)\left(\sum_{i=1}^{N} C_i Y_i\right)/N}{\sum_{i=1}^{N} C_i X_i^2 - \left(\sum_{i=1}^{N} C_i X_i\right)^2/N} \tag{A4.4}$$

and

$$\beta = \left\{\sum_{i=1}^{N} C_i Y_i - \alpha \sum_{i=1}^{N} C_i X_i\right\}/N \ . \tag{A4.5}$$

We now discuss the χ^2-test. [We shall restrict the discussion to the analysis of the spin-glass susceptibility, χ_{SG}; the other quantities mentioned in Chapter IV are analysed in an analogous way.] So, we measure $\chi_{SG}(T_i) \pm \varepsilon_i$ $(i = 1,\ldots,N)$, where ε_i is the sample error. As mentioned in Chapter IV, (4.95), we are interested in the quality of the fit of the data to

$$\chi_{SG} = \chi_0 + \frac{A}{(T - T_0)^{\gamma_{SG}}} \tag{A4.6}$$

where χ_0, A, T_0 and γ_{SG} are unknown parameters. One first sets $\chi_0 = \tilde{\chi}_0$ and rewrites (A4.6) as

$$\ln(\chi_{SG} - \tilde{\chi}_0) = \ln A - \gamma_{SG} \ln(T - T_0). \tag{A4.7}$$

One then chooses $T_0 = T_0'$ and defines

$$Y = \ln (\chi_{SG} - \tilde{\chi}_0) \tag{A4.8}$$

and

$$X = \ln (T - T_0') \ , \tag{A4.9}$$

thereby transforming (A4.6) to

$$Y = \ln A - \gamma_{SG} X. \tag{A.10}$$

Using the method outlined above, a weighted line of best fit to (A4.10) is calculated; this has $A = A'$ and $\gamma_{SG} = \gamma'_{SG}$, say.

The "goodness-of-fit" of the data to

$$\tilde{\chi}_{SG} \equiv \tilde{\chi}_0 + \frac{A'}{(T - T'_0)^{\gamma_{SG}}} \tag{A.11}$$

is now evaluated by calculating the χ^2 value, which is defined by

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{\chi_{SG}(T_i) - \tilde{\chi}_{SG}}{\varepsilon_i} \right)^2 \tag{A.12}$$

In (A4.12) $\chi_{SG}(T_i)$ is the experimental value of χ_{SG} at T_i and $\tilde{\chi}_{SG}$ is the value of (A4.11) with $T = T_i$. The above procedure [from (A4.8) to (A4.12)] is repeated for different values of T_0 ($= T''_0, \ldots$, say) but the same value of χ_0 ($= \tilde{\chi}_0$) until a minimum in χ^2 is located. In this way, for a given χ_0 we allow for variations in all three of the other adjustable parameters. One now repeats the entire procedure for different values of χ_0 ($= \chi''_0, \ldots$, say). Hence, we obtain χ^2 as a function of the background χ_0 —— $\chi^2(\chi_0)$.

By fixing T_0 and allowing for variations in χ_0, A and γ_{SG} we also evaluate $\chi^2(T_0)$. Further, for any fixed T_0, we can define

$$Y = \chi_{SG} \tag{A4.13}$$

and

$$X = T - T_0 \tag{A4.14}$$

to rewrite (A4.6) as

$$Y = \chi_0 + A/X^{\gamma_{SG}} , \qquad (A4.15)$$

thereby enabling one to use the above method to evaluate χ^2 (γ_{SG}). [See Chapter IV for plots of χ^2.]

In general, one rejects the fit at the α-level of significance - which corresponds to a $100(1 - \alpha)\%$ confidence level - if [Spiegel 1961]

$$P\{\chi^2_{n-r} \geq S\} \leq \alpha , \qquad (A4.16)$$

where n is the number of data points, r is the number of fitting parameters, that is those parameters that are estimated from the data [n - r is known as the number of degrees of freedom] and S is the critical value of a χ^2 random variable with (n-r) degrees of freedom, which is found from statistical tables [Spiegel 1961].

As a rule of thumb, we only accept fits which give rise to values of χ^2 less than or equal to $2\chi^2_{min}$, where χ^2_{min} is the absolute minimum in χ^2, or by the 75% confidence level, whichever is smaller. Now, as the latter requires us to reject a fit if

$$P\{\chi^2_{n-r} \geq S\} \leq 0.25 \qquad (A4.17)$$

and, as we allow all adjustable parameters to vary, n - r = N in our case, we are interested in the critical value, $S_{critical}$, resulting from

$$P\{\chi^2_N \geq S_{critical}\} = 0.25 \qquad (A4.18)$$

where N = 1,2,... (the number of data points). In Table A4.1 we show some of the critical values, $S_{critical}$ [Spiegel 1961].

Table A4.1

CRITICAL VALUES OF A χ^2 RANDOM VARIABLE

N	$S_{critical}$
1	1.36
2	2.82
3	4.15
4	5.44
5	6.68
6	7.90
7	9.09
8	10.28
9	11.45
10	12.61
11	13.77
12	14.91

Thus, if we are examining the goodness-of-fit of 11 data points, say, we reject the fit at this level if the χ^2 value as calculated above exceeds 13.77.

APPENDIX V

THE DISTRIBUTED ARRAY PROCESSOR

The Monte Carlo simulations discussed in Chapter IV were performed on the ICL Distributed Array Processor (DAP) at Queen Mary College. In this appendix we outline some of the salient features of this computer.

The DAP [Bowler 1983], which is specific to the ICL 2900 series mainframe, can, unlike a conventional serial processor, perform the same operation simultaneously on different data items. In Chapter IV we utilise this facility to perform Monte Carlo simulations of nearest neighbour X-Y spin-glasses.

The main feature of the DAP, illustrated in Figure A5.1a, is a 64×64 matrix of processing elements. Each processing element has a 4 Kbit store chip and is capable of operating independently; the DAP, effectively a 2 Mbyte (8 bits ≡ 1 byte) store, is simply the sum total of all 4096 processing elements.

The high-level language one uses on the DAP is DAP Fortran which is an extension of 2900 Fortran. In DAP Fortran all data values have a particular mode which can be scalar, vector or matrix. Whereas a value with a scalar mode corresponds to an ordinary Fortran scalar, values with vector and matrix modes are arrays of 64 and 64×64 components respectively. The most important feature of the DAP is the capability to process in parallel the component values of vectors and matrices. A data value in DAP Fortran may be of type integer, real, logical or character. Integer values are held in 32 bits, the first of which indicates the sign; real values are held in 32 bit 2900 floating point format; and logical data are held as a single bit.

In passing, we note two special features of DAP Fortran which were used extensively throughout the computations. One such feature is that of 'logical masking', which enables operations and assignments to be performed conditional upon a logical mask defined over the whole 64×64 matrix of processing elements. This facility was used to map the two- and three-dimensional lattices in question on to the two-dimensional array of processing elements of the DAP and also to enforce the periodic boundary conditions (see below). In the actual computations themselves, use was made of the other important feature, namely that of 'shifting'. This allows one to perform calculations requiring the values of a number of processing elements at each processing element.

As DAP Fortran has no input/output facilities, the DAP program has to be accessed via a 2900 Fortran routine, that is one has a host program - run on the host ICL 2900 mainframe - containing the DAP program as a subroutine, all input/output being performed within the 2900 routine. Further, all data is passed between 2900 Fortran programs and DAP Fortran programs in the form of labelled COMMON blocks.

The unique nature of the DAP requires a rather complicated compilation procedure. The compilation is carried out in stages, each of which uses a particular ICL supplied 'macro', that is 2900 'System Control Language' commands.

The host 2900 Fortran program is compiled using the standard Fortran compiler, the FORT macro, which produces an 'Object Module Format'. Each of the DAP Fortran subroutines is first compiled by the DAP Fortran compiler, the DAPFORT macro, which generates an 'Assembler Macro Format'; the output from the DAPFORT macro

is not an executable code. The DAP assembler uses the DAPASM macro to convert the Assembler Macro Format into a DAP executable code. However, the output from the assembler, known as 'Consolidator Input Format', requires certain 'fix-ups' to be performed. This stage is carried out by the DAP Consolidator and produces a loadable file in 'Object Module Format'.

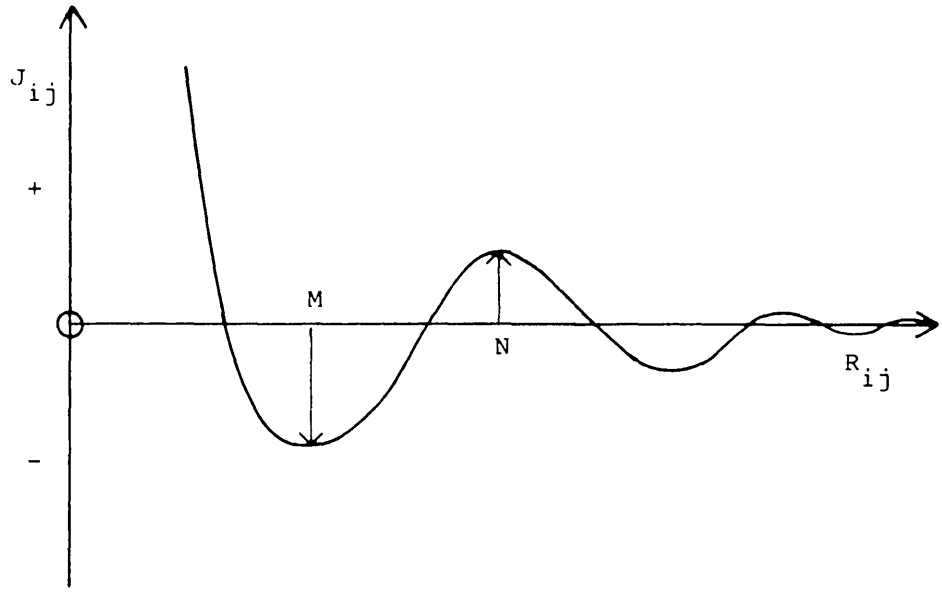
The complete program - the host 2900 Fortran program and the DAP Fortran subroutines - is loaded and started by the RUNDAP macro.

As we want to perform Monte Carlo simulations in two- and three-dimensions, our first problem is to map our lattices on to the two-dimensional matrix of processing elements comprising the DAP. We use logical masks to cover the processing elements with a chequerboard of .FALSE. (black) and .TRUE. (white) values. In Figure A5.1b we indicate the map used in the simulations. This map has the advantage that we can simulate both two- and three-dimensions with the same computer program. Note that for clarity Figure A5.1b is restricted to a 16×16 matrix, whereas the DAP is actually of size 64×64. The blank and shaded squares form the two sub-lattices mentioned in Chapter IV. As indicated in Figure A5.1b, the chequerboard effectively partitions the 64×64 array into 16 independent blocks of size 16×16. We employ logical masks to enforce periodic boundary conditions within each block. So, when considering a two-dimensional lattice, we can simulate simultaneously 16 samples, each of size 16^2. For the three-dimensional lattice, on the other hand, we connect up the blocks using periodic boundary conditions (see Figure A5.1b) to simulate just one sample of size 16^3.

Finally, for any given job, one is restricted to a maximum of 1 hour on the DAP; this time limit imposes a lower bound on the temperatures we are able to simulate. [See Chapter IV for an indication of the speed of the program used.]

FIGURE 1.1a

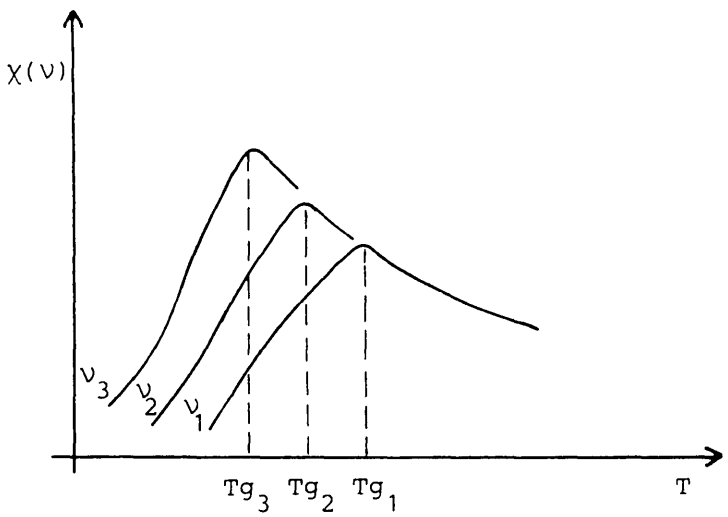
THE RKKY INTERACTION



Consider a given spin at the origin O. Then another spin at R_{ij} = OM will experience an antiferromagnetic interaction, whereas a spin at R_{ij} = ON will have a ferromagnetic coupling.

FIGURE 1.1b

THE FREQUENCY DEPENDENCE OF THE ac SUSCEPTIBILITY



A schematic representation of the frequency, ν, dependence of the ac susceptibility. One has

$$Tg_3 < Tg_2 < Tg_1$$

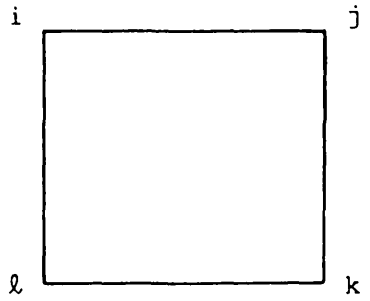
and

$$\nu_3 < \nu_2 < \nu_1 .$$

(arbitrary units are employed).

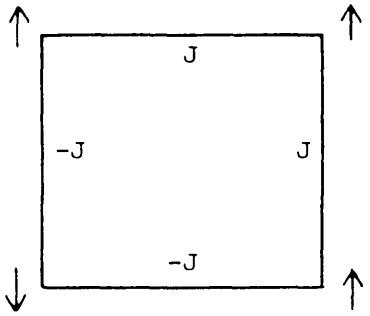
FIGURE 1.2

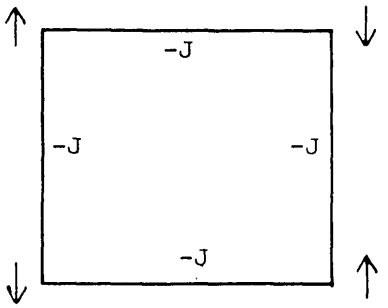
COMPETITION BETWEEN BONDS



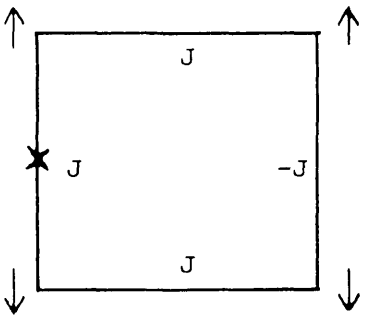
Consider this plaquette with a spin at each vertex.

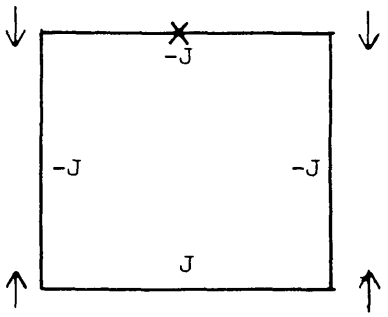
a)





b)

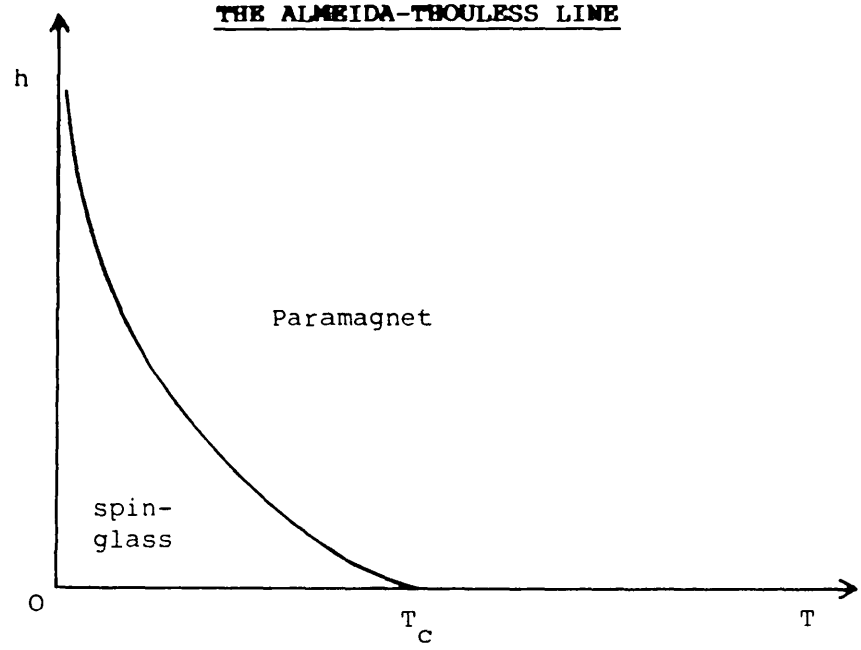




In case (a) one can satisfy all the bonds, that is spins connected by positive bonds are parallel while those connected by negative bonds are antiparallel. In case (b), however, one bond (indicated by a cross) remains unsatisfied. We call the plaquettes in the latter case "frustrated".

FIGURE 1.3a

THE ALMEIDA-THOULESS LINE



The replica symmetry ansatz breaks down in the spin-glass phase.

Note: [Almeida & Thouless 1978]

i) when $h = 0$, $T_c = J$;

ii) for $h \simeq 0$, $T \to T_c$ the equation of the line is

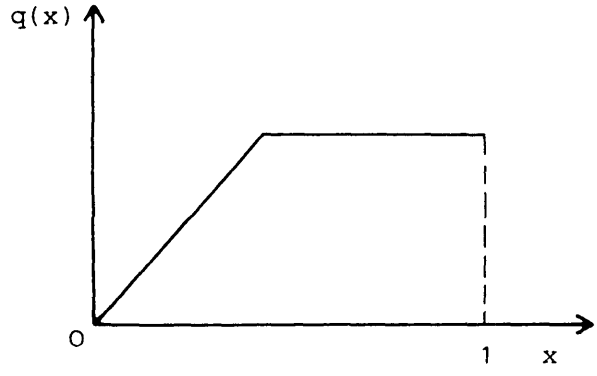
$$[h/J]^2 = \frac{4}{3}\,[1 - T/T_c]^3;$$

iii) while for $h >> 1$, $T \to 0$ one has

$$T = \frac{4}{3}\,(2\pi)^{-1/2}\, e^{-h^2/2}.$$

FIGURE 1.3b

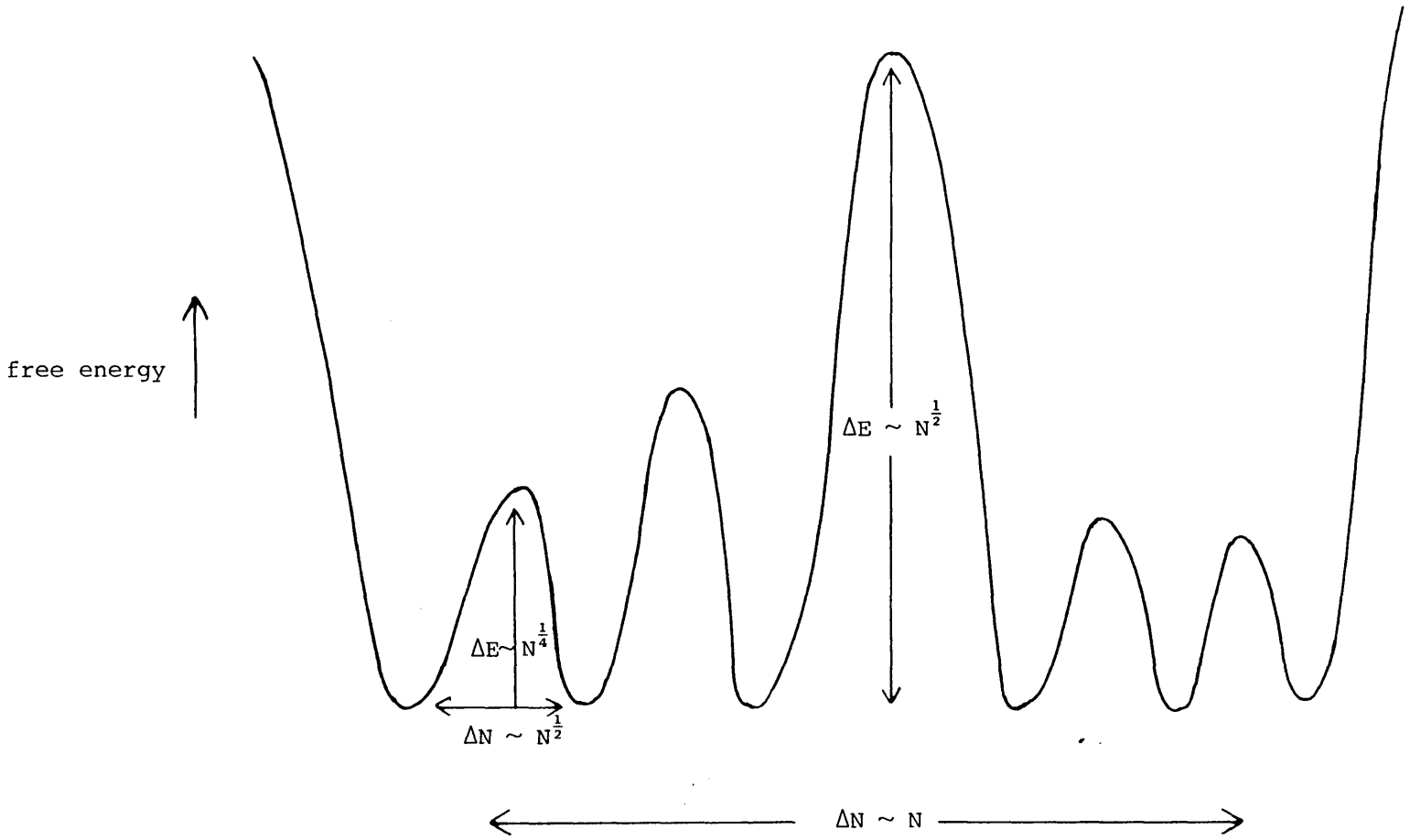
q(x) for h = 0 and T < T_c



We note: $q(0) = 0$ and

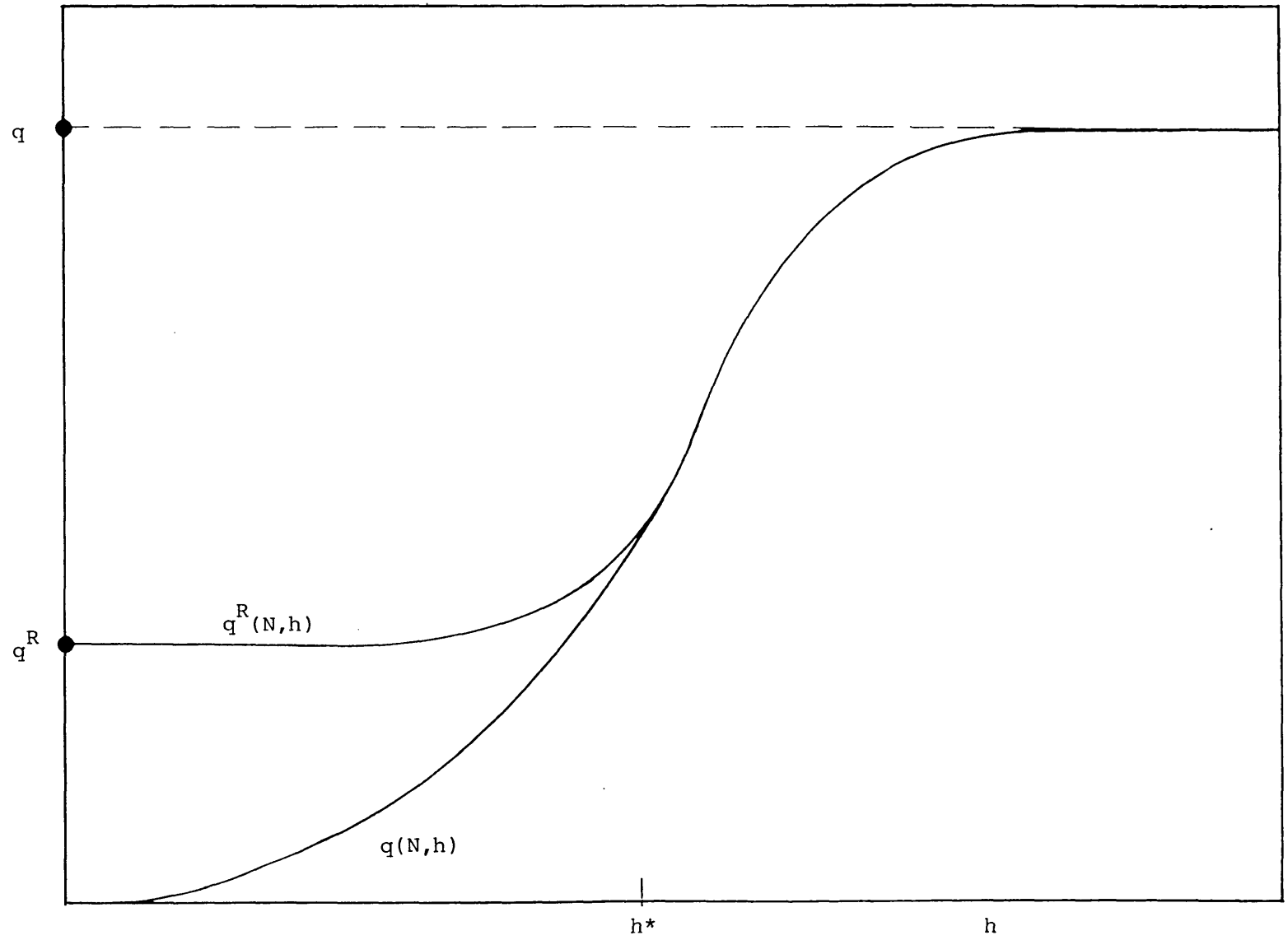
$$\operatorname{Max}_{\{x:0\leqslant x\leqslant 1\}} q(x) = q(1).$$

FIGURE 2.1 A schematic representation of the free energy in phase space for the SK model



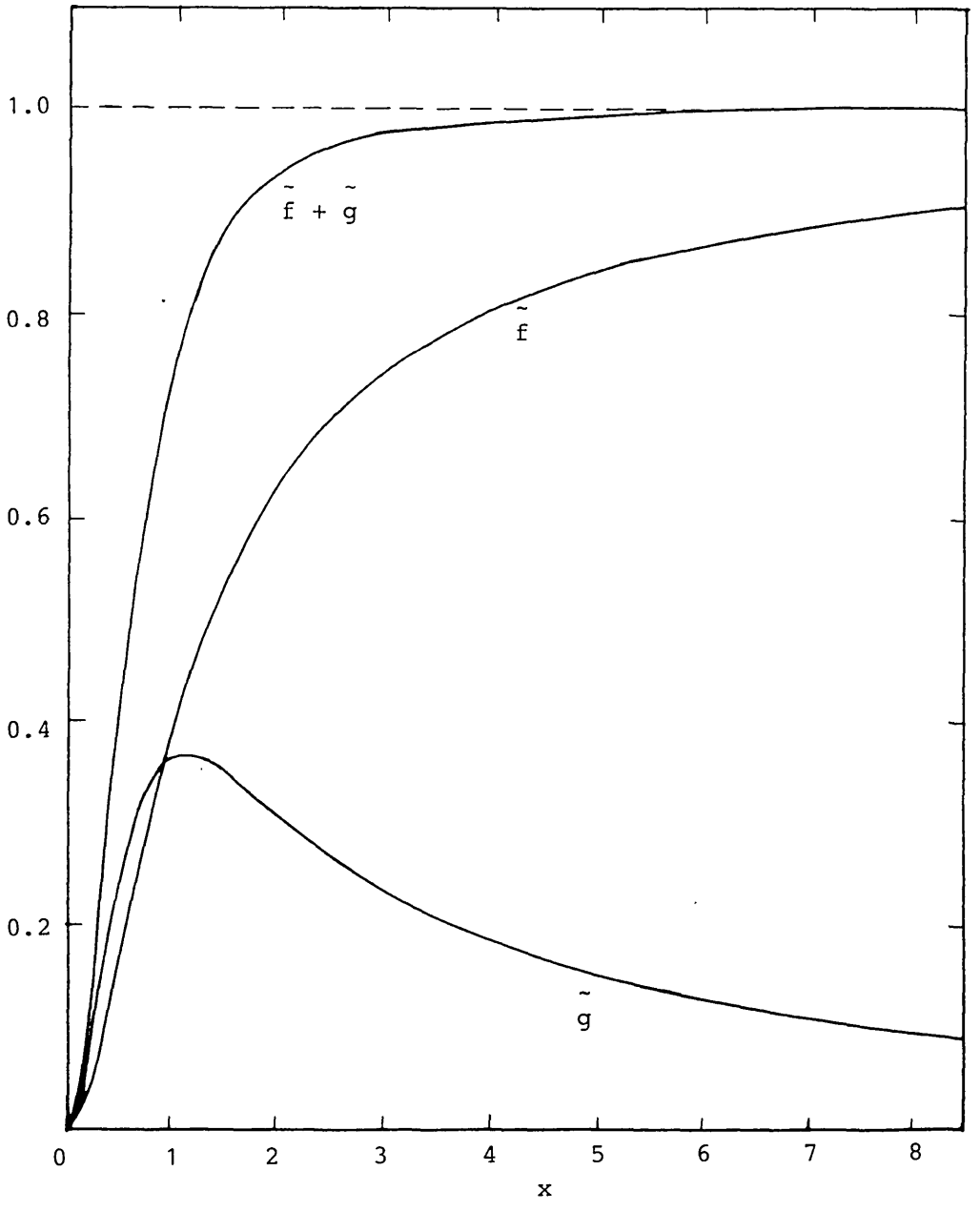
There is considerable structure in each well. In order to surmount the central free energy barrier all N spins have to be flipped, whereas to get over the smaller barriers one needs to flip of order $N^{\frac{1}{2}}$ spins. The minima correspond to metastable states.

FIGURE 2.2 A sketch of the possible behaviour of $q(N,h)$ and $q^R(N,h)$ with h



h* is defined by (2.17), q is defined by (2.14a) and q^R by (2.50b). Clearly, in this case $q > q^R > 0$.

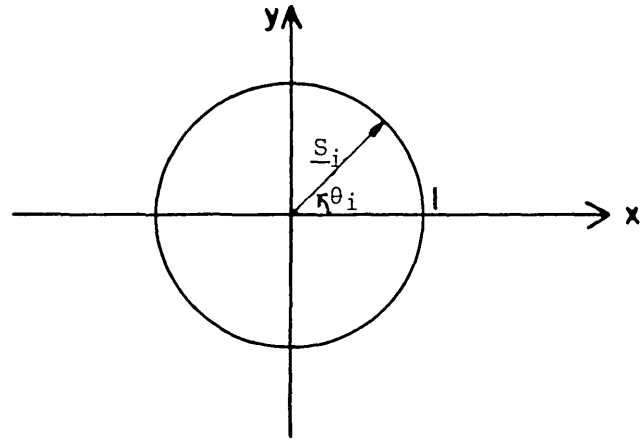
FIGURE 2.3 A plot of $\tilde{f}(x)$, $\tilde{g}(x)$ and $\tilde{f}(x) + \tilde{g}(x)$



The functions $\tilde{f}(x)$ and $\tilde{g}(x)$ are related by $\tilde{g}(x) = x\tilde{df}/dx$. As we can see, the sum of the two functions approaches its asymptotic value faster than $\tilde{f}(x)$ or $\tilde{g}(x)$ separately approach their asymptotic values.

FIGURE 4.1a

A PLANAR SPIN

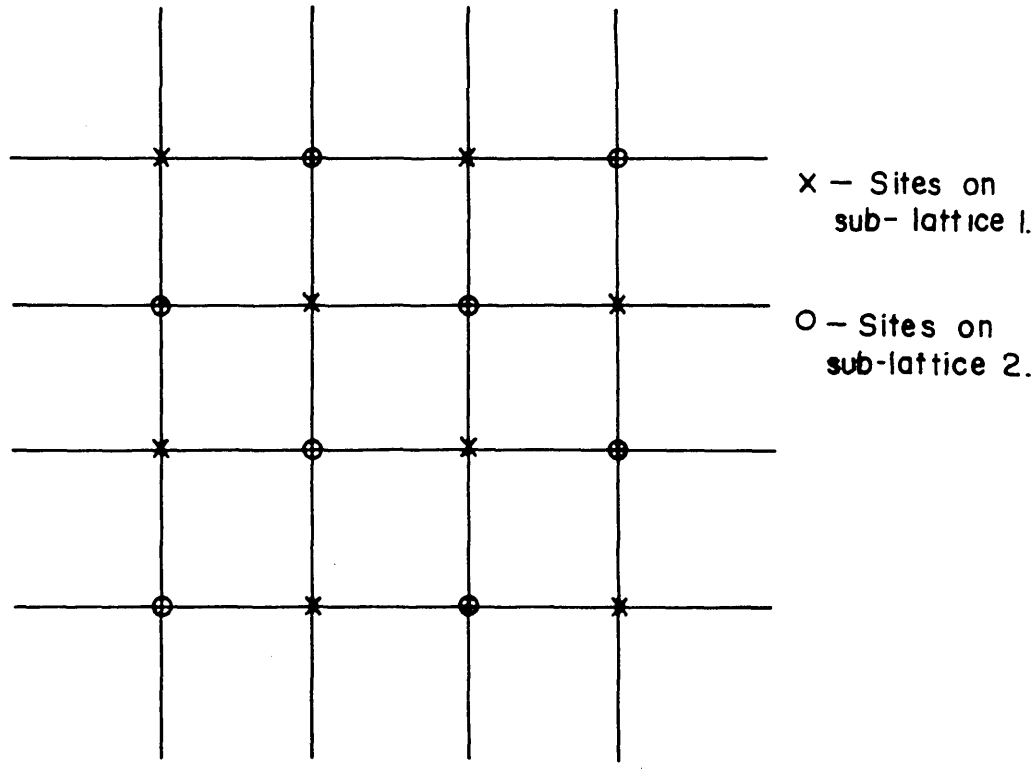


We assume a continuous spin symmetry : $\underline{S}_i = (\cos\theta_i, \sin\theta_i)$

$\equiv (S_i^1, S_i^2)$

FIGURE 4.1b

THE TWO-DIMENSIONAL LATTICE



A 4 x 4 portion of the square lattice . We can test simultaneously all of the site on either of the sub-lattices

FIGURE 4.2 Typical behaviour of q(t)

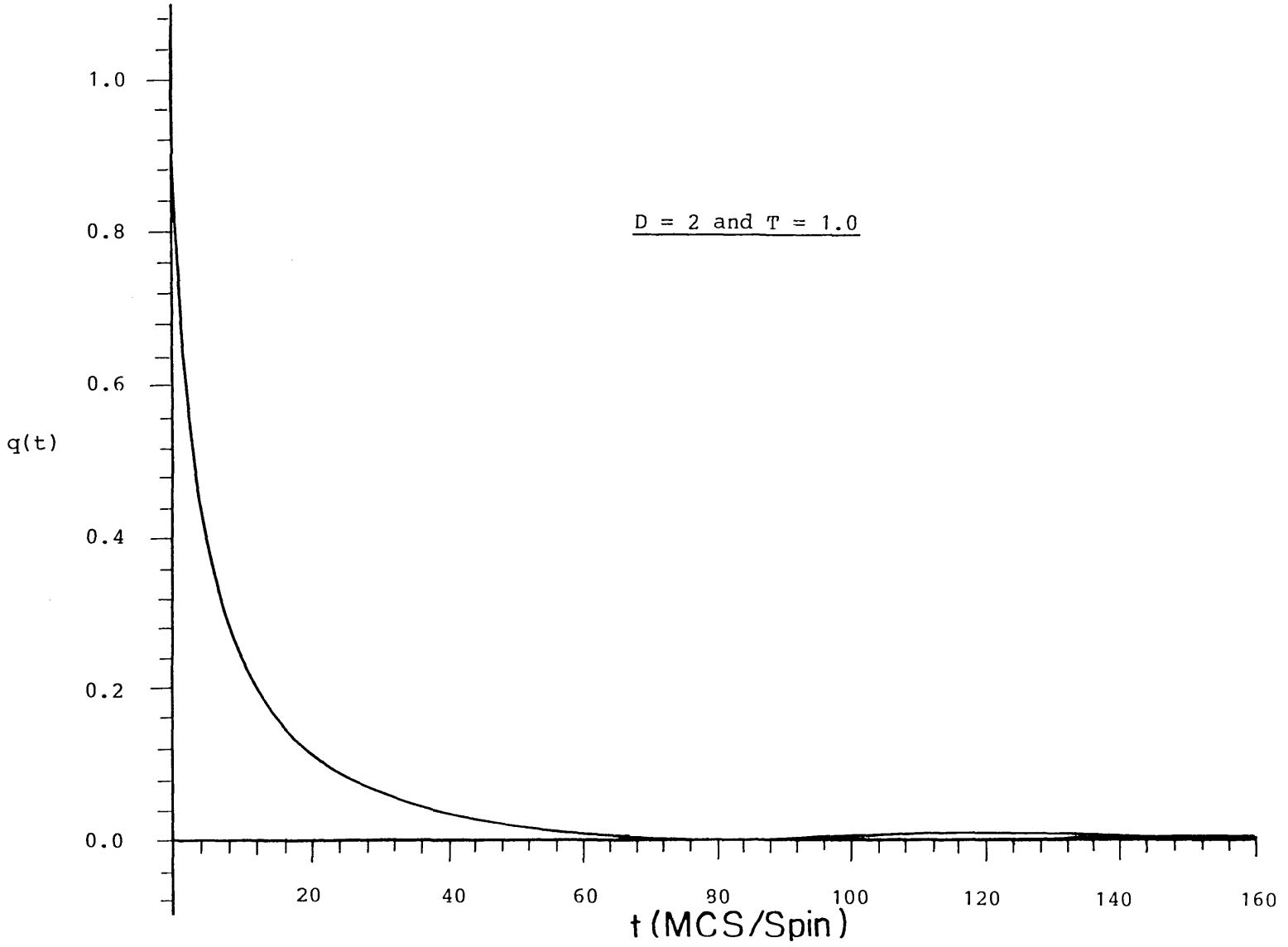
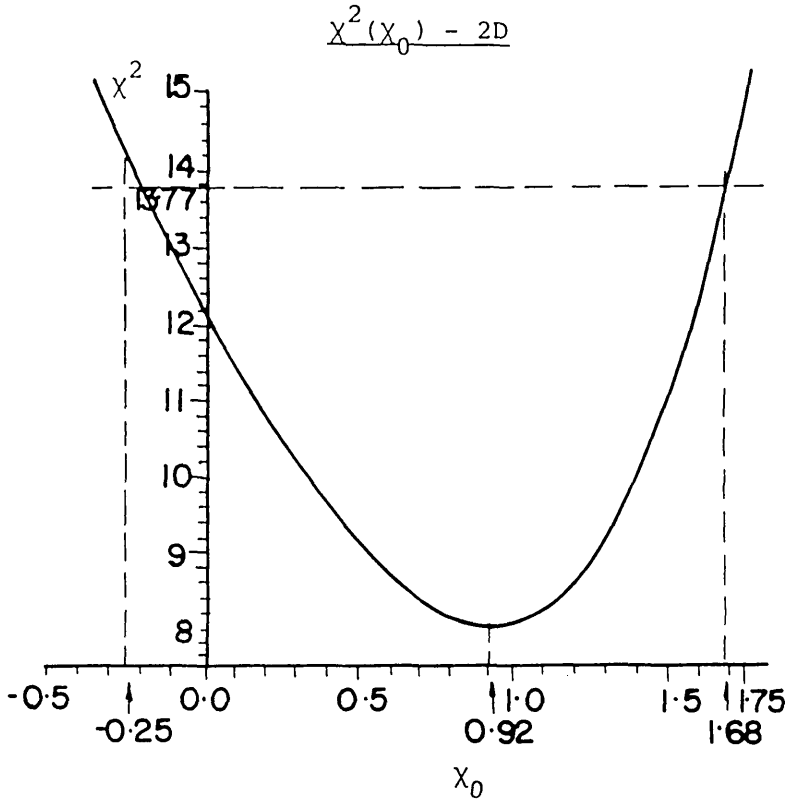
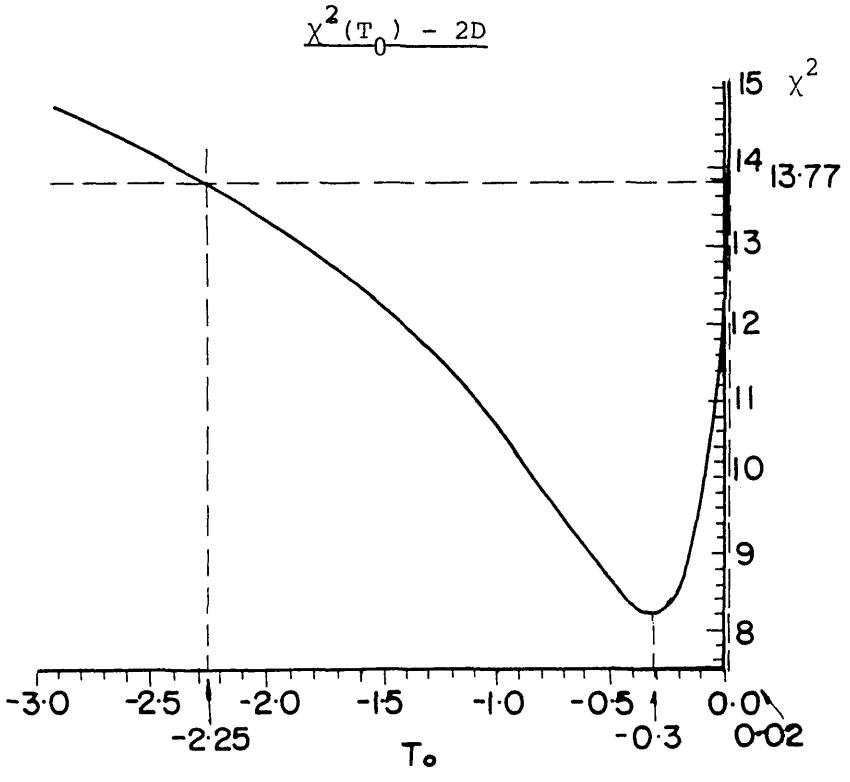


FIGURE 4·3a



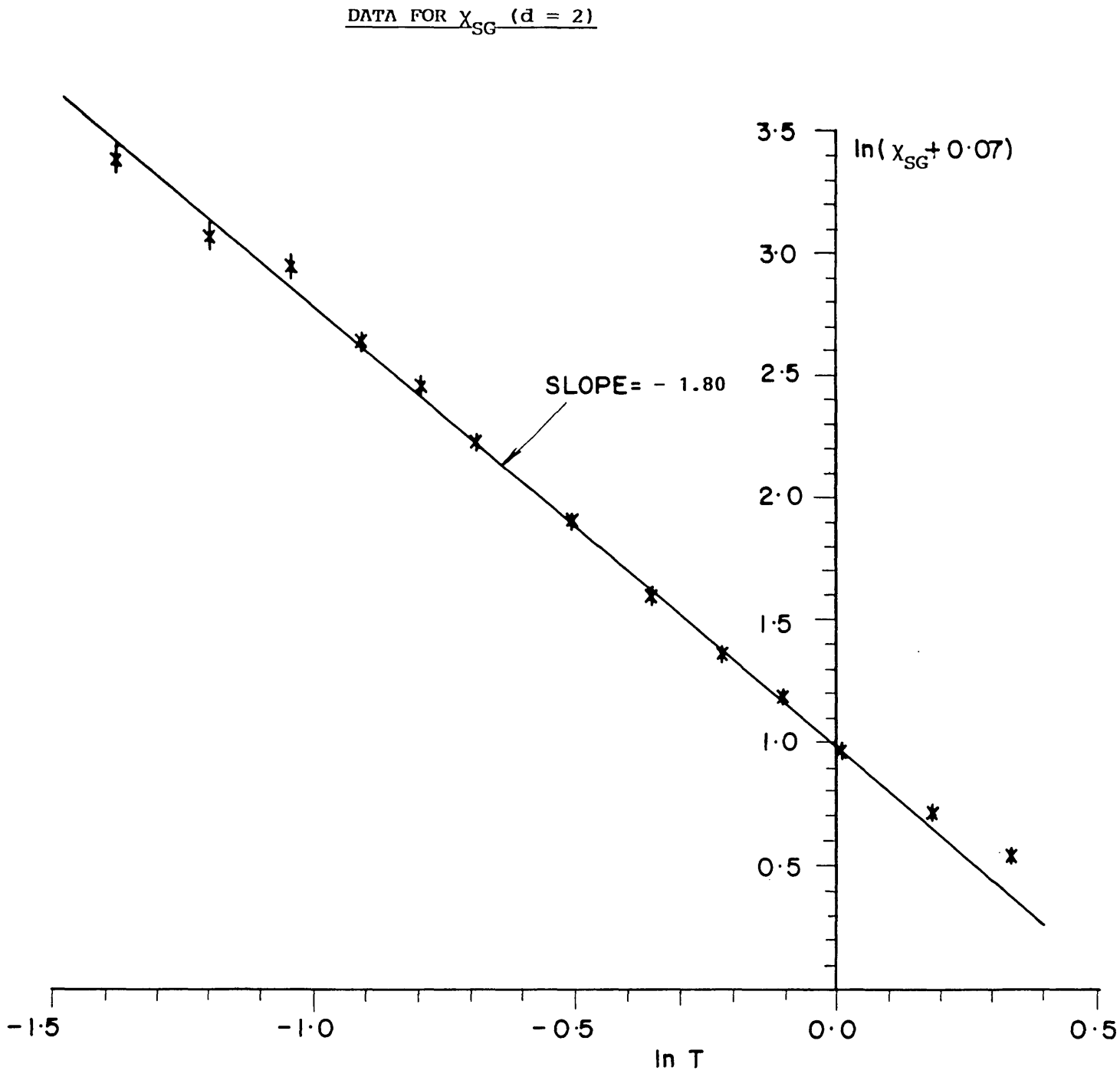
AS THE "CUT-OFF" IS 13·77 (SEE APPENDIX IV), WE HAVE A GOOD FIT FOR $-0{\cdot}25 \leq \chi_0 \leq 1{\cdot}68$

FIGURE 4·3b



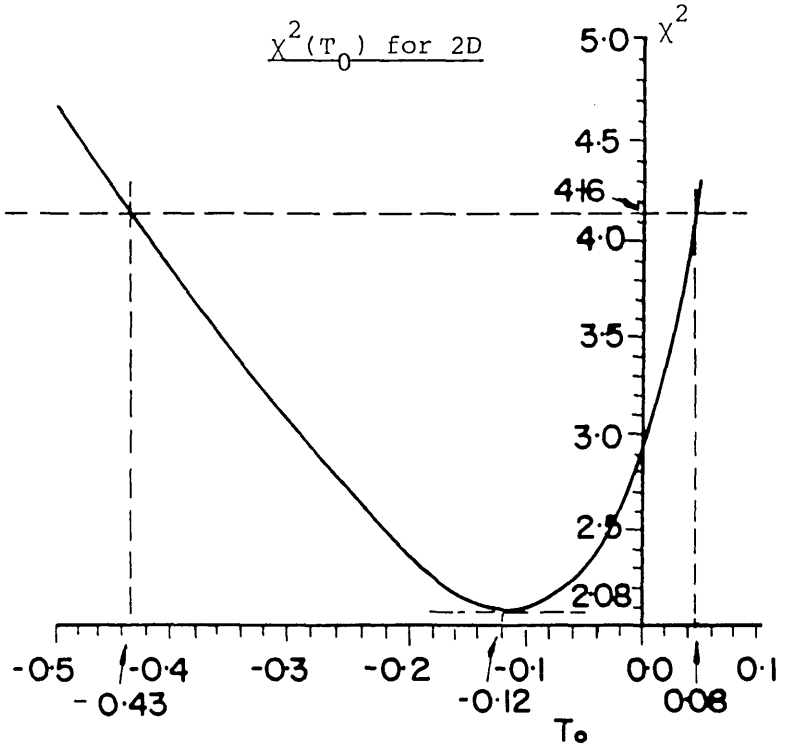
SO WE HAVE A GOOD FIT FOR $-2{\cdot}25 \leq T_0 \leq 0{\cdot}02$

FIGURE 4·4



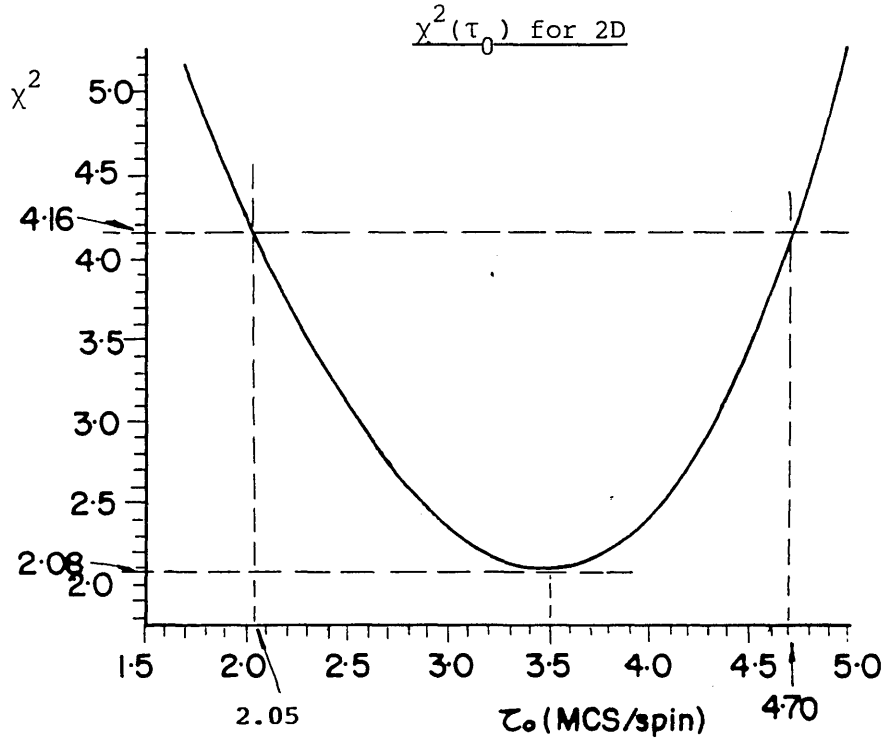
ABOVE WE PLOT THE DATA FOR χ_{SG} ASSUMING THAT $T_c=0$; WE ALSO INDICATE THE CONSEQUENT LINE OF BEST FIT (SEE TEXT). TEMPERATURE IS GIVEN IN UNITS OF J.

FIGURE 4·5a



AN ACCEPTABLE FIT FOR $-0{\cdot}43 \leq T_0 \leq 0{\cdot}05$

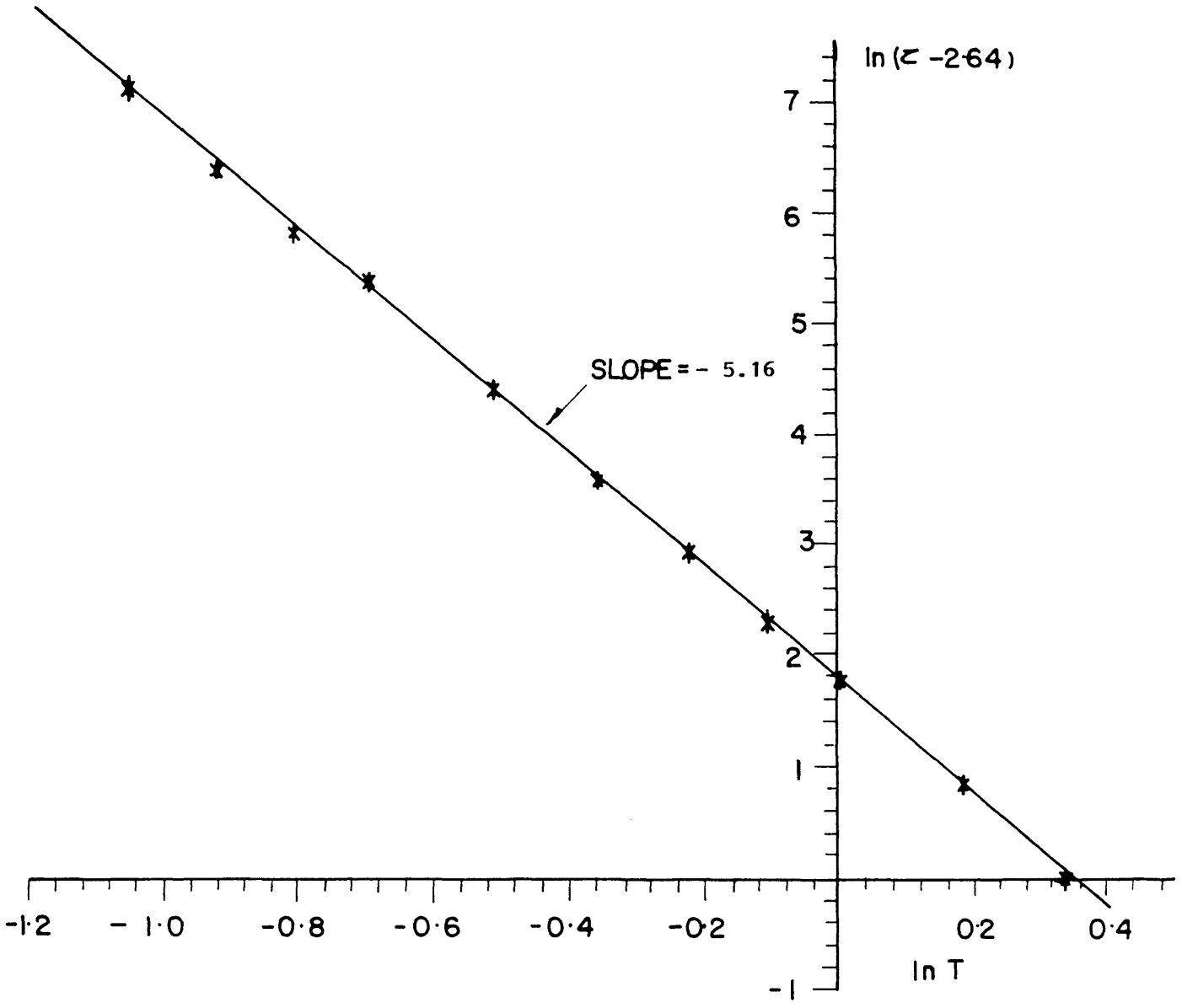
FIGURE 4·5b



A GOOD FIT FOR $2{\cdot}05 \leq \tau_0 \leq 4{\cdot}70$

FIGURE 4·6

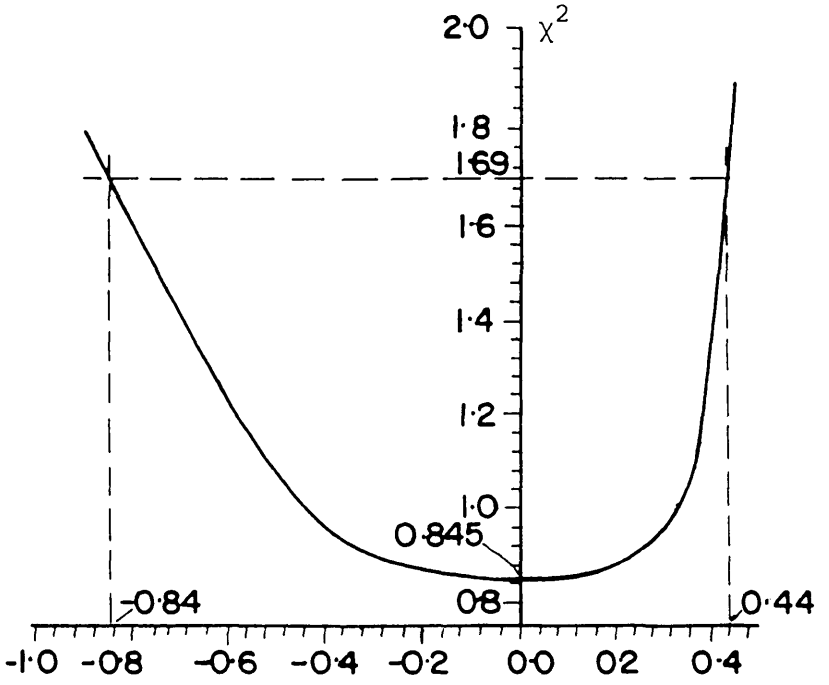
DATA FOR τ (d = 2)



A PLOT OF ln (τ -2·64) VERSUS ln T ; THE LINE OF BEST FIT HAS GRADIENT = - 5.16

FIGURE 4·7a

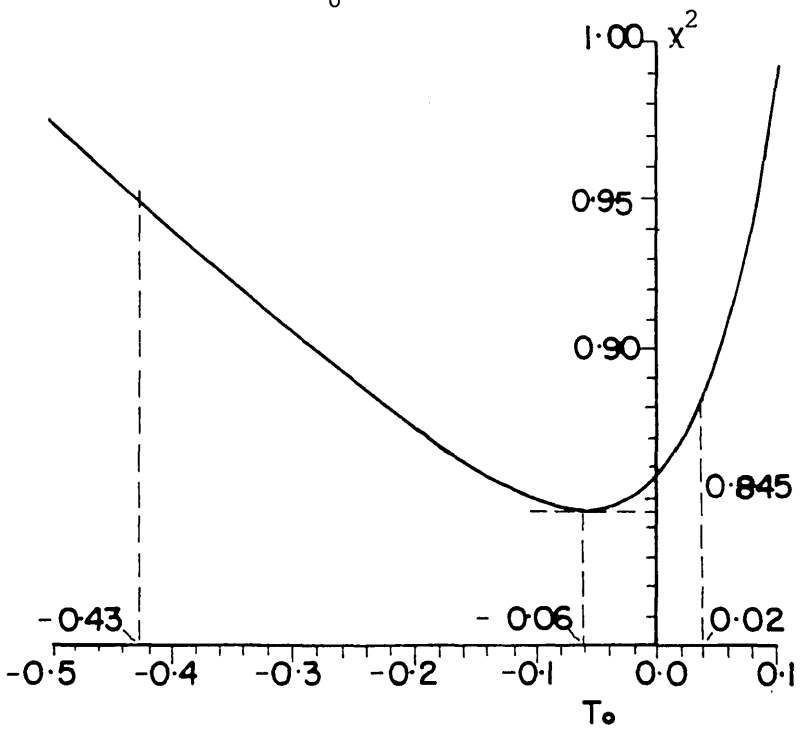
$\chi^2(\xi_0)$ in two-dimensions



An acceptable fit for $-0{\cdot}84 \leq \xi_0 \leq 0{\cdot}44$

FIGURE 4·7b

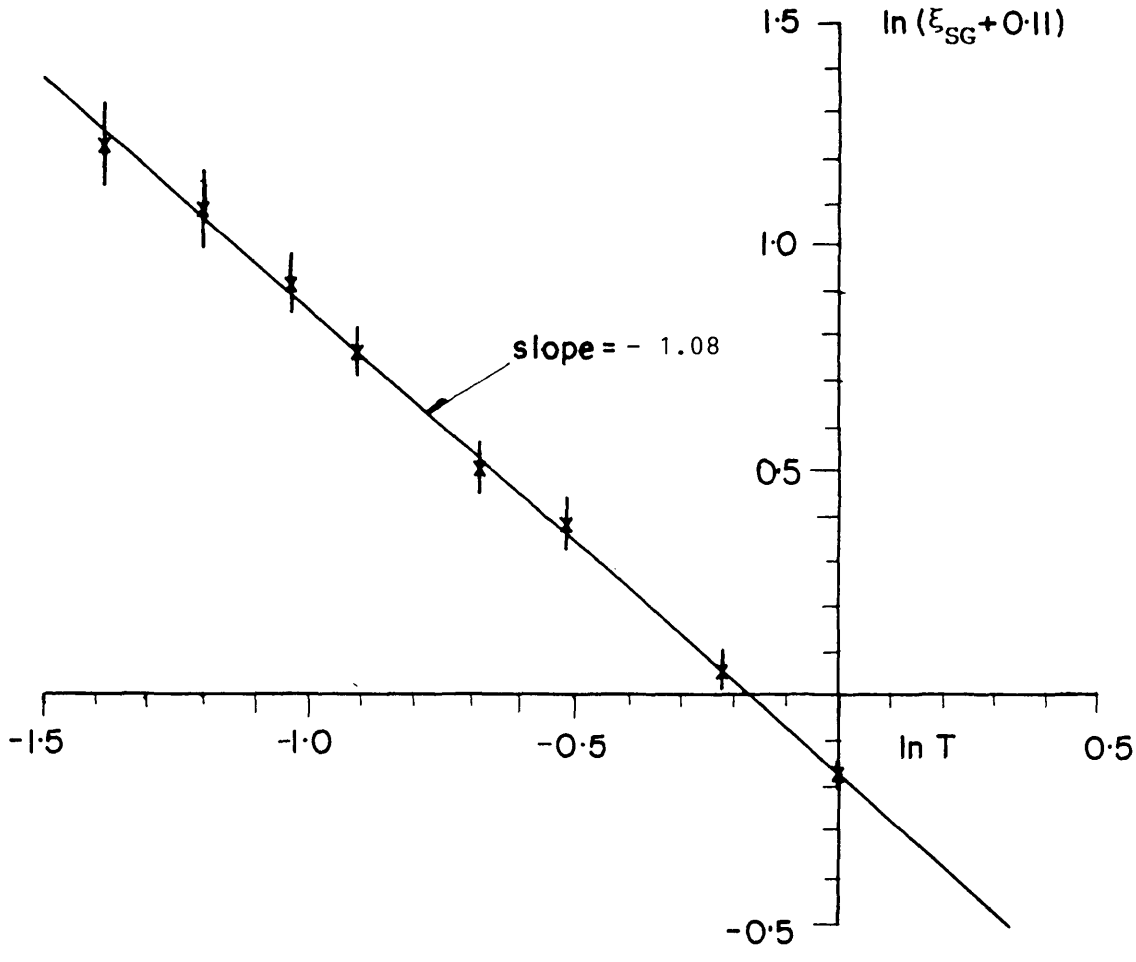
$\chi^2(T_0)$ in two-dimensions



This curve is extremely shallow and we get a good fit for all attempted values of T_0

FIGURE 4.8

DATA FOR ξ_{SG} (d = 2)



Data for ξ_{SG} plotted as $\ln(\xi_{SG}+0.11)$ versus ln T.

The straight line shown has gradient - 1.08.

FIGURE 4.9a

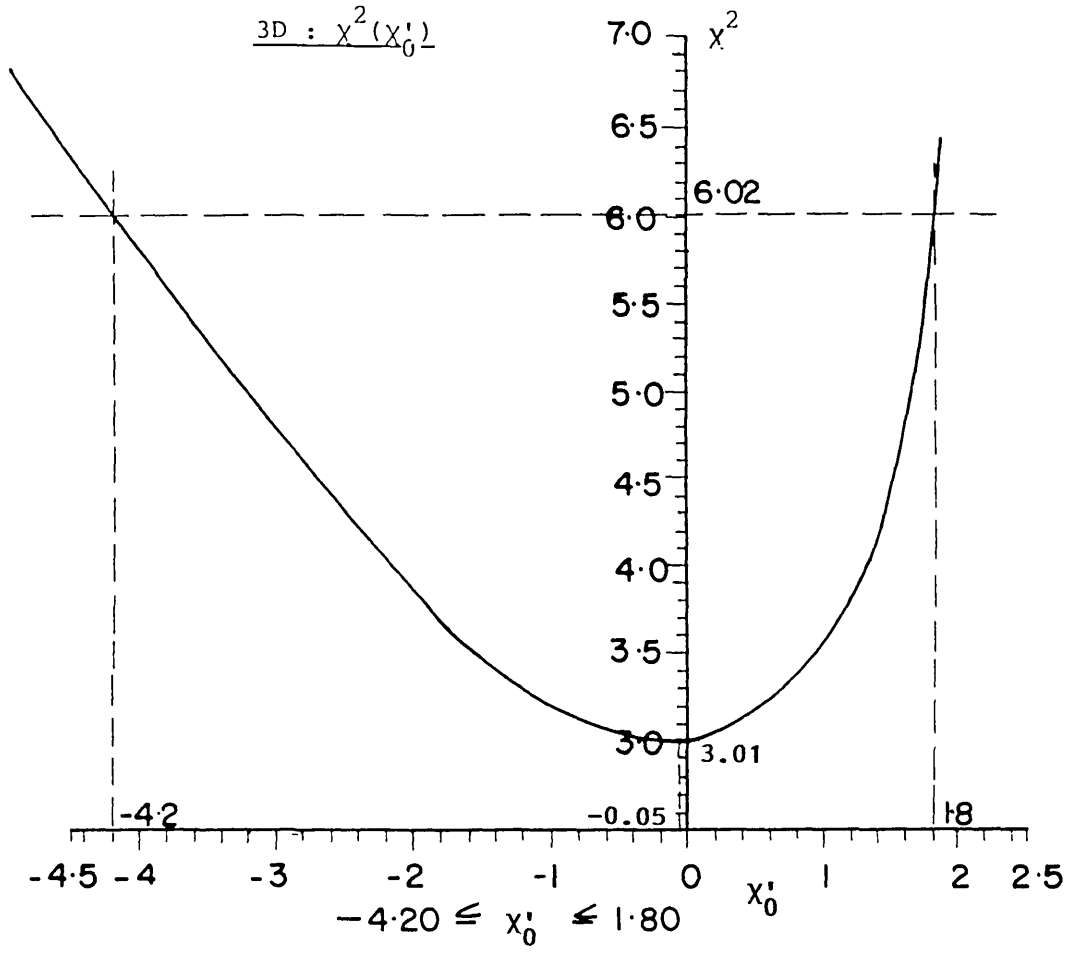


FIGURE 4.9b

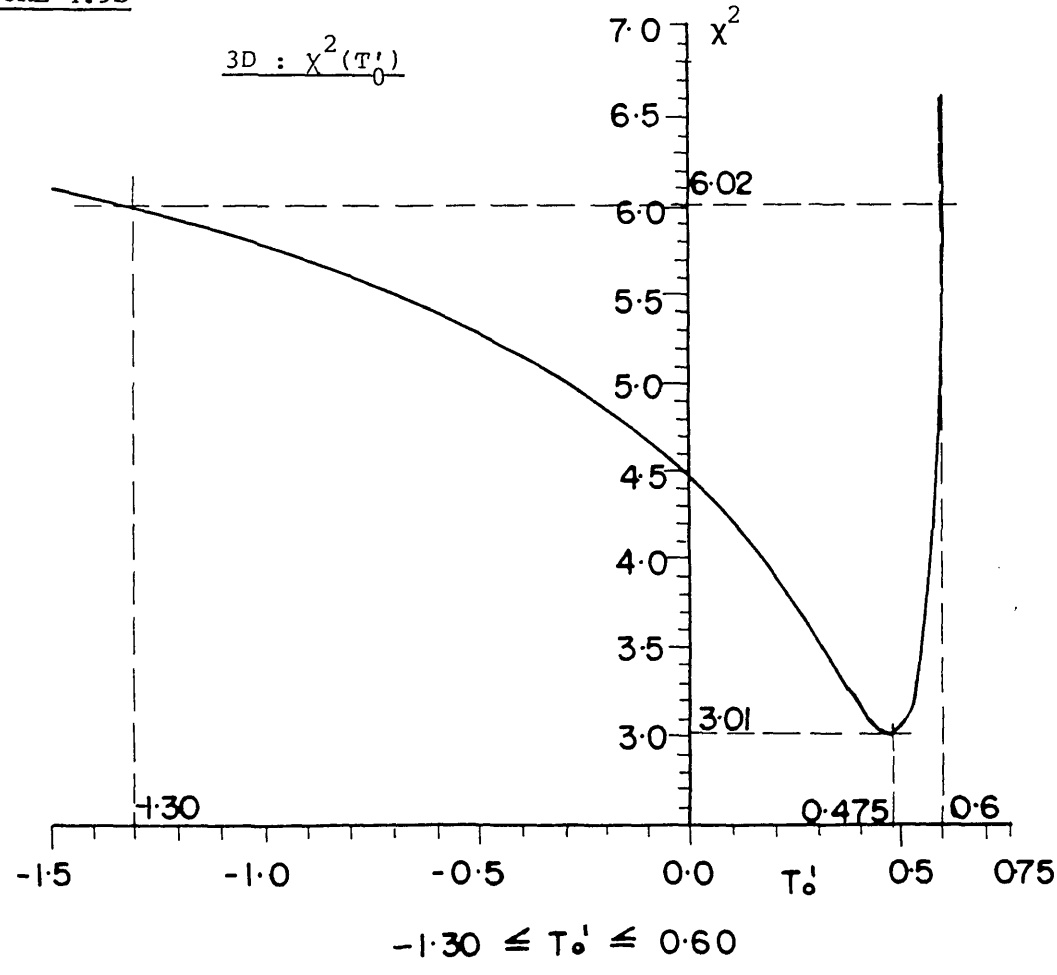


FIGURE 4.10a A plot of the data for χ_{SG} with $T_c = 0$

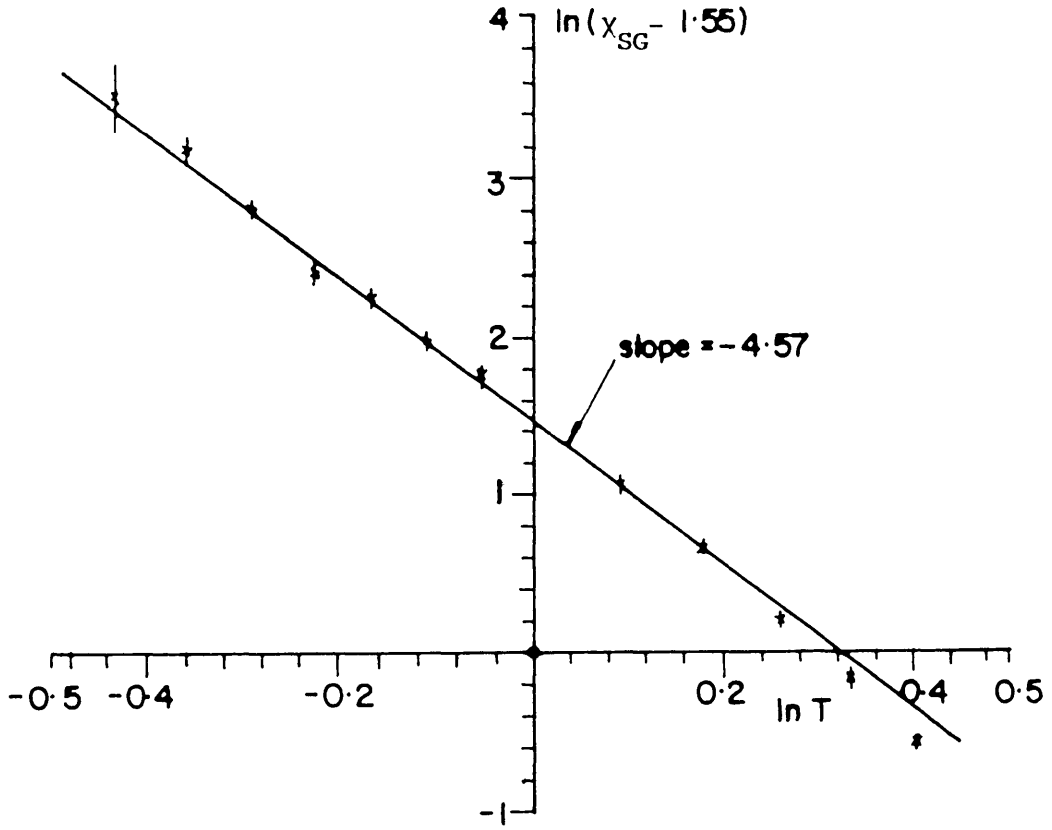


FIGURE 4.10b A plot of the data for χ_{SG} with $T_c = 0.45$

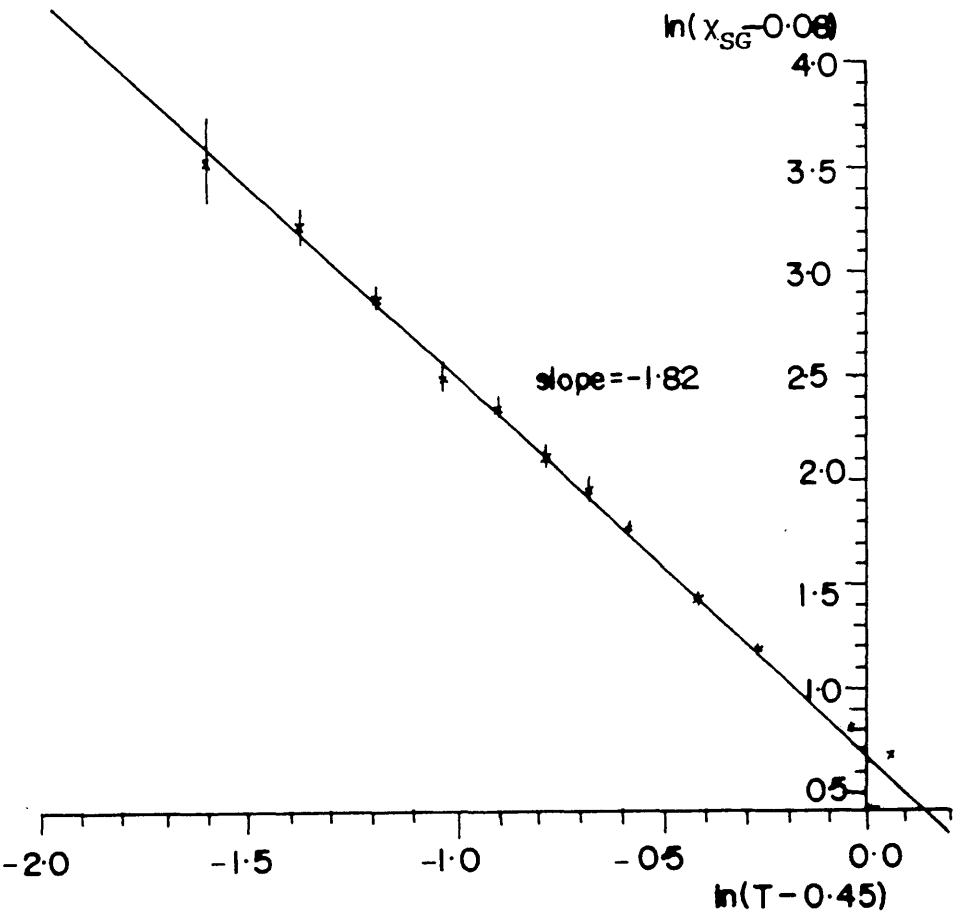
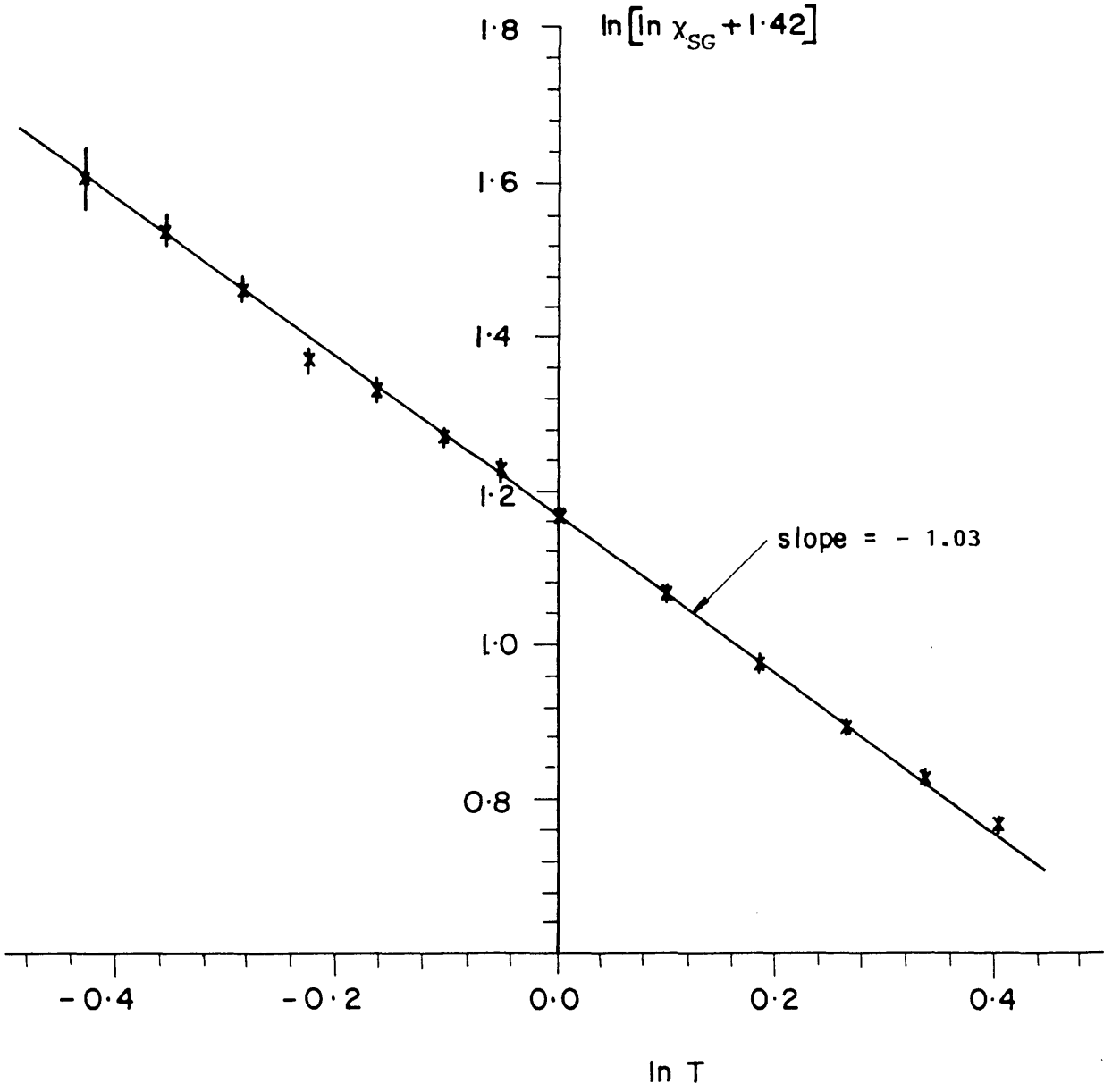
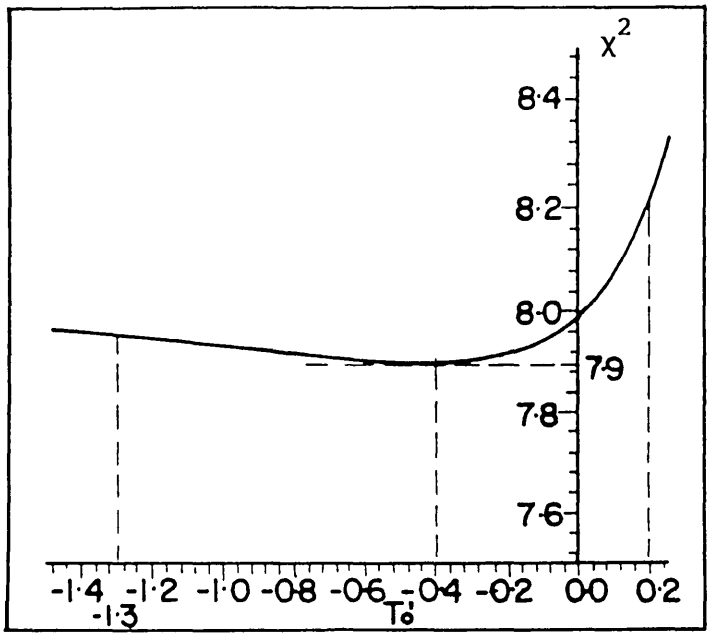


FIGURE 4.11

ln [ln χ_{SG} + 1·42] versus ln T



The data plotted assuming that the L C D for the X - Y spin-glass is three. See text and equations (4.115) and (4.116).



χ^2 (T_o') for $\mathcal{C}$ (3D)

FIGURE 4·12a

The quality of the fit of the data to equation (4.117a). We have that

$-1.3 \leq T_o' \leq 0.2$

and

$0.11 \leq \tau_0 \leq 1.54$

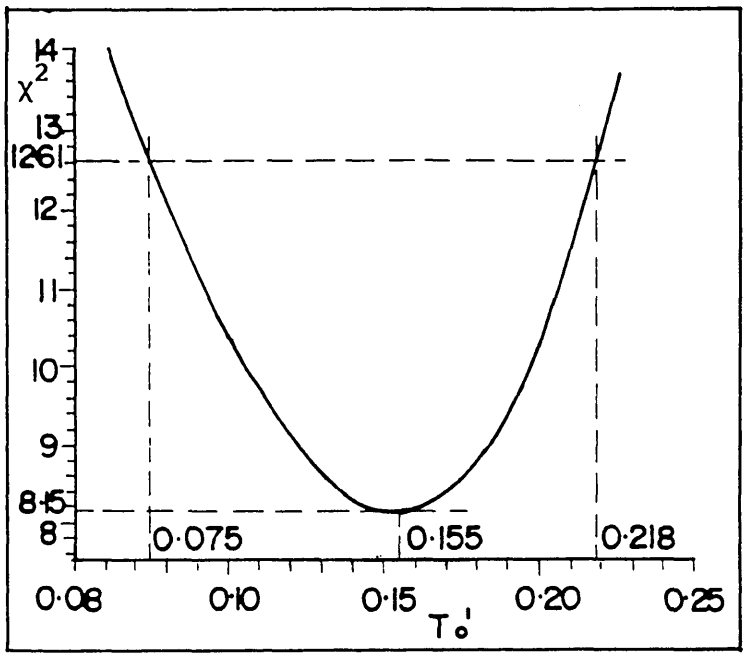


FIGURE 4·12b

The range of values of T_0' for which the Vogel-Fulcher law (4.117b) gives a good fit:

$0.075 \leq T_o' \leq 0.218$

At the best fit one has

$T_o' = 0.155$, $\tau_o = 0.16$ and

$E = 4.52$

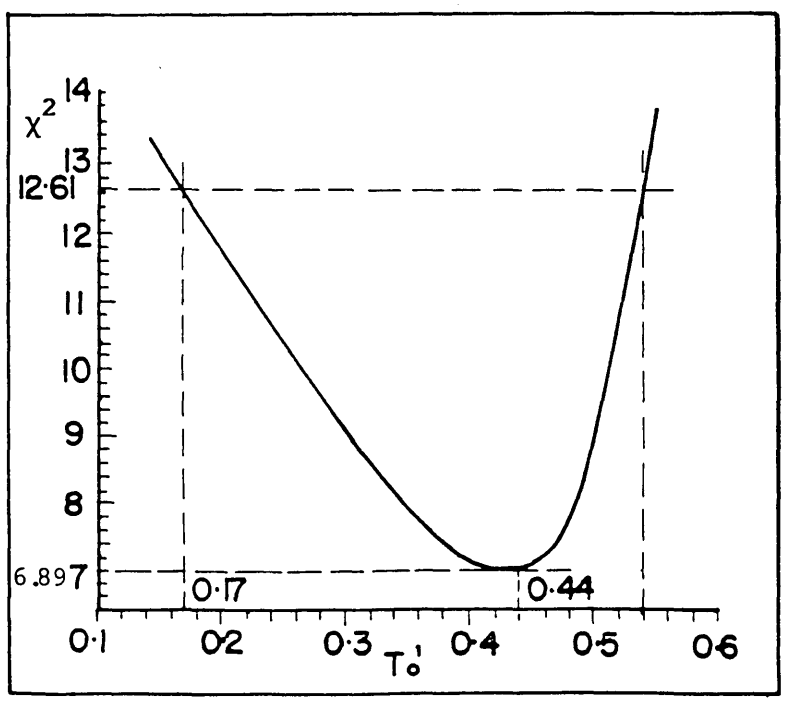


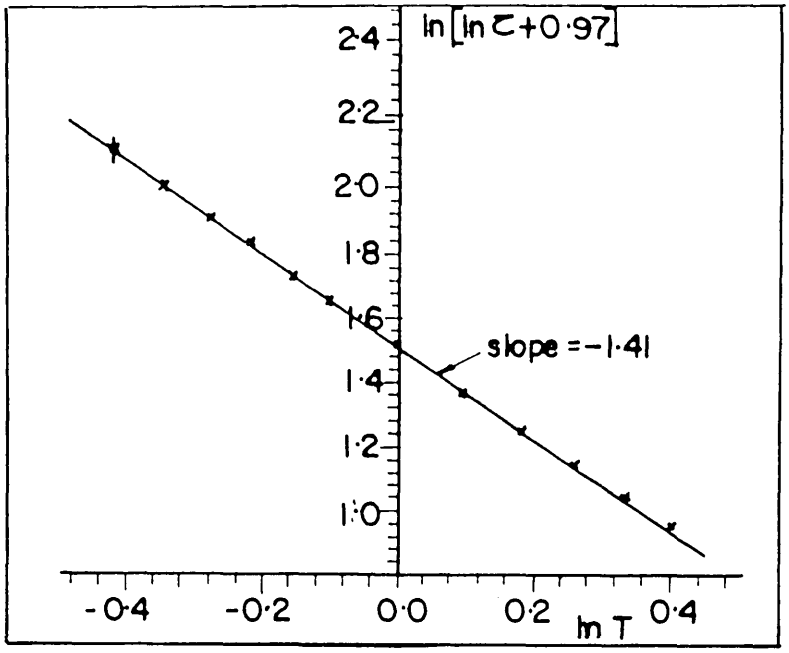
FIGURE 4·12C

The fit of the data to (4.117c). This time we have that

$0.17 \leq T_0' \leq 0.54$

and

$-0.30 \leq \tau_0 \leq 5.95$



PLOTS OF THE DATA FOR τ (3D)

FIGURE 4.13a

The data plotted assuming that (4.117a) holds with $T_c = 0{\cdot}0$ With this fit we find that the energy barriers $\simeq 4{\cdot}48$ (in units of J)

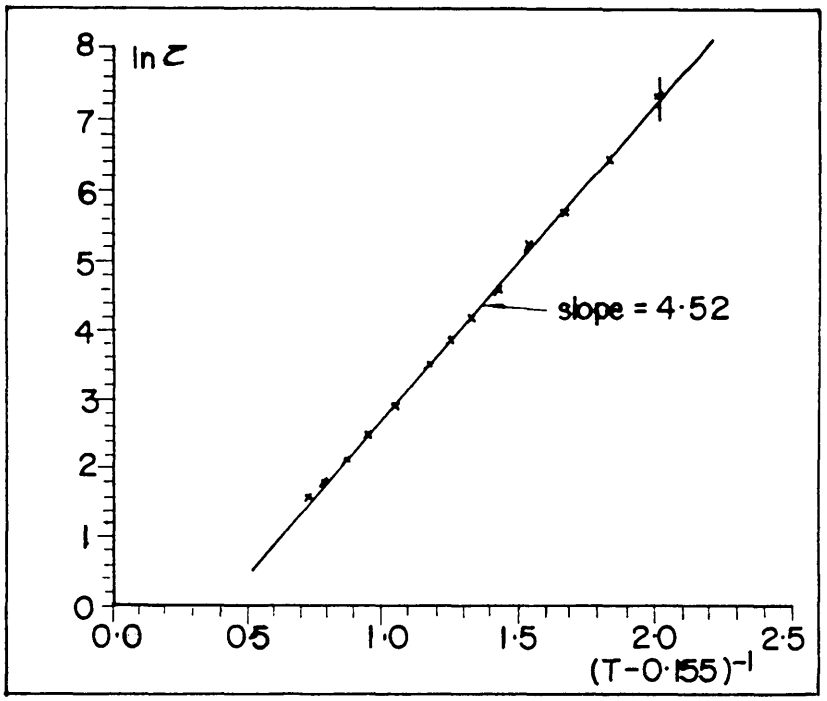


FIGURE 4.13b

The best fit assuming that the Vogel-Fulcher law (4.117b) holds. The freezing temperature is estimated to be 0·155 (in units of J).

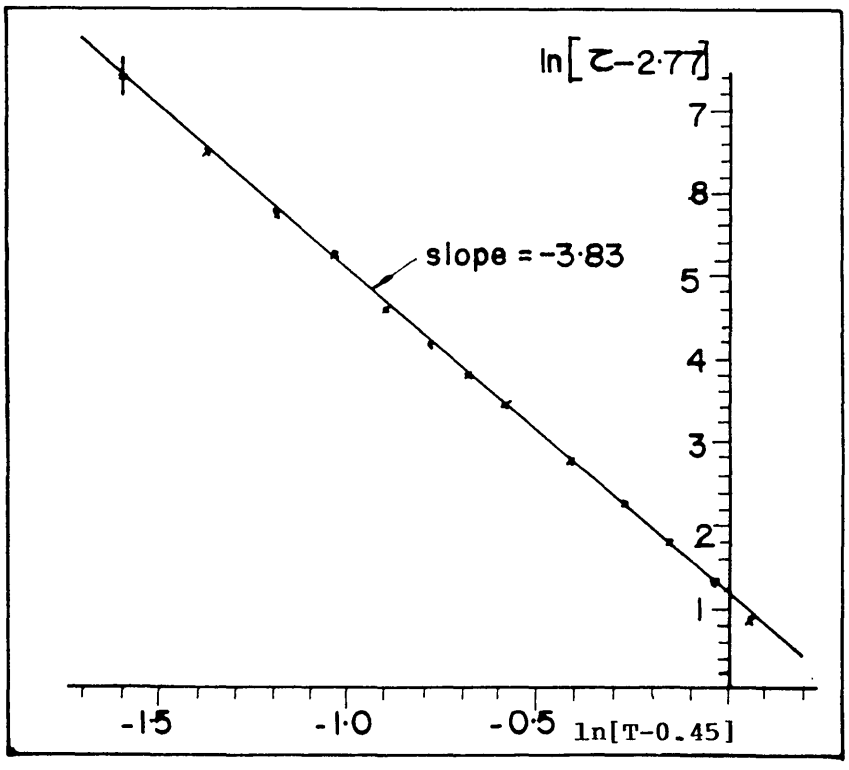
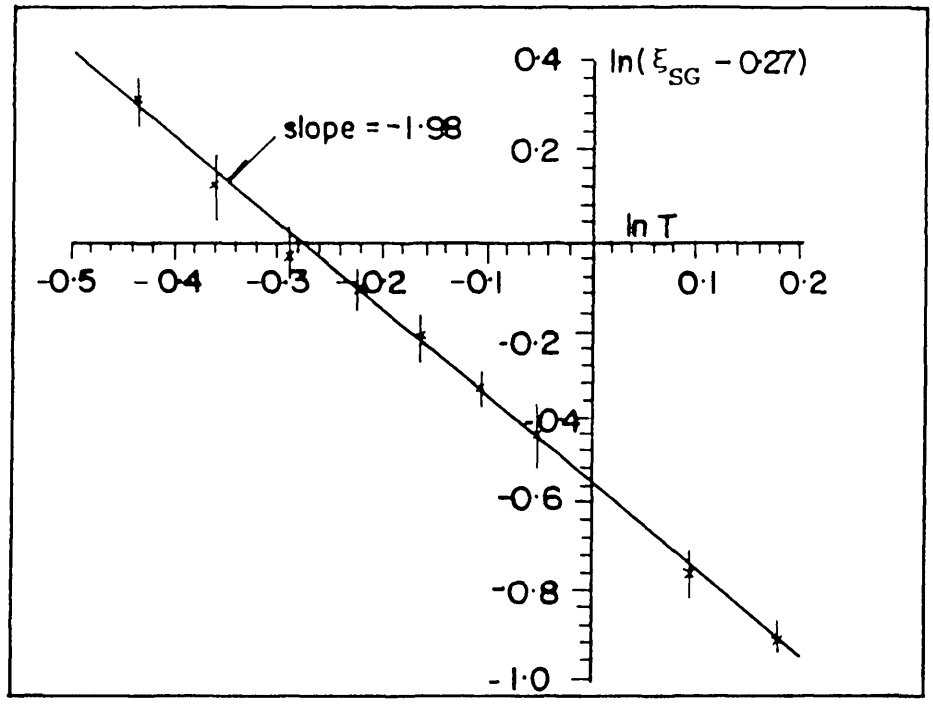


FIGURE 4.13c

The data can also be fitted by (4.117c). Here we plot $\ln[\tau - \tau_0]$ against $\ln[T - T_c]$ with $\tau_0 = 2{\cdot}77$ and $T_c = 0{\cdot}45$

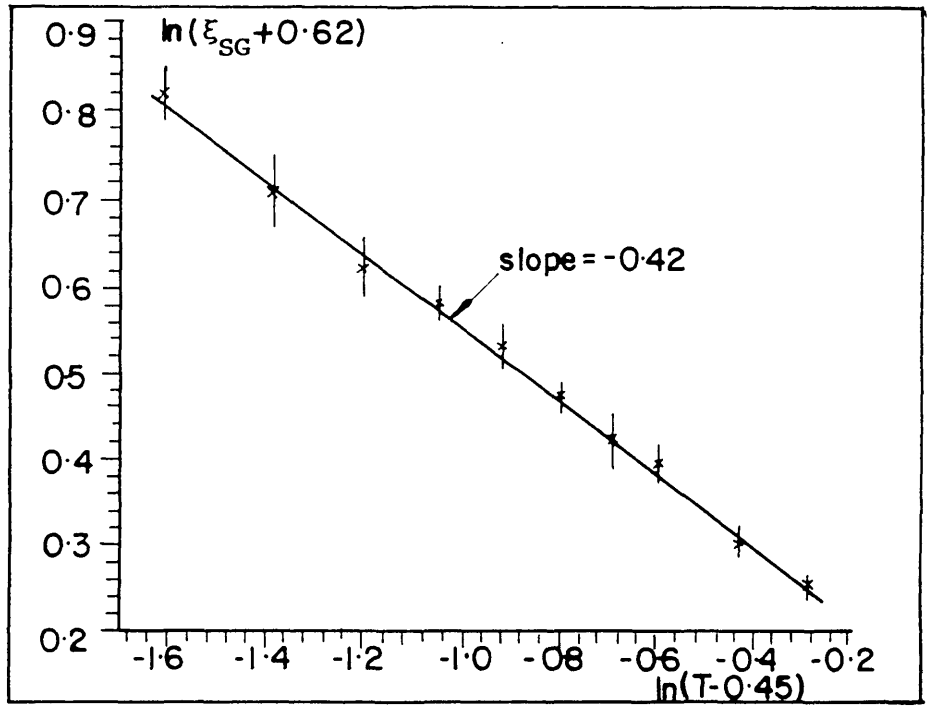
PLOTS OF ξ_{SG} FOR 3D

FIGURE 4·14a



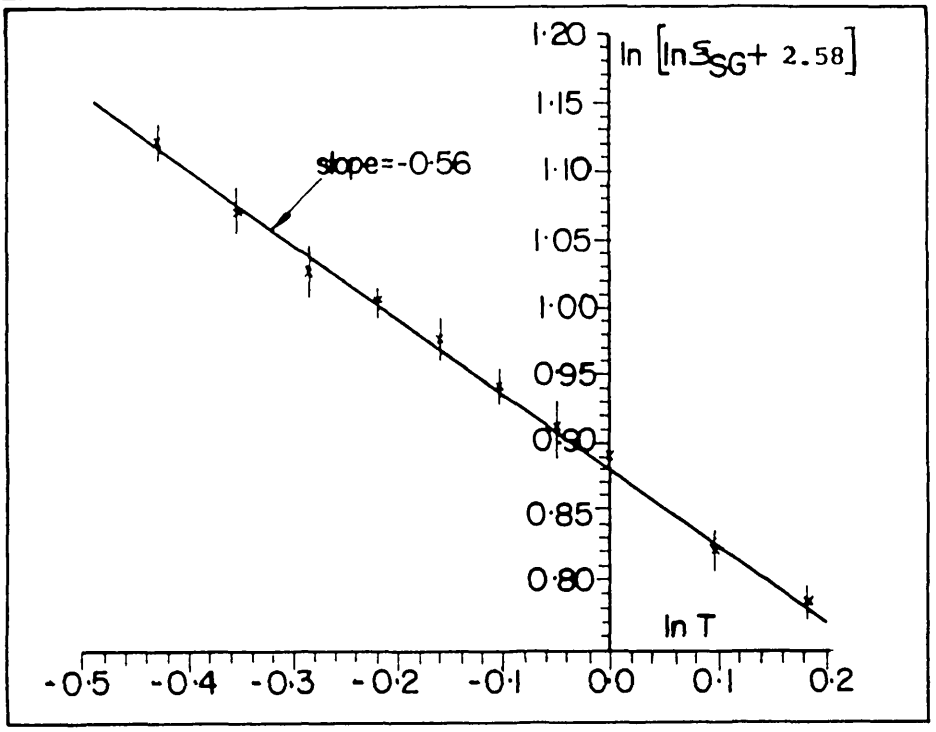
A Plot of the data assuming that $T_c = 0{\cdot}0$. The other parameters in (4.122) are $\xi_0' = 0{\cdot}27$, $D' = 0{\cdot}58$ and $\nu_{SG} = 1{\cdot}98 \mp 0{\cdot}54$

FIGURE 4·14b



We also plot the data assuming that $T_c = 0{\cdot}45$ ($\xi_0' = -0.62$, $D' = 1{\cdot}14$, $\nu_{SG} = 0{\cdot}42 \mp 0{\cdot}21$)

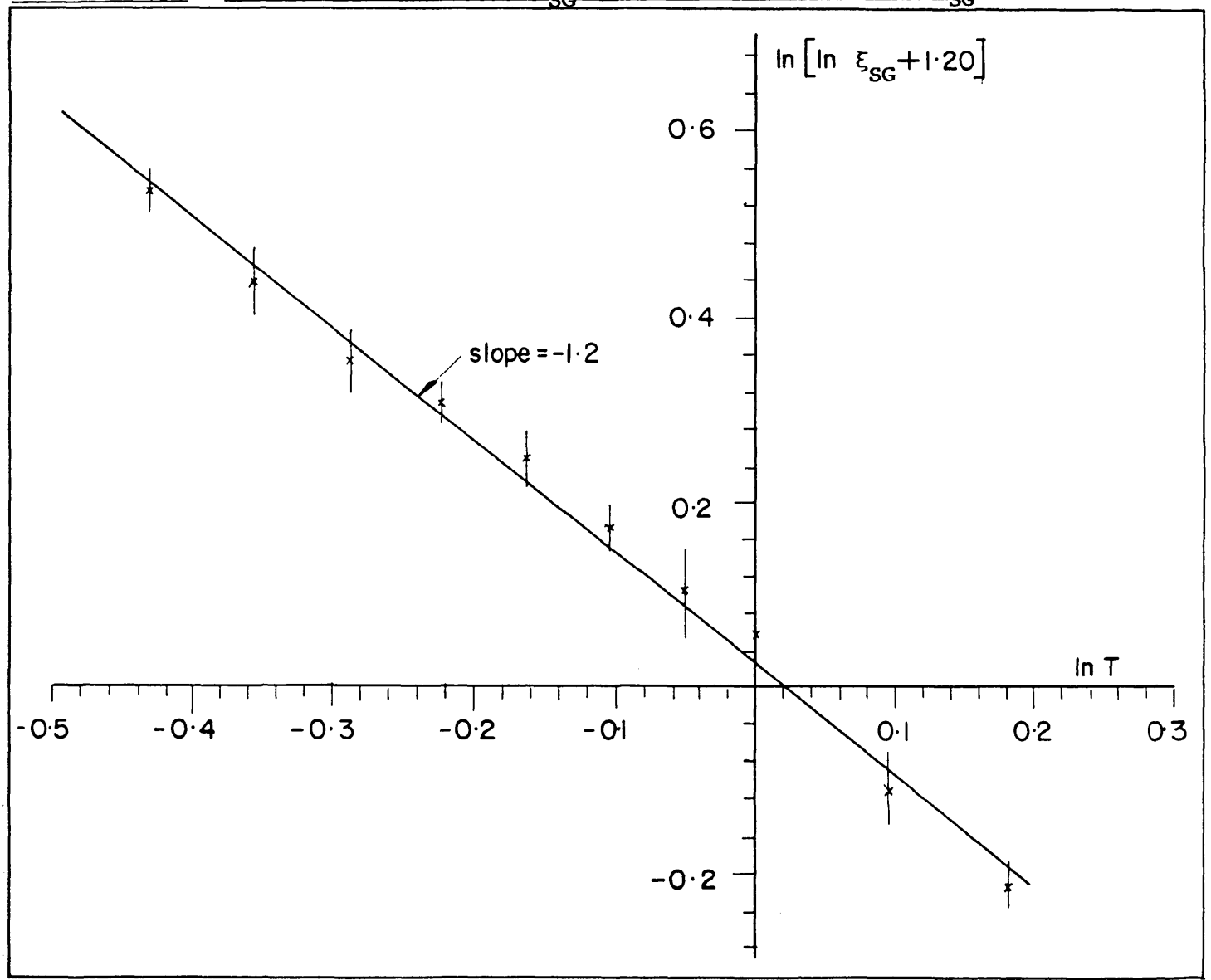
FIGURE 4·15a



Here we plot the data assuming that the LCD = 3 (4.123). The best fit is obtained for $\tilde{\xi}_0 = 0{\cdot}08$, $\tilde{D} = 2{\cdot}41$ and $\ell_{SG} = 0{\cdot}56 \mp 0{\cdot}48$

A PLOT OF THE DATA FOR ξ_{SG} ASSUMING THAT LCD = 3

FIGURE 4·15b A PLOT OF THE DATA FOR ξ_{SG} ASSUMING THAT LCD = 3 AND $\rho_{SG} = 1.2$



A plot of the data with the exponent ℓ_{SG} set to 1·2. One then has $\tilde{\xi}_0 = 0{\cdot}30$, $\tilde{D} = 1{\cdot}03$ and $\tilde{\chi}^2 = 4{\cdot}10$

FIGURE A5.1a

The DAP

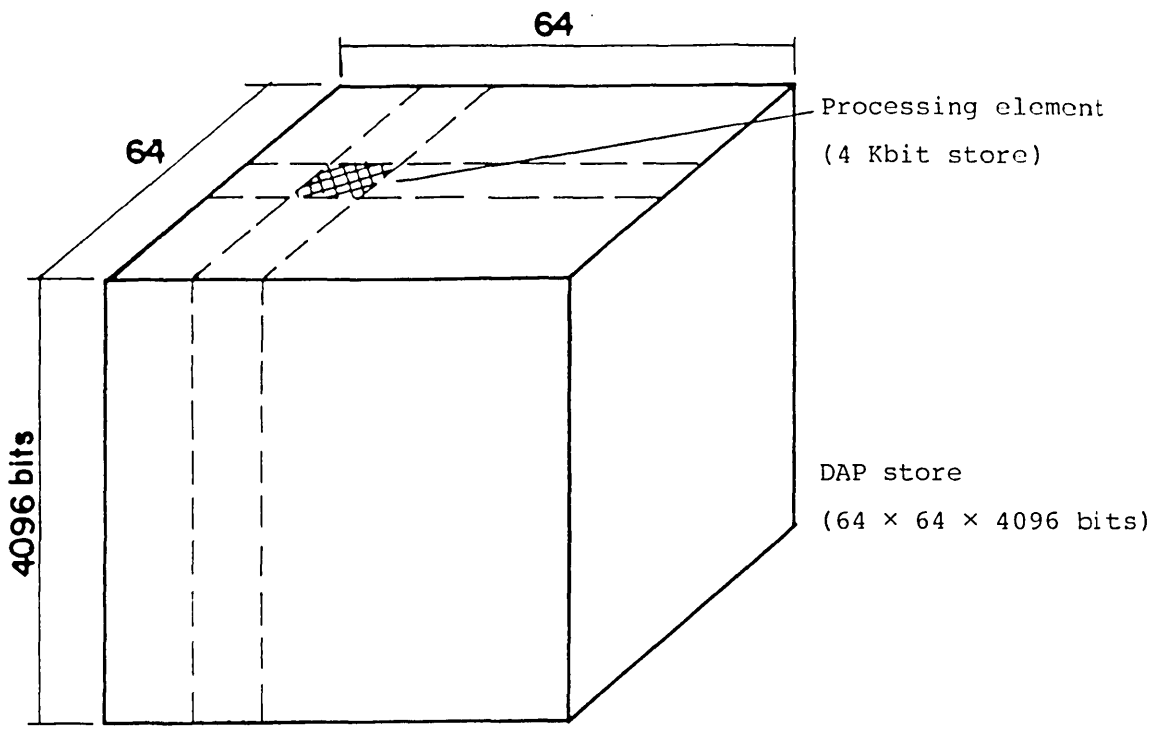
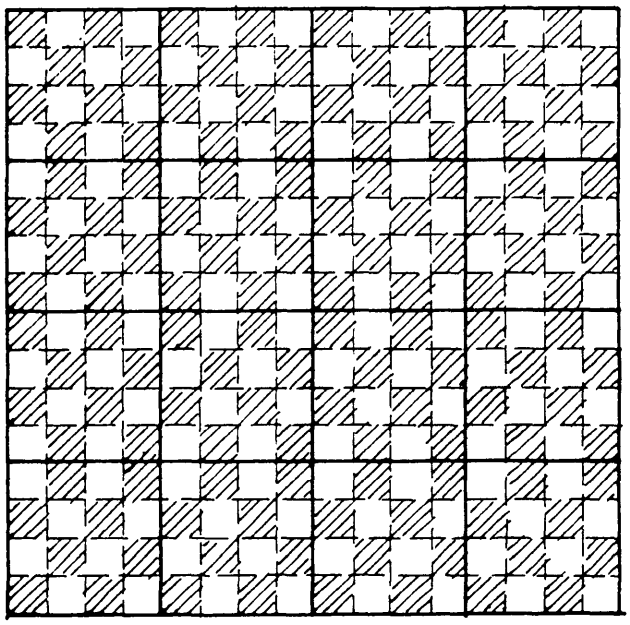


FIGURE A5.1b

The Map



16 x 16

1	5	9	13
2	6	10	14
3	7	11	15
4	8	12	16

On the left we indicate (on a 16 × 16) matrix) the mapping used to simulate 2D and 3D lattices on the DAP.

The DAP is effectively partitioned into 16 blocks as shown. Periodic boundary conditions are imposed in both directions within each block. For a 2D lattice we simulate 16 independent samples. A 3D lattice is constructed by connecting up the blocks as shown, that is block 1, which forms the uppermost plane, is connected to block 2, which is connected to block 3,..., which is connected to block 16, which is connected to block 1. Thus we are able to consider just one sample in 3D.

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