Dynamic linear response of the SK spin glass coupled microscopically to a bath

T Plefka

Theoretische Festkörperphysik, TU Darmstadt, D 64289 Darmstadt, Germany

E-mail: timm@arnold.fkp.physik.tu-darmstadt.de

Abstract
The dynamic linear response theory of a general Ising model weakly coupled
to a heat bath is derived by employing the quantum statistical theory of Mori,
treating the Hamiltonian of the spin bath coupling as a perturbation, and
applying the Markovian approximation. Both the dynamic susceptibility and
the relaxation function are expressed in terms of the static susceptibility and the
static internal field distribution function. For the special case of the SK spin
glass, this internal field distribution can be related to the solutions of the TAP
equations in the entire temperature region. Application of this new relation and
the use of numerical solutions of the modified TAP equations lead, for finite but
large systems, to explicit results for the distribution function and for dynamic
linear response functions. A detailed discussion is presented which includes
finite-size effects. Due to the derived temperature dependence of the Onsager–
Casimir coefficients, a frequency-dependent shift of the cusp temperature of
the real part of the dynamic susceptibility is found.

PACS numbers: 75.10.Nr, 05.50.+q, 87.10.+e

1. Introduction

The Ising model of Sherrington–Kirkpatrick (SK) [1] with quenched random bonds is the
most important representative of a class of long-ranged models that describe spin glasses (see,
in general, [2–4]). For the static analysis of this model, two complementary but conceptually
different approaches exist. The first approach uses the replica method [1] and the breaking of
the replica symmetry [5] to calculate bond-averaged quantities. The approach of Thouless–
Anderson–Palmer (TAP) [6] is based on more conventional techniques and does not perform
this bond average as it is expected that macroscopic physical quantities will be independent of
the particular configuration in the thermodynamic limit.

Although the TAP equations are well established [2, 3, 7] they are still a field of current
interest. It is suspected that not all aspects of this approach have yet been worked out.

Recently, the author [8] has re-analysed the stability of these equations and has shown that unstable states cannot be described by the original TAP equations. Therefore, he proposed modified TAP equations which turned out to be useful for explicit numerical calculations of the characteristic features of the SK model of finite sizes [9].

Dynamical questions are of great importance for the physics of spin glasses (for reviews see [2–4]). Therefore numerous dynamical extensions have been added to the SK model. Following the early dynamical approaches [1, 10] Glauber dynamics has been used by various authors [8, 11, 12]. In addition, Langevin dynamics has been employed in the studies [13] mostly for the soft spin version of the SK model. Both the Langevin and the Glauber dynamics are basically phenomenological and can at best be justified partially by microscopic arguments. Note that this also applies to the work of Szamel [12] although this approach is formulated in the 'spirit' of the microscopic Mori theory.

The aim of this paper is to present a compete microscopic analysis of the dynamical linear response for the SK model coupled to a bath. An adequate tool for this purpose is the general theory of Mori [14, 15]. This quantum-statistical approach is used in the present work and is worked out not only for the SK model but also for a general Ising model. Such a treatment is obvious and straightforward. Nevertheless, to the author's knowledge it has not been published previously.

As usual, the results of the Mori theory are expressed in terms of static equilibrium quantities. Together with the static isothermal susceptibility, it is the internal field distribution function [18, 19] which fully determines the dynamical linear response. At this point, we restrict the approach to the SK model. It is shown that the internal field distribution function can be related to the solutions of the TAP equations. Employing the approximate TAP solutions [9], all the quantities of the linear response theory can be numerically calculated in the entire temperature regime for all external fields.

Thomsen *et al* [18, 19] showed that an exact and complete description of the thermodynamics of Ising models can be formulated in terms of the internal field distribution function. Thus as a by-product the presented results of this function are of some interest, independent of the dynamical linear response problems.

Following a description of the microscopic Hamiltonian, the Mori approach for a general Ising system is performed in section 2. The internal magnetic field distribution function for the SK model is treated in section 3. Both the analytical and numerical results for the field distribution function, the dynamic susceptibility and the response function are explicitly presented in section 4. Finally, some concluding remarks can be found in section 5.

2. Linear response for a general Ising system

2.1. The microscopic system

A system of N spins s_i with $s = \frac{1}{2}$ is considered in the presence of external fields H_i. The spins interact via an arbitrary Ising spin–spin interaction J_{ij} $(=J_{ji})$ and are described by the spin Hamiltonian

$$\mathcal{H}^S = -\frac{1}{2} \sum_{i,j} J_{ij} S_i S_j - \sum_i H_i S_i = -2 \sum_{i,j} J_{ij} s_i^z s_j^z - 2 \sum_i H_i s_i^z \tag{1}$$

where $J_{ii} = 0$ is presumed. Both quantum spin-$\frac{1}{2}$ operators s_i^z and Ising spins S_i $\left(= 2s_i^z\right)$ are used simultaneously in this work. Note that at this stage the bonds J_{ij} are quite general.

The assembly of spins is weakly coupled to a bath described by the Hamiltonian $\mathcal{H}^B$ via a spin bath interaction,

$$\mathcal{H}^{SB} = \sum_i B_i s_i = \sum_i \frac{1}{2} (B_i^+ s_i^- + B_i^- s_i^+) + B_i^z s_i^z \tag{2}$$

where the operators B_i represent variables of the bath system. Thus the total Hamiltonian is given by

$$\mathcal{H} = \mathcal{H}^0 + \mathcal{H}^{SB} \qquad \text{with} \quad \mathcal{H}^0 = \mathcal{H}^B + \mathcal{H}^S. \tag{3}$$

There is no need for an explicit specification of the bath Hamiltonian $\mathcal{H}^B$ and the bath operators B_i. As shown below, it is just the absorptive part $\chi_B''(\omega)$ of the dynamic bath susceptibility

$$\chi_B(\omega) = \chi_B'(\omega) + \mathrm{i}\chi_B''(\omega) = -\mathrm{i} \int_0^\infty \langle [B_i^-, \mathrm{e}^{\mathrm{i}\mathrm{L}^B t} B_i^+] \rangle_{(B)} \, \mathrm{e}^{\mathrm{i}\omega t} \, \mathrm{d}t \tag{4}$$

which enters the calculation and is assumed to be known. In equation (4) $\langle \ldots \rangle_{(B)}$ represents the canonical thermal expectation value with respect to $\mathcal{H}^B$ and L^B denotes the Liouville operator defined by $\mathrm{L}^B A = [\mathcal{H}^B, A]$. For later use, note that $\chi_B''(\omega)$ may be rewritten as

$$\chi_B''(\omega) = \pm\pi (\mathrm{e}^{\pm\beta\omega} - 1)\langle B_i^\mp \delta(\mathrm{L}^B \pm \omega) B_i^\pm \rangle_{(B)} \tag{5}$$

which can easily be shown or found in the literature [15]. In writing equation (4), it is assumed that the bath susceptibilities do not depend on the site i. This assumption is not essential and an extension to the general case is straightforward.

Let τ_B and τ_S be the relaxation times of the bath and the spin system respectively. Then it is natural to assume a fast relaxation to thermal equilibrium for the bath system compared to the spin system which implies

$$\tau_B \ll \tau_S. \tag{6}$$

For the explicit determination of linear response quantities (see section 4) the bath susceptibility $\chi_B''(\omega)$ enters for $\omega\tau_S \approx 1$. This implies $\omega\tau_B \ll 1$ and

$$\chi_B''(\omega) \approx \mathrm{const}\,\omega \qquad \text{for} \quad \omega \ll \tau_B^{-1} \tag{7}$$

can be used in the generic case for the explicit calculations below. If the simple form $\chi_B(\omega) = \chi_B(1 - \mathrm{i}\omega/\tau_B)$ is presumed, the constant of proportionality is given by $\mathrm{const} = \chi_B/\tau_B$, which may in principle be temperature dependent. This dependence is neglected in this work by assuming a slow variation on scale determined by the spin glass temperature. This assumption is to a certain extent arbitrary but can be justified for special cases. Such a case is the Korringa mechanism, where the bath and the B_i are identified as the conduction electrons and itinerant spin density operators respectively.

2.2. Mori formalism for the dynamic susceptibility

The linear response of the magnetizations

$$\langle S_i \rangle(t) - \langle S_i \rangle = \sum_j \chi_{ij}(\omega) h_j^{ex} \, \mathrm{e}^{\mathrm{i}\omega t} \qquad t \geqslant 0 \tag{8}$$

due to small time-dependent external fields $h_i^{ex}\,\Theta(t)\,\mathrm{e}^{\mathrm{i}\omega t}$ is governed by the dynamic susceptibility matrix $\chi(\omega)$ which is given by the Kubo formula written in the Liouville space [14, 15]

$$\chi_{ij}(\omega) = \beta(\tilde{S}_i | \mathrm{L}\{\mathrm{L} + \omega + \mathrm{i}\eta\}^{-1} | \tilde{S}_j) \qquad \eta \to +0 \tag{9}$$

with $\tilde{A} = A - \langle A \rangle$. In the Liouville space, the operators A of the state space are considered as vectors $|A)$ with the temperature dependent Mori scalar product

$$(A|B) = \frac{1}{\beta} \int_0^\beta d\lambda \langle A^\dagger e^{-\lambda \mathcal{H}} B e^{\lambda \mathcal{H}} \rangle = \frac{1}{\beta} \langle A^\dagger (1 - e^{-\beta L}) L^{-1} B \rangle \qquad (10)$$

where $\langle \cdots \rangle$ is the canonical thermal expectation value with respect to $\mathcal{H}$. Operators in the Liouville space, like the Liouville operator

$$L|A) = |[\mathcal{H}, A]) \qquad (11)$$

will be written in roman type[1].

Introducing the projection operator in Liouville space,

$$P = \beta \sum_{ij} |\tilde{S}_i) \chi_{ij}^{-1} (\tilde{S}_j| \qquad \text{with} \quad \chi_{ij} = \beta(\tilde{S}_i|\tilde{S}_j) \qquad (12)$$

and applying the standard Mori projection procedure [14, 15] leads to

$$\chi^{-1}(\omega) = \chi^{-1} - i\omega \beta^{-1} L^{-1}(\omega) \qquad (13)$$

with

$$L_{ij}(\omega) = L'_{ij}(\omega) + iL''_{ij}(\omega) = i(S_i | LQ\{QLQ + \omega + i\eta\}^{-1} QL|S_j) \qquad (14)$$

and $Q = 1 - P$. The matrices χ and L represent the static isothermal susceptibility matrix and the dynamic Onsager–Casimir matrix respectively. Note that the vectors $|\tilde{S}_i)$ which span the subspace P commute. Thus the frequency matrix vanishes in the present case.

According to the standard approach [15] for a sufficiently weak coupling $\mathcal{H}^{SB}$, the Markovian approximation $L(\omega) \approx L'(0)$ can be applied in equation (13). Furthermore, the leading-order perturbation theory expressions can be used for both χ and $L'(0)$ in (13). The static isothermal susceptibility matrix is of the order zero and approximated by

$$\chi_{ij} = \beta \langle \tilde{S}_i \tilde{S}_j \rangle_{(S)} = \beta(\langle S_i S_j \rangle_{(S)} - m_i m_j) \qquad (15)$$

where $m_i = \langle S_i \rangle_{(S)}$ and $\langle \cdots \rangle_{(S)}$ is the canonical thermal expectation value with respect to the Ising Hamiltonian (1).

Setting $L = L'(0)$ the lowest order of this matrix is the second order in the perturbation and is given by

$$L_{ij} = \pi (Q^0 L^{SB} S_i \mid \delta(Q^0 L^0 Q^0) Q^0 L^{SB} S_j)_{(0)} = \pi (L^{SB} S_i \mid \delta(L^0) L^{SB} S_j)_{(0)} \qquad (16)$$

where L^{SB} and L^0 are the Liouville operators related to $\mathcal{H}^{SB}$ and $\mathcal{H}^0$ respectively. The index (0) denotes the Mori product taken with $\mathcal{H}^0$ alone and the projector Q^0 is defined with the latter Mori product. The projector Q^0 drops out, since S_i commutes with $\mathcal{H}^0$ and thus $(\tilde{S}_i|L^{SB} S_j) = i\langle \tilde{S}_j [\mathcal{H}^{SB}, S_j] \rangle_{(0)} = 0$ holds, where, in addition, the second equation of (10) was used. Recalling $J_{ii} = 0$, one finds that

$$\delta(L^0) B_i^\pm s_i^\mp = s_i^\mp \delta(L^B \pm 2H_i \pm 2X_i) B_i^\pm \qquad (17)$$

where the operator of the internal field X_i at the site i is given by

$$X_i = \sum_j J_{ij} S_j. \qquad (18)$$

Using equation (17) we find $L_{ij} = L_{ii} \delta_{ij}$ with

$$L_{ii} = \frac{\pi}{2} \langle (1 - S_i) B_i^+ \delta(L^B - 2H_i - 2X_i) B_i^- + (1 + S_i) B_i^- \delta(L^B + 2H_i + 2X_i) B_i^+ \rangle_{(0)}. \qquad (19)$$

---

[1] The details of the Mori approach including the justifications and the general discussion of the approximations can be found in [15]. The notation of the present work widely agrees with [15]. Here both the Boltzmann constant and $\hbar$ are set equal to 1.

Let O be any operator in the unitary space of the spins not involving site i. Then

$$\langle S_i O \rangle_{(S)} = \left\langle \frac{\mathrm{Tr}_i\, S_i O \exp(-\beta H_i - \beta X_i)}{\mathrm{Tr}_i \exp(-\beta H_i - \beta X_i)} \right\rangle_{(S)} = \langle O \tanh \beta (H_i + X_i) \rangle_{(S)} \quad (20)$$

can be obtained [19]. Applying this relation to equation (19) and using (5) finally yields for the dynamic susceptibility matrix

$$\chi^{-1}(\omega) = \chi^{-1} - \mathrm{i}\omega(\beta L)^{-1} \qquad \text{with} \quad L_{ij} = \delta_{ij} \left\langle \frac{\chi_B''(2H_i + 2X_i)}{\sinh \beta (2H_i + 2X_i)} \right\rangle_{(S)} \quad (21)$$

where the static isothermal susceptibility matrix χ and the internal field operators X_i are given by equations (15) and (18) respectively.

To complete the analytic investigations for the general Ising case, the local-field probability distribution functions

$$P_i(h) = \langle \delta(h - H_i - X_i) \rangle_{(S)} = \langle \delta(h - H_i - \Sigma_j J_{ij} S_j) \rangle_{(S)} \quad (22)$$

are introduced which permit the L_{ii} to be rewritten as

$$L_{ii} = \int P_i(h) \frac{\chi_B''(2h)}{\sinh(\beta 2h)}\, \mathrm{d}h. \quad (23)$$

From the definition, the relations

$$\int P_i(h)\, \mathrm{d}h = 1 \qquad \int h P_i(h)\, \mathrm{d}h = H_i + \sum_j J_{ij} m_j \qquad \int \tanh(\beta h) P_i(h)\, \mathrm{d}h = m_i$$

$$(24)$$

immediately result, where the last relation is based on equation (20) with $O = 1$.

With the result (21) we have found a very compact form of the dynamic susceptibility matrix $\chi(\omega)$. This result is not restricted to the SK model and holds for all Ising models. According to equations (21) and (23) the dynamic susceptibility $\chi(\omega)$ can be explicitly calculated provided that the static susceptibility χ and the internal magnetic field distribution functions $P_i(h)$ are known.

Knowledge of the linear dynamic susceptibility $\chi(\omega)$ implies knowledge of all the other response functions. Let us consider the linear relaxation functions $\Phi(t)$ which describe the linear response $\langle \tilde{S}_i \rangle(t) = \sum_j [\Phi_{ij}(t) - \chi_{ij}] h_j^{ex}$ for $t \geqslant 0$ due to small changes of the external fields $-h_j^{ex} \Theta(t)$. According to the general response theory, $\Phi(t)$ is given by

$$\Phi_{ij}(t) = \beta(\tilde{S}_i | \tilde{S}_j(t)) \quad (25)$$

and is approximated by

$$\frac{\mathrm{d}\Phi(t)}{\mathrm{d}t} = -\beta L \chi^{-1} \Phi(t) \qquad \text{or by} \qquad \Phi(t) = \chi \exp(-\chi^{-1}\beta L t). \quad (26)$$

The remaining quantity of interest in linear response theory is the response function matrix which equals $-\dot{\Phi}(t)$. Due to this simple relation, the response function matrix is not considered further in this work.

The results (26) can be compared in detail with the work of Szamel [12] which represents both the most recent and the nearest approach to the subject of this paper. Comparing equation (26) for the case $H_i = 0$ with equation (13) of the first paper of [12] clearly shows that the values $(1 - \langle S_i \tanh \beta X_i \rangle_{(S)})$ or according to relation (20) the values $(1 - \langle \tanh^2 \beta X_i \rangle_{(S)})$ are used for the L_{ii} instead of the correct values given in equation (21). Thus in general both approaches disagree.

The work of Szamel and other former work [11] is based on the phenomenological Glauber dynamics. Microscopic derivation [16, 17] of this master-equation (in the form of [12]) leads to the transition rates

$$w_i = (1 - S_i \tanh \beta X_i) \frac{\chi_B''(2X_i)}{4 \tanh \beta X_i} \tag{27}$$

for the $H_i = 0$ case. In the work of Szamel, the values for the rates $(1 - S_i \tanh \beta X_i)/2$ were used which can only be justified for the special, rather unrealistic case that the bath susceptibility $\chi_B''(\omega)$ is proportional to $\tanh(\beta\omega/2)$. Thus, for a general agreement with the present approach, the correct transition rates (27) have to be used in the master-equation treatment.

Microscopically unjustified rates of the form of [12] are widely used to analyse the dynamics of Ising models for various physical questions. Provided that the characteristic width of the distribution $P(h)$ is of the order of the temperature T or larger than T, a modified master-equation approach with the rates (27) will lead to significant changes. Note that for (standard) mean field treatments these effects are absent. In these cases, $P(h)$ is a δ-function and the modifications reduce to a factor which can be eliminated by scaling the time. For the spin glasses at low temperatures, however, the exact form of the transition rates is essential, as worked out in the following for the SK model.

3. Internal field distribution function for the SK spin glass

For the rest of the paper, we consider exclusively the special case of the SK model. In this case, the bonds J_{ij} are independent random variables with zero means and standard deviations $N^{-\frac{1}{2}}$. This scaling fixes the spin glass temperature to $T = 1$. The smallness and the randomness enter basically into the approach of this section where a tractable form for the field distribution $P_i(x)$ of the SK model is deduced.

This approach uses techniques similar to the derivations of the TAP equations [2, 6, 8]. The spin Hamiltonian (1) is rewritten as $\mathcal{H}^S = -(H_i + X_i)S_i + \hat{\mathcal{H}}_i$ where $\hat{\mathcal{H}}_i$ describes an $N - 1$ spin system with the spin S_i removed from the original spin system. Using the relation $\delta(h - H_i - X_i) \exp[\beta(H_i + X_i)S_i] = \delta(h - H_i - X_i) \exp(\beta h S_i)$ and the Fourier representation of the δ-function and taking the trace over the site i,

$$P_i(h) = \frac{\cosh(\beta h)}{i\pi Z} \int_{-\infty}^{\infty} \hat{Z}_i(k) \, e^{-ik(h - H_i)} \, dk \qquad \text{with}$$

$$\hat{Z}_i(k) = \hat{\mathrm{Tr}}_i \, \exp \left\{ ik \sum_j J_{ij} S_j - \beta \hat{\mathcal{H}}_i \right\} \tag{28}$$

is obtained. The partition function of the original spin system is denoted by Z and $\hat{\mathrm{Tr}}_i$ stands for the trace of the $N - 1$ spin system.

The quantity $\hat{Z}_i(k)$ represents a partition function of the $N - 1$ spin system in the presence of additional imaginary fields $ik\beta^{-1}J_{ij}$. Due to the smallness of the J_{ij}, the cumulant expansion can be performed which yields to leading order in N^{-1} [2, 6, 8]

$$\ln \hat{Z}_i(k) = \ln \hat{Z}_i(0) + ik \sum_j J_{ij} \hat{m}_j - \frac{k^2}{2\beta} \sum_{jl} J_{ij} \hat{\chi}_{jl} J_{li} \tag{29}$$

where $\hat{m}_j = \beta^{-1} \partial \ln \hat{Z}_i(0) / \partial H_j$ and $\hat{\chi}_{jl} = \partial \hat{m}_j / \partial H_l$ are the local magnetizations and the static susceptibilities of the $N-1$ spin system, respectively. Following again the former approaches [2, 6, 8], the double sum in equation (29) is replaced by the local static susceptibility

$$\chi_l = \frac{1}{N} \sum_j \chi_{jj} = \frac{1}{N} \sum_j \frac{\partial m_j}{\partial H_j}. \tag{30}$$

With the result (29) the integration in equation (28) can be performed yielding

$$P_i(h) = \sqrt{\frac{\beta}{2\pi \chi_l}} \frac{\cosh(\beta h)}{\cosh\left(\beta H_i^{\text{eff}}\right)} \exp\left\{-\frac{\beta \chi_l}{2}\right\} \exp\left\{-\frac{\beta \left(h - H_i^{\text{eff}}\right)^2}{2\chi_l}\right\} \tag{31}$$

where the factors independent of h are determined from the normalization condition $1 = \int P_i(h) \, dh$ and the local effective field $H_i^{\text{eff}} = H_i + \sum_j J_{ij} \hat{m}_j$ was introduced. The latter two relations of equation (24) yield

$$H_i^{\text{eff}} = H_i + \sum_j J_{ij} m_j - m_j \chi_l \qquad \text{and} \qquad m_i = \tanh\left(\beta H_i^{\text{eff}}\right) \tag{32}$$

which are employed to rewrite equation (31) as function of h, m_i and χ_l,

$$P_i(h) = \sqrt{\frac{\beta \left(1 - m_i^2\right)}{2\pi \chi_l}} \cosh(\beta h) \exp\left\{-\frac{\beta \chi_l}{2}\right\} \exp\left\{-\frac{\beta (h - \beta^{-1} \operatorname{arctanh} m_i)^2}{2\chi_l}\right\}. \tag{33}$$

Note that equations (32) are the well known TAP equations if the local static susceptibility χ_l is specified. In this work, the modified version [8] of these equations is used which yields

$$\chi_l = \frac{1}{N} \sum_i \frac{\beta \left(1 - m_i^2\right)}{1 + \Gamma^2 \beta^2 \left(1 - m_i^2\right)^2} \tag{34}$$

with

$$\Gamma = 0 \qquad \text{for} \quad 1 - \frac{\beta^2}{N} \sum_i \left(1 - m_i^2\right)^2 \geqslant 0 \tag{35}$$

$$1 = \frac{1}{N} \sum_i \frac{\beta^2 \left(1 - m_i^2\right)^2}{1 + \Gamma^2 \beta^2 \left(1 - m_i^2\right)^2} \qquad \text{for} \quad 1 - \frac{\beta^2}{N} \sum_i \left(1 - m_i^2\right)^2 \leqslant 0. \tag{36}$$

As worked out in [8], for the stable states the modified TAP equations are equivalent to the original ones in the thermodynamic limit and differences result only for unstable states. For finite systems, the complete temperature and field dependence of the solutions of the modified equations are known [9], in contrast to the original TAP equations.

With the knowledge of these solutions, the total internal field distribution function defined as

$$P(h) = \frac{1}{N} \sum_i P_i(h) \tag{37}$$

can be calculated according to equation (31) or (33). In zero field above the spin glass temperature, the distribution function reduces to

$$P(h) = P_i(h) = \frac{1}{\sqrt{2\pi}} \cosh(\beta h) \exp\left\{-\frac{\beta^2 + h^2}{2}\right\} \qquad \text{for} \quad T \geqslant 1, H_i = 0. \tag{38}$$

The latter result for the special case has already been obtained by Thomsen *et al* [19]. However, to the best of the authors' knowledge, the general results of this section have previously not been published.
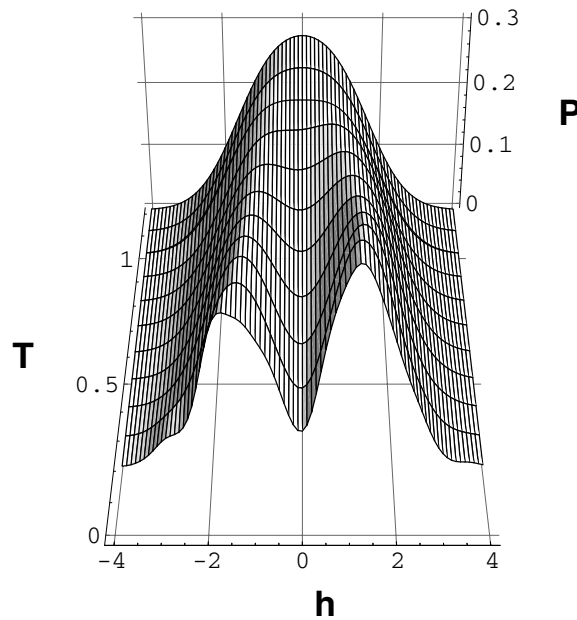
Figure 1. Temperature dependence of the internal field distribution function $P(h)$ of the SK spin glass for temperatures T below and above the spin glass temperature $T = 1$ for zero external field.

4. Discussion and numerical results

4.1. Internal field distribution function

The static properties of Ising models can be entirely formulated in terms of the internal field distribution function $P(h)$ [18, 19]. Due to this general importance, some discussion of $P(h)$ for the SK model is presented.

For zero magnetic field, the temperature dependence of $P(h)$ is shown in figure 1. Above the spin glass temperature $T = 1$ the exact result (38) is plotted. Below the spin glass temperature, the figure is based on equation (33) and on the numerical results of [9]. In the plot, the local magnetizations m_i for the state of lowest free energy of an $N = 225$ system (sample I) are used. On the scale of figure 1 both regimes $T \geqslant 1$ and $T \leqslant 1$ fit smoothly together. The distribution function $P(h)$ bifurcates from a one-peak structure to a two-peak structure at the spin glass temperature. With decreasing temperature, the minimum located at $h = 0$ becomes deeper and finally reaches the value $P(h = 0) = 0$ for zero temperature within numeric precision. This behaviour also applies to the metastable states. Moreover, the variations for the different states are small and seem to become negligible in the thermodynamic limit. This is remarkable and is an indication for self averaging of $P(h)$. These findings, as well as the general temperature dependence of $P(h)$, are in agreement with Monte Carlo simulations of [19].

The discussion is completed by figure 2 where $P(h)$ is shown for a system with a homogenous external field $H = 0.5$. No exact results are known for this case and thus the plot is based on numerical data everywhere. Again the data of sample I of [9] are used. Now the distribution $P(h)$ is asymmetric but again a bifurcation to a two-peak structure is found when the spin glass regime is entered. This occurs at the Almeida–Thouless (AT) temperature
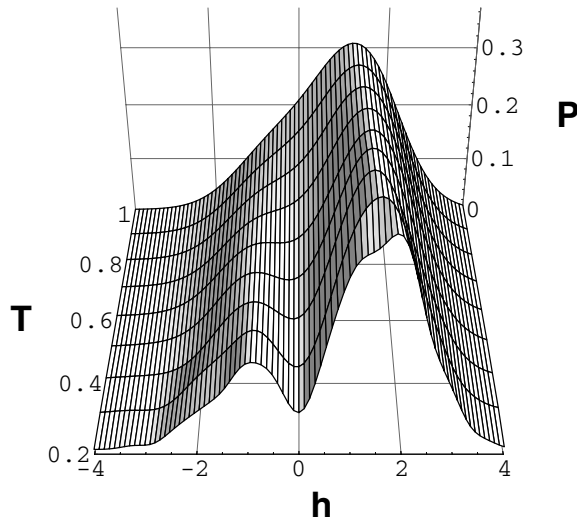
Figure 2. Temperature dependence of internal field distribution function $P(h)$ of the SK spin glass in the presence of a homogenous external field $H = 0.5$. The (numerical) AT temperature is $T = 0.577$.

[20] which is determined from $T^2 = N^{-1} \sum_i \left(1 - m_i^2\right)^2$ and which leads to the numerical value of $T = 0.577$ for the sample under consideration. These results indicate that the spin glass regime is also characterized by a two-peak structure of $P(h)$ for the case where a finite external field is present.

Certainly, in the numerical results finite-size effects are present. The most obvious feature is the asymmetry of $P(h)$ in figure 1. Thus the investigations of the finite-size effects [9] are extended to the distribution function $P(h)$ and averages over a few tens of independent samples are performed keeping N and T fixed. For the averages, the asymmetry of $P(h)$ for the case $H = 0$ reduces both with increasing number of samples and with increasing N. This represents some numerical evidence that the asymmetry is indeed an artefact due to the finite system size.

In this context, we recall that in zero magnetic field for each solution of the TAP equation (32) a further solution can be constructed trivially by changing the sign of all m_i. According to equation (31) the distributions corresponding to these two solutions are given by $P(h)$ and $P(-h)$ respectively. The means of these two distributions exhibit considerably smaller sample-to-sample variations than the individual $P(h)$. This can in principle be used to construct improved approximations of $P(h)$ for the thermodynamic limit. The TAP approach, however, does not use any averaging and thus we avoid this procedure. Moreover, the asymmetry of figure 1 indicates the order of magnitude of the finite-size effects.

4.2. Dynamic susceptibility

We focus on the local dynamic susceptibility which is defined as

$$\chi_l(\omega) = \chi_l'(\omega) + i\chi_l''(\omega) = N^{-1} \operatorname{Tr} \chi(\omega) = N^{-1} \operatorname{Tr}\{\chi^{-1} - i\omega(\beta \boldsymbol{L})^{-1}\}^{-1} \tag{39}$$

and which is a quantity of both theoretical and experimental interest. Employing the results of section 4.1 and the approximation (7) (setting const $= 1$ which fixes the time scale) the Onsager

coefficient L_{ii} can be numerically determined according to equation (23). Furthermore, using the well-known expression for the static isothermal susceptibility

$$\chi_{ij}^{-1} = \left\{ \left[\beta \left(1 - m_i^2 \right) \right]^{-1} + \chi_l \right\} \delta_{ij} - J_{ij} \tag{40}$$

with χ_l given by equations (34)–(36), all terms of equation (21) are explicitly known and the dynamic susceptibility matrix $\chi(\omega)$ is obtained by numerical matrix inversion. From this the local susceptibility $\chi_l(\omega)$ is finally calculated.

There exists another method to determine $\chi_l(\omega)$ which is based on the theorem of Pastur [21][2]. This theorem immediately leads to the identity (compare [8])

$$\chi_l(\omega) = N^{-1} \sum_i \left\{ \left[\beta \left(1 - m_i^2 \right) \right]^{-1} + \chi_l - i\omega (\beta L_{ii})^{-1} - \chi_l(\omega) \right\}^{-1} \tag{41}$$

and $\chi_l(\omega)$ is obtained as a solution of equation (41) satisfying $\omega \chi_l''(\omega) \geqslant 0$. In the paramagnetic regime and in the absence of external magnetic fields, this equation leads to the analytic result

$$\chi_l(\omega) = \frac{\beta + \beta^{-1} - i\omega \beta^{-1} L^{-1}}{2} + \sqrt{\frac{(\beta + \beta^{-1} - i\omega \beta^{-1} L^{-1})^2}{4} - 1} \qquad T \geqslant 1, H_i = 0 \tag{42}$$

where the Onsager coefficient $L_{ii} = L(T)$ is temperature dependent and given by

$$L(T) = \exp(-\beta^2/2) \frac{1}{\sqrt{2\pi}} \int \frac{h \exp(-h^2/2)}{\sinh \beta h} \, dh \tag{43}$$

using equations (23) and (38). Note that for $T \gg 1$ equation (42) reduces to $\chi_l = \beta(1 - i\omega\beta)^{-1}$ which implies a relaxation time proportional to β, as is the case for the Korringa relaxation of single magnetic moments dissolved in a metal. Note further that the result (42) partially agrees with the work of Kinzel and Fischer [3, 10] who, however, have not obtained the temperature dependence of $L(T)$. Near the spin glass temperature, both approaches agree and yield $\chi_l(\omega) = 1 + i\sqrt{|\omega|}$ at $T = 1$.

With reference to the definition of Γ [8, 9],

$$\chi_l(\omega) \mid_{\omega \to \pm 0} = \chi_l \pm i\Gamma \tag{44}$$

results from equation (41). Thus the quantities χ_l and Γ, which enter formally in derivation of the modified TAP equations, are related to the real and the imaginary parts of the isolated susceptibility $\chi_l(\omega \to 0)$. Recalling that frequently there are situations in physics where the isolated and the isothermal susceptibilities differ (for some general discussion see [15]) this result gives some additional insight into the approach leading to the modified TAP equations [8, 9].

In figure 3 both the analytical and the numerical results for χ_l are presented for the zero external field case. For the numerical parts again the lowest free energy state of sample I from [9] with $N = 225$ is used. The two different methods lead to similar results but deviate increasingly for small frequencies ω. It is remarkable that the results of figure 3 show some overall similarity to real, experimental data [3, 4]. One of these features is the frequency dependence of the cusp temperature of $\chi_l'(T, \omega = \text{const})$. In the present approach, the shift results simply from the temperature dependence of the Onsager coefficients.

The deviations appearing in figure 3 for small frequencies are caused by the finite size of the system. According to equation (21) L is positive definite. Thus the matrix $A = (\beta L)^{\frac{1}{2}}$ is

---

[2] Actually, a slight generalization of this theorem is needed to incorporate the term $i\omega\beta^{-1}L^{-1}$. Such a generalization can be easily added to the method of Bray and Moore [22].
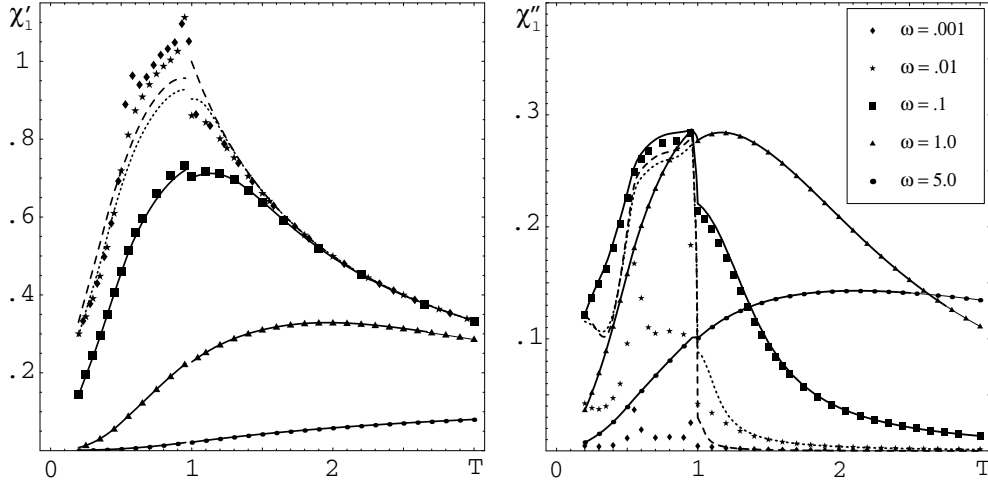
Figure 3. Temperature dependence of the real part, $\chi'_l(\omega)$, and the imaginary part, $\chi''_l(\omega)$, of the local dynamic susceptibility $\chi_l(\omega)$ in zero external field for different frequencies. The data points are calculated by numerical inversion of equation (40) for a system of $N = 225$ spins (compare text). The lines represent the results calculated from equation (41) via the theorem of Pastur. For $T < 1$ they are again based on the numerical data of the $N = 225$ spin system. For $T > 1$ the lines give the analytic result of equation (42) in the thermodynamic limit. The dashed line, the dotted line and the full lines correspond to $\omega = 0.001$, $\omega = 0.01$ and $\omega = 0.1, 1.0, 5.0$ respectively. For $\omega = 0.001$ some data points exist which are outside the plot range of $\chi'_l(\omega)$.

well defined and $\chi^{-1}(\omega)$ can be rewritten as $\chi^{-1}(\omega) = A^{-1}(A\chi^{-1}A - \mathrm{i}\omega)A^{-1}$. Use of the diagonal representation of $A\chi^{-1}A$ leads to

$$\chi_l(\omega) = N^{-1} \sum_\alpha \langle u_\alpha|A^2|u_\alpha\rangle(\delta_\alpha - \mathrm{i}\omega)^{-1} \qquad \text{where} \quad A\chi^{-1}A|u_\alpha\rangle = \delta_\alpha|u_\alpha\rangle \qquad (45)$$

which shows that $\chi_l(\omega)$ can be written as a superposition of Lorentzian functions with relaxation rates δ_α given by the eigenvalues of $A\chi^{-1}A$. In the spin glass regime, the minimum value $\delta_{\min}$ of all rates δ_α is small (the numerical value for the data used in figure 3 is of the order 0.03) for finite N and tends to zero in the thermodynamic limit [8, 9, 22]. For frequencies $\omega < \delta_{\min}$ the susceptibility $\chi_l(\omega)$ sensitively depends on the small eigenvalues according to equation (45) and thus finite-size effects mainly show up for small ω for the data obtained by direct matrix inversion. According to figure 3 the deviations are moderate for those results which use the theorem of Pastur. This indicates that the use of this theorem for finite N partly smooths out the finite-size effects.

4.3. Relaxation function

The local relaxation function can be written as

$$\Phi_l(t) = N^{-1} \operatorname{Tr} \Phi(t) = N^{-1} \sum_\alpha \langle u_\alpha|A^2|u_\alpha\rangle \delta_\alpha^{-1} \mathrm{e}^{(-\delta_\alpha t)} \qquad (46)$$

where equation (26) and the eigenvalue equation (45) were used. Again the superposition of the contributions resulting from the different rates δ_α (or relaxation times δ_α^{-1}) can be identified. The local relaxation function satisfies $\Phi_l(t) \leqslant \Phi_l(0) = \chi_l$ and thus is well behaved in the
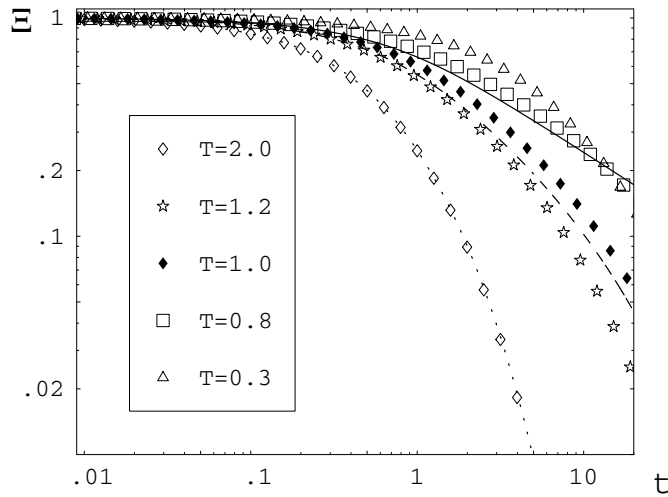
Figure 4. Time t dependence of the reduced local relaxation function $\Xi(t) = \Phi_l(t)/\Phi_l(0)$ in a double log scale for different temperatures T in zero external field. The data points correspond to the numerical results of a sample with $N = 225$ spins. The lines represent the results in the thermodynamic limit given by equation (47). The full, the dashed and the dotted lines correspond to $T = 1.0$, 1.2 and 2.0 respectively.

thermodynamic limit even for the case when δ_{min} tends to zero. For vanishing external fields, $\Phi_l(t)$ can be given analytically,

$$\Phi_l(t) = \frac{2}{\pi} \int_{-1}^{1} dx \frac{\sqrt{1-x^2}}{\beta + \beta^{-1} - 2x} \exp[-(1 + \beta^2 - 2\beta x)L(T)] \qquad T \geqslant 1, H_i = 0 \qquad (47)$$

in the paramagnetic regime [1]. As already noted, the temperature dependence of $L(T)$ differs from [1, 12] and is given by equation (43).

In figure 4 the numerical results for the local relaxation function $\Phi_l(t)$ are plotted (again for the state with lowest free energy of sample I of [9]) together with the analytic results (47). The plot clearly exhibits the slowing down at the spin glass temperature and the presence of the slow dynamics in the spin glass regime. Comparing the numerical and the analytical results above the spin glass temperature, the deviations increase for the long time behaviour when approaching the spin glass regime. As already discussed above, these finite-size effects result from the finite value of δ_{min} and limit the numerical results to the region $t \ll \delta_{min} \approx 30$ near and below the spin glass temperature.

5. Conclusions

Two questions are studied from a more general point of view in the present work. First of all, the linear response theory for an arbitrary Ising model which is microscopically and weakly coupled to a bath is investigated using the theory of Mori and applying the standard approximations. This approach seems to be natural and conservative and could have been carried out some decades ago. Nevertheless the results are remarkable, as the entire dynamical response of any Ising model is completely determined by the internal field distribution function, by the static isothermal susceptibility and—as the only characteristic feature of the bath—by a bath dynamic susceptibility. Due to the simple structure, this part of the present work may be of interest for other models than the SK model.

The relation to former approaches has been worked out in some detail at the end of section 2. It is the use of microscopically unjustified transition rates in these master-equations which causes the differences in the present investigation.

The second question is exclusively related to the SK model and represents the study of the internal field distribution function showing how this function is related to the solutions of the TAP equations. The obtained relationship opens the possibility of explicitly calculating further quantities of interest for the SK model, such as the inelastic-neutron-scattering cross section [18].

Another tool to obtain the final results for the dynamic linear response functions of the SK model is the explicit knowledge of the solutions of the modified TAP equations. This again demonstrates the importance of the modified TAP approach.

The present work is limited to the dynamics in linear approximation near the thermodynamic equilibrium. It is, however, well known that in the physics of spin glasses nonlinear dynamical effects and the linear response in out-of-equilibrium situations are of great importance [4]. Thus an extension of the present microscopic approach to nonlinear dynamics would be of great use to treat these effects on a well-founded basis. Such an approach based on the theory of Robertson or Nakajima–Zwanzig (see e.g. [15]) is in progress and will be published elsewhere [16].

Acknowledgments

References

[1] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **32** 1972
    Kirkpatrick S and Sherrington D 1978 *Phys. Rev.* B **17** 4384
[2] Mezard M, Parisi G and Virasoro M A 1987 *Spin Glass Theory and Beyond* (Singapore: World Scientific) and references therein
[3] Fisher K H and Hertz J A 1991 *Spin Glasses* (Cambridge: Cambridge University Press) and references therein
[4] Yong A P (ed) 1997 *Spin Glasses and Random Fields* (Singapore: World Scientific) and references therein
[5] Parisi G 1979 *Phys. Rev. Lett.* **43** 1754
    Parisi G 1980 *J. Phys. A: Math. Gen.* **13** 1101
    Parisi G 1980 *J. Phys. A: Math. Gen.* **13** 1887
[6] Thouless D J, Anderson P W and Palmer R G 1977 *Phil. Mag.* **35** 593
[7] Plefka T 1982 *J. Phys. A: Math. Gen.* **15** 1971
[8] Plefka T 2002 *Europhys. Lett.* **58** 892
[9] Plefka T 2002 *Phys. Rev.* B **65** 224206
[10] Kinzel W and Fischer K H 1977 *Solid State Commun.* **23** 687
[11] Fisher K H and Kinzel W 1983 *Solid State Commun.* **46** 309
    Sommers H J 1987 *Phys. Rev. Lett.* **58** 1268
    Łusakowski A 1991 *Phys. Rev. Lett.* **66** 2543
    Coolen A C C and Sherrington D 1993 *Phys. Rev. Lett.* **71** 3886
    Coolen A C C and Sherrington D 1994 *J. Phys. A: Math. Gen.* **27** 7687
    Laughton S N, Coolen A C C and Sherrington D 1996 *J. Phys. A: Math. Gen.* **29** 763
    Nishimori H and Yamanna M 1996 *J. Phys. Soc. Japan* **65** 3
    Yamanna M, Nishimori H, Kadowaki T and Sherrington D 1997 *J. Phys. Soc. Japan* **66** 1962
[12] Szamel G 1998 *J. Phys. A: Math. Gen.* **31** 10045
    Szamel G 1998 *J. Phys. A: Math. Gen.* **31** 10053
[13] Sompolinsky H 1981 *Phys. Rev. Lett.* **47** 935
    Sompolinsky H and Zippelius A 1981 *Phys. Rev. Lett.* **47** 359
    Sompolinsky H and Zippelius A 1982 *Phys. Rev.* B **25** 6860

Horner H 1984 *Z. Phys.* B **57** 29

Horner H 1984 *Z. Phys.* B **57** 39

Cugliandolo L F and Kurchan J 1994 *J. Phys. A: Math. Gen.* **27** 5749

[14] Mori H 1965 *Prog. Theor. Phys. (Kyoto)* **34** 399

[15] Fick E and Sauermann G 1990 *The Quantum Statistics of Dynamic Processes* (Berlin: Springer)

[16] Plefka T 2002 in preparation

[17] Just W 2002 Private communication

[18] Thomsen M, Thorpe M F, Choy T C and Sherrington D 1984 *Phys. Rev.* B **30** 250

[19] Thomsen M, Thorpe M F, Choy T C, Sherrington D and Sommers H-J 1986 *Phys. Rev.* B **33** 1931

[20] de Almeida J R L and Thouless D J 1978 *J. Phys. C: Solid State Phys.* **11** 983

[21] Pastur L A 1974 *Russ. Math. Surv.* **28** 1

[22] Bray A J and Moore M A 1979 *J. Phys. C: Solid State Phys.* **12** L441