Dynamics of Ising models coupled microscopically to bath systems

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Abstract. – Based on the Robertson theory the nonlinear dynamics of general Ising systems coupled microscopically to bath systems is investigated leading to two complimentary approaches. Within the master equation approach microscopically founded transition rates are presented which essentially differ from the usual phenomenological rates. The second approach leads to coupled equations of motion for the local magnetizations and the exchange energy. Simple examples are discussed and the general results are applied to the Sherrington-Kirkpatrick spin glass model.

Introduction. – Ising spin models are probably the simplest interacting many particle systems to which many equilibrium and non-equilibrium phenomena found in nature can be mapped. In many cases the analysis of these models exhibit the basic features and consequently lead to a first understanding of the reality. Therefore numerous investigations employing Ising models exist in literature and are the subject of research activities. In addition to the questions in physics various problems arising in other fields (biology, social science, information theory, etc.) are treated on the basis of Ising models.

Ising spin systems do not exhibit an intrinsic dynamics. Thus the kinetics of these models is exclusively caused by couplings to bath systems of the environment. Forty years ago Glauber [1] suggested a phenomenological master equation for a one-dimensional chain of Ising spins with nearest neighbor interactions. Generalized to other spin arrangements and to other types of interactions (for a review see [2]) the approach of Glauber has been nearly exclusively used to describe the dynamics of the Ising spin systems. Note that the above comment also applies to the numerous Monte Carlo simulations performed on various models in the last decades [3].

The transition rates of these phenomenological equations are required to satisfy detailed balance which guaranties relaxation to equilibrium for non driven systems. But this requirement is not sufficient to fix the rates completely. Therefore ad hoc assumptions have to be employed which lead to the claim [2] that kinetic Ising models should not be regarded as faithful representations of processes occurring in real systems.

It is microscopic quantum-statistical investigations which can remove the arbitrarily of the phenomenological equations. The tools for such a purpose are known since nearly half a century ago [4] and many general approaches exist. The application of these general theories...
in Ising models, however, are rare. A first approach of Heims [5] uses a very special and thus artificial spin-bath interaction. Further approaches, both based on special realizations of the heat bath, are presented by Martin [6] and recently by Park et al. [7].

All these microscopic approaches find transition rates different from [1]. A recent investigation for the linear response of a general Ising model [8] based on the Mori theory results in the same conclusion. It is the aim of the present letter to calculate the transition rates under general aspects and to work out the generic behavior for the general non-linear case. Thus neither specific Ising models nor specific realizations of the baths are presumed. The Ising spins may even interact with more than one bath to include problems like those treated in [9]. Calculations are performed on the bases of the Robertson theory [10,11], although equivalent result [12] are obtained by employing [4] or the Nakajima-Zwanzig approach [11].

With rare exceptions like the original problem of Glauber [1], analytical solutions of the master equations are not known and therefore approximations have to be employed. The typical procedure involves the elimination of fast degrees of freedom in the master equation. This leads to a reduced description and equations of motion result for the slow or relevant variables. The latter equations, in many cases, can directly be found by the Robertson theory. Thus both, the master equation and the equation of motion of such reduced descriptions can simultaneously be derived which justifies the above choice of the method.

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

$$H^S = -2 \sum_i H_i s_i^z + H^{ex}, \quad H^{ex} = -2 \sum_{i,j} J_{ij} s_i^z s_j^z$$

where $J_{ii} = 0$ is presumed. Both quantum spin $\frac{1}{2}$ operators $s_i$ with $\hbar = 1$ and Ising spins $S_i (= 2s_i^z)$ are used simultaneously.

The assembly of spins interact via spin bath interactions $B_{\alpha} s_i$ with a system consisting of $N_B$ adiabatically isolated baths $H^B_{\alpha}$. Thus the total Hamiltonian of the system is described by

$$\mathcal{H} = \mathcal{H}^0 + \mathcal{H}^{SB}, \quad \mathcal{H}^0 = \mathcal{H}^S + \mathcal{H}^B, \quad \mathcal{H}^B = \sum_{\alpha} \mathcal{H}^B_{\alpha}, \quad \mathcal{H}^{SB} = \frac{1}{2} (B^{+}_{\alpha} s_i^+ + B^{-}_{\alpha} s_i^-) + B^z_{\alpha} s_i^z.$$  

During the dynamic evolution of the spin system thermal equilibrium is presumed for each individual bath system $\mathcal{H}^B_{\alpha}$ leading to the statistical operator

$$R^B = \exp(-\sum_{\alpha} \beta_{\alpha} \mathcal{H}^B_{\alpha})/\text{Tr} \exp(-\sum_{\alpha} \beta_{\alpha} \mathcal{H}^B_{\alpha}).$$

These requirements on the bath systems can be realized by sufficient large bath heat capacities and by faster relaxation of the bath system. Thus $\tau_B \ll \tau_S$ where $\tau_B$ and $\tau_S$ are the characteristic relaxation times of the bath and the spin system respectively. In general all the temperatures $\beta_{\alpha}$ are different. Due to couplings to additional reservoirs the $\beta_{\alpha}$ may even be time dependent. Thus the $\beta_{\alpha}(t)$ - together with $H_i(t)$ - are preset quantities. Both the $\beta_{\alpha}(t)$ and the $H_i(t)$ are presumed to have negligible variations on the fast time scale $\tau_S$.  

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(1) This interaction represents the most general one spin coupling to the bath. Note that the contribution $B^+_i s_i^+$ has no effect and that the coupling of $B^0_i s_i^z$ or similar two spin couplings will lead to spatial correlations via $H^{SB}$. Such a behavior may be possible but is certainly not the generic case.

(2) Eq. (4) is an approximation which requires this presumption for the $H_i(t)$. 


With these requirements there is no need for an explicit specification of the bath Hamiltonian \( H^B \) and the bath operators \( B_{\alpha i} \). As shown below, it is just the absorptive part \( \chi''_{\alpha i}(\omega) \) of the dynamic bath susceptibility

\[
\chi_{\alpha i}(\omega) = \chi'_{\alpha i}(\omega) + i \chi''_{\alpha i}(\omega) = -i \int_0^\infty \langle [B_{\alpha i}^-, e^{iH_B t} B_{\alpha i}^+] B \rangle e^{i\omega t} dt ,
\]

which enters the calculation for values \( \omega \tau_S \approx 1 \). Expectation values with respect to \( R^B \) are represented by \( \langle \ldots \rangle_B \) and \( L^B \) denotes the Liouvillian defined by \( L^B A = [H^B, A] \). It is assumed that \( \langle B_{\alpha i} \rangle_B = 0 \) holds, which can always be achieved by a renormalization of the terms of the Hamiltonian. Note that \( \omega \tau_S \approx 1 \) implies \( \omega \tau_B \ll 1 \) and the first term of the low frequency expansion of \( \chi''_{\alpha i} \) can be used. Apart from interesting exceptions (compare [7]) this yields in the generic case

\[
\chi''_{\alpha i}(\omega) \approx \text{const } \omega \quad \text{for} \quad \omega \ll \tau_B^{-1}
\]

where the constant of proportionality may depend on \( \beta_{\alpha} \).

**Calculation:** Let \( A^k(S_1, \ldots, S_N) \) be a fixed but arbitrary set of variables which are functions of the Ising spins \( S_i \). This set is assumed to give a sufficient dynamical description of some physical question and will be called observation level according to [11]. Without further specification of the observation level at this stage the general approach of Robertson [10, 11] is applied employing the usual perturbation treatment up to the second order in \( H^S B \) and the standard Markovian approximation [13]. As all variables \( A^k \) commute with \( H^0 \) this leads to

\[
\frac{d}{dt} \langle A^k \rangle_t = - \int_0^\infty d\tau \langle [U(t, t - \tau) H^S B, [H^S B, A^k]] \rangle_t , \quad U(t, t - \tau) = \exp(-i\tau[L^S(t) + L^B(t)])
\]

where the Liouvillians \( L^S \) and \( L^B \) are associated to \( H^S \) and to \( H^B \), respectively. The time dependent expectation values \( \langle \ldots \rangle_t \) are performed with the generalized canonical statistical operator

\[
R_t = R^S_t R^B \quad \text{with} \quad R^S_t = \exp(V)/\text{Tr}_S \exp(V) \quad \text{and} \quad V = \sum_k \lambda^k_t A^k
\]

where the time dependent Lagrange parameters \( \lambda^k_t \) are implicitly determined by

\[
\langle A^k \rangle_t = \text{Tr}_S A^k R^S_t .
\]

Note that the system of eqs. (10) and (11) represent a closed set of nonlinear differential eqs. for the expectation values \( \langle A^k \rangle_t \) and the Lagrange parameters \( \lambda^k_t \). Thus together with the initial values for the \( \langle A^k \rangle_t \) (or with the initial values for \( \lambda^k \)) the time dependence of all quantities are completely determined by this set of equations.

Analog to [8] eq. (6) can be brought in a more convenient form. Using again \( \chi_{\alpha i}(\omega) = \chi'_{\alpha i}(\omega) + \pi (e^{\pm \beta_{\alpha} \omega} - 1) \langle B_{\alpha i}^\pm (H^B \pm \omega) B_{\alpha i}^\mp \rangle_B \) this leads to

\[
\frac{d}{dt} \langle A^k \rangle_t = \sum_{\alpha i} \langle \Gamma_{\alpha i} \{ \tanh(\beta_{\alpha} H_i + \beta_{\alpha} X_i) - S_i \} A^k \rangle_t \quad \text{with} \quad \Gamma_{\alpha i} = \frac{\chi''_{\alpha i}(2H_i + 2X_i)}{2 \tanh(\beta_{\alpha} H_i + \beta_{\alpha} X_i)} .
\]
For all functions $F$ of the $N$ Ising spins $F_i$ is defined as

$$ F_i = \frac{1}{2}\text{Tr}_i S_i F(S_1, \ldots, S_N) $$

which enter in the calculation from $[s_i^+, F] = \mp 2s_i^+ F_i$. The operators of the internal field at sites $i$ are

$$ X_i = -\mathcal{H}_i^{ex} = \sum_j J_{ij} S_j. $$

In the step leading to eq. (10) the relation (14) was used which holds for any operator $O$ of the Ising spins not involving the spin $S_i$.

Eqs. (10) and (11) represent in a compact form the most general results of this work. These results are valid for any observation level which has to be specified for concrete physical problems. As already pointed out, all slow variables of the specific problem have been included.

One can also see that via eq. (10) a second requirement on the set of variables results. Being, in principle, arbitrary the initial value of $R_i$ is assumed to have the special form of eq. (10).

By an extension of the observation level, however, this second requirement can always be satisfied for any given initial state.

Here two special observation levels will be discussed. First, the observation level is analyzed which leads to the master equations and contains all functions $F(S_1, \ldots, S_N)$ of the $N$ Ising spins. Obviously all of the above requirements are satisfied. The second observation level is spanned by all Ising spins $S_1, \ldots, S_N$ and by the interaction $\mathcal{H}^{ex}$. This choice implies that all thermal equilibrium states of the spin system are possible initial states. Consequently this observation level leads to a dynamical description of a standard thermodynamic system and is therefore denoted as standard system in the following.

**Master equation.** — Let the $|\sigma\rangle$ be the common eigenvectors of the $S_i$ where $\sigma = \{\sigma_1, \ldots, \sigma_N\}$ denotes the configuration of the spin system with the possible values $\sigma_i = \pm 1$. Then the observation level is spanned by all the $2^N$ projectors $|\sigma\rangle\langle\sigma|$. Introducing the notation $\sigma^{(i)} = \{\sigma_1, \ldots, \sigma_i, \ldots, \sigma_N\}$, the relation $\langle\sigma|\langle\sigma|_i = \sigma_i/2 (|\sigma\rangle\langle\sigma| + |\sigma^{(i)}\rangle\langle\sigma^{(i)}|)$ holds. Eq. (11) immediately leads to the master equation

$$ \frac{d}{dt} p_\sigma = -\sum_i \left( W_i^{\sigma}_{\sigma} p_\sigma - W_i^{\sigma^{(i)}}_{\sigma^{(i)}} p_\sigma^{(i)} \right) $$

for the occupation probabilities $p_\sigma = \langle\sigma|\rho_i^{eq}|\sigma\rangle$. The transition rates $W_i^{\sigma}$ are given by

$$ W_i^{\sigma} = \sum_{\alpha} \frac{C_{\alpha}}{2} (1 - \sigma_i \tanh(\beta_\alpha H_i^{\sigma})) = \sum_{\alpha} \frac{\chi''_{\alpha}(2\sigma_i H_i^{\sigma})}{4\exp(2\beta_\alpha \sigma_i H_i^{\sigma}) - 1} $$

with

$$ C_{\alpha} = \frac{\chi''_{\alpha}(2 H_i^{\sigma})}{4 \tanh(\beta_\alpha H_i^{\sigma})} \quad \text{and} \quad H_i^{\sigma} = H_i + \sum_j J_{ij}\sigma_j. $$

The rates $W_i^{\sigma}$ are consistent with the results of (11) but disagree with the usual ad hoc assumption of phenomenological kinetic Ising models (11) which uses constant values of coefficient $C_{\alpha}$ independent of the configuration $\sigma$. Thus for a faithful representation of processes occurring in real systems the full $\sigma$ dependence of the $C_{\alpha}$ has in general be used.
Standard system. — This observation level will be characterized by \( V = -\lambda_{ex} H^{ex} + \sum_i \lambda_i S_i \) which leads to \( V [t] = \lambda_i + \lambda_{ex} X_i \). Introducing the internal local-field probability functions
\[
w_i(x) = \langle \delta(x - X_i) \rangle_t = \frac{\text{Tr} \delta(x - \sum_j J_{ij} S_j) \exp(V)}{\text{Tr} \exp(V)}
\]
and employing again the relation (10), the expectation values of the magnetizations \( m_i = \langle S_i \rangle_t \) and the exchange energy \( U^{ex} = \langle H^{ex} \rangle_t \) can be written as (compare 11)
\[
m_i = \int dx w_i(x) \tanh(\lambda_i + \lambda_{ex} x), \quad U^{ex} = -\frac{1}{2} \sum_i \int dx w_i(x) \tanh(\lambda_i + \lambda_{ex} x)
\]
and the eqs. (12) leads to
\[
\frac{d}{dt} m_i = -\sum_i \int dx w_i(x) \lambda_i \frac{\tanh(\lambda_i + \lambda_{ex} x)}{\tanh(\lambda_i H_i + \lambda_{ex} x)} - 1
\]
\[
\frac{d}{dt} U^{ex} = \sum_{ij} \int dx w_i(x) \lambda_{ij} \frac{\tanh(\lambda_i + \lambda_{ex} x)}{\tanh(\lambda_i H_i + \lambda_{ex} x)} - 1.
\]

The set of nonlinear equations (19-21) for the dynamic variables \( m_i \) and \( U^{ex} \) together with the associated time dependent Lagrange parameters \( \lambda_i \) and \( \lambda_{ex} \) is closed and is expected to give an adequate description for many physical systems and situations.

Note that the internal local-field distribution functions \( w_i(x) \) govern the set of nonlinear equations of motion. Indeed all the terms of these set of equations can explicitly be calculated from the knowledge of the \( w_i(x) \). These findings generalize the previous results, that the \( w_i(x) \) determine the statics 14 and the dynamical linear response 8 of an arbitrary Ising model. In that previous work the distributions \( w_i(x) \) have explicitly been calculated for various specific physical models including both ferromagnetic and disordered systems. Consequently for all those models the nonlinear equation of motion can easily be obtained from the eqs. (19-21).

Application to the SK spin glass. — The latter procedure will be illustrated for infinite range spin glass model of Sherrington and Kirkpatrick 15 16. In the SK model 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 \( T = 1 \). Employing the modified TAP approach 15 18
\[
w_i^{SK}(x) = \frac{1}{\sqrt{2\pi \Delta}} \frac{\cosh(\lambda_i + \lambda_{ex} x)}{\cosh(\lambda_i + \lambda_{ex} H_i^{ex})} \exp \left\{ -\frac{(x - H_i^{ex})^2 + (\lambda_{ex} \Delta)^2}{2\Delta} \right\}
\]
holds 15 with
\[
H_i^{ex} = \sum_j J_{ij} m_j - \lambda_{ex} m_i \Delta \quad \text{and with} \quad \Delta = \frac{1}{N} \sum_i \frac{(1 - m_i^2)}{1 + \Gamma^2 \lambda_{ex}^2 (1 - m_i^2)^2},
\]
where \( \Gamma \) is determined from
\[
\Gamma = 0 \quad \text{for} \quad 1 - \frac{\lambda_{ex}^2}{N} \sum_i (1 - m_i^2)^2 \geq 0
\]
\[
1 = \frac{1}{N} \sum_i \frac{\lambda_{ex}^2 (1 - m_i^2)^2}{1 + \Gamma^2 \lambda_{ex}^2 (1 - m_i^2)^2} \quad \text{for} \quad 1 - \frac{\lambda_{ex}^2}{N} \sum_i (1 - m_i^2)^2 \leq 0.
\]

With the eqs. (22-24) the equations of motion (19-21) are explicit provided the system of baths is specified. For the case of one singular bath and identical spin bath couplings the sums over
α drop out in eqs. (20, 21) and only one bath temperature β remains. The resulting equations are expected to describe the complete non linear dynamics of the SK spin glass including temperature quenches, memory and ageing effects [17].

A complete discussion of these interesting effects is beyond the scope of this work and is a subject of further research. In the following, I focus on the discussion of the special situations when the exchange system is in equilibrium with the bath, implying λ_{ex} = β_B. This situation can physically be realized by allowing only changes of the fields H_i. Setting λ_{ex} = β_B = β eq. (20) yields Glauber type equations of motion

$$\dot{m}_i = -\gamma(\beta, H_i^{eff}, \Delta) [m_i - \tanh \beta H_i^{eff}] \quad , \quad H_i^{eff} = H_i + \sum_j J_{ij} m_j - m_i \beta \Delta$$  \hspace{1cm} (26)

with the relaxation rates

$$\gamma(\beta, H, \Delta) = \frac{\cosh \beta H}{\sqrt{2\pi}} \int dz \exp \left\{ -\frac{\beta^2 \Delta + z^2}{2} \right\} \frac{\chi''_B(2H + 2\sqrt{\Delta} z)}{2 \sinh \beta(H + \sqrt{\Delta} z)} > 0$$ \hspace{1cm} (27)

where Δ has to be determined from eq. (23-25) (with λ_{ex} replaced by β). On a phenomenological basis - with γ replaced by a constant - equations of motions of this kind have been used since the early days in spin glass research [19]. Moreover the author himself had used such equations to find numerically the solutions of the static TAP equations [18, 20]. Note that eq. (27) implies relaxation to the static TAP equations independent of the values of γ(β, H^{eff}, Δ). Thus the phenomenological equations can be used instead of the microscopic results to calculate static properties and these results justify the procedure used in [18, 20] to calculate the solutions of the TAP equations.

For all dynamic quantities, however, the full form of γ(β, H^{eff}, Δ) has to be used. First examples are the dynamic susceptibility and the relaxation function as presented already in [20]. Note that a result of [20], the frequency-dependent shift of the cusp temperature of the real part of the susceptibility, is basically a consequence of γ(β, H^{eff}, Δ). In this context the general result [11] should be recalled that the linear approximation of the Robertson theory leads the Mori theory. Consequently all the linear response theory results of [20] can also be obtained from the of eqs. (26) and (27) by linearizing around the thermal equilibrium which can easily be checked.

Discussion. - The consequences of the results of this letter are further illustrated on simple physical situations. First one singular spin coupled to a bath with temperature β is considered. This implies no spin spin interaction at all. Both the master equation and the standard system approach of this letter leads to the equation of motion $\dot{m} = -\gamma_1(m - \tanh \beta H)$ for the magnetization m with $\gamma_1 = \frac{1}{2} \chi''_B(2H) \coth \beta H$. For a static field the magnetization m relaxes to the equilibrium value tanh βH with the well known (see e.g. [11]) longitudinal relaxation rate γ1. Note the latter result is not found if instead of eq. (17) the usual ad hoc assumptions of the kinetic Ising model are used.

Next the original system of Glauber, an infinite chain of Ising spins with next neighbor ferromagnetic interactions is considered which is coupled to one bath with a temperature β. The transition rates (17) satisfy the detailed balance relation and therefore relaxation to the thermal equilibrium results within the master equation approach. The same consequences apply for the standard system approach. Indeed the equilibrium values of the Lagrange parameter $\lambda_i = H_i$ and λ_{ex} = β describe a fixed point of the eqs. (20) and (21). It is obvious that nether the transition rates (17) nor the details of distribution functions $w_i$ enter in thermal expectation values. Note that these arguments apply to all undriven Ising system which are coupled to one singular bath. Thus all this systems relax to thermal equilibrium.
taking in account that the fixed points are always stable. This can easily be checked by a linear stability analysis.

For situations, however, where two or more bates with different temperatures $\beta_\alpha$ are present the values of stationary solutions depend on the transition rates or on the details of the distribution functions $w_i(x)$. Thus for example the non equilibrium stationary states of Schmittmann and Schmüser can not be accepted as a realistic solution for their interesting model of a one dimensional Ising chain coupled to two bath systems as the analysis is based on the phenomenological rates and not on the physical rates.

Finally it is pointed out that the results of the present work will always effect the details of the dynamic evolution apart form situations where the hight temperature approximation can be used. In general more complicated expressions are found compared to the phenomenological results. This even applies to the original model of Glauber. For this kinetic Ising model the equations of motion for the time correlation function partly separate which enables the explicit calculation of the complete dynamics. Such a simplifying separation does not occur for the microscopical master equation. Thus the solution is not known and is hard to find as already pointed out in [1].

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