Selfconsistent Approximations in Mori's Theory

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Abstract

The constitutive quantities in Mori's theory, the residual forces, are expanded in terms of time dependent correlation functions and products of operators at $t = 0$, where it is assumed that the time derivatives of the observables are given by products of them. As a first consequence the Heisenberg dynamics of the observables are obtained as an expansion of the same type. The dynamic equations for correlation functions result to be selfconsistent nonlinear equations of the type known from mode–mode coupling approximations. The approach yields a neccessary condition for the validity of the presented equations. As a third consequence the static correlations can be calculated from fluctuation–dissipation theorems, if the observables obey a Lie algebra. For a simple spin model the convergence of the expansion is studied. As a further test, dynamic and static correlations are calculated for a Heisenberg ferromagnet at low temperatures, where the results are compared to those of a Holstein Primakoff treatment.

Keywords: projection operator technique; residual forces; Heisenberg dynamics; relaxation functions
PACS: 05.20.-y; 05.40.+j

[1] supported by Deutsche Forschungsgemeinschaft

Preprint submitted to Elsevier Science *21 January 1998*

1 Introduction

In Mori's theory [1] the dynamics of a set of relevant observables in the Heisenberg picture are transformed to an equation of motion of the Langevin type showing a systematic part and a residual (stochastic) force as it is suggested by the phenomenological theory of Brownian motion. The great success of Mori's theory is due to the fact that the rewritten equations of motion allow for excellent approximations in calculating linear response functions which are determined by the systematic part of Mori's equations.

In treating the systematic part of the equation the main problem is to get an adequate approximation for the integral kernel given by the correlation functions of the residual forces. For its evaluation mainly two methods have been very successful: A simple perturbation theoretical calculation (for an introduction see [2]) and a factorization procedure into correlation functions of the observables (mode–mode coupling, e.g. [3,4] and references therein).

From a general point of view, the basic quantity in Mori's theory is the residual force. The purpose of the present paper is to point out that for a large class of systems of interacting particles or spins, one can find a systematic approach for the residual force itself, thus being able to go beyond the calculation of linear response functions in terms of static correlation functions: From the residual force one can deduce approximations for

i) the Heisenberg dynamics of the relevant operators
ii) the dynamic correlation functions of the observables
iii) the static correlations

We will show that for systems as interacting spins, where the time derivatives of the relevant observables G are given by a superposition of products of the observables

$$[\mathcal{H}, G] = V^{(1)}G + V^{(2)}GG + V^{(3)}GGG + \cdots \tag{1.1}$$

one can expand the residual force in terms of the dynamic correlation functions. This leads to an approximation scheme for the points (i) and (ii), and together with a Lie algebra for the observables to point (iii). In using this scheme one can see that the calculated Heisenberg dynamics do not have divergent secular terms which occur in a simple perturbation treatment. The dynamics of the correlation functions are governed by a set of nonlinear equations which are close to the usual mode–mode coupling equations. The static correlations in these equations can be expressed by dissipation–fluctuation relations and the Heisenberg dynamics which are given by the dynamic correlation functions and operators at time $t = 0$. Thus all quantities in principle can be calculated from the bare interactions $V^{(1)}, V^{(2)}, \ldots$.

As already mentioned the essential condition for our treatment is that the time derivatives $[\mathcal{H}, G]$ of the relevant observables are given by the products of the observables (Eq.(1.1)). Additionally we exploit the unitarity of the time evolution in Hilbert space which written with the Liouvillian

$$\exp(iLt)\,(GG) = (\exp(iLt)\,G)\,(\exp(iLt)\,G) \quad , \tag{1.2}$$

is not automatically included in a Liouville space calculation, since G and GG are just two different elements of the space.

It is to be expected that our expansion scheme could be generalized to the case where in Eq.(1.1) additional contributions have to be taken into account which are not products of the chosen set. But this extension is beyond the scope of our paper. Our principal interest is to show that besides of linear response, Mori's theory provides a powerful tool to find selfconsistent approximations for the time dependence of the Heisenberg operators $G(t)$, thus leading to the possibility of calculating higher order response functions or expectation values for relaxation processes beyond linear response.

Our paper is organized as follows: In section 2, after having given a short summary of Mori's theory, we present a formal expansion of the residual forces in terms of the dynamic correlation functions, and then discuss the approximation scheme for the points (i)–(iii).

In section 3 we want to illustrate the formal results of section 2 from different points of view. First we will study the accuracy of the approximations by treating a simple model which can be solved exactly. Secondly, we will show how the formalism can be applied to a physical system, and will compare the results to other approaches.

2 Expansion into powers of correlation functions

2.1 Summary of Mori's theory

To summarize Mori's theory we take the notation of [2]. The theory starts with a scalar product in Liouville space given by

$$(A|B) = \beta^{-1} \int_0^\beta d\lambda \langle A^\dagger B(i\lambda)\rangle_\beta \quad , \tag{2.1}$$

where $B(t)$ denotes the time evolution in the Heisenberg picture. Projecting the observables $G_\mu(t)$ onto the space spanned by all the G_ν with

$$P\,G_\nu = (1-Q)G_\nu = G_\nu \quad , \tag{2.2}$$

and onto the orthogonal space, one obtains the Langevin operator for the column vectors $\dot{G}(t)$ in the form

$$\dot{G}(t) = i\,G(t)\Omega - \int_0^t G(t-t')\;(G|G)^{-1}(f|f(t'))dt' + f(t) \quad , \tag{2.3}$$

where $f(t)$ is the column vector of the residual forces with the property

$$Qf(t) = f(t) \quad . \tag{2.4}$$

The abbreviations mean

$$(G(t)\Omega)_\mu = \sum_\nu G_\nu(t)\Omega_{\nu\mu} \tag{2.5}$$

$$\Big((G|G)^{-1}(f|f(t)\Big)_{\nu\mu} = \sum_\lambda (G|G)^{-1}_{\nu\lambda}(f_\lambda|f_\mu(t)) \quad , \tag{2.6}$$

and the frequency matrix is given by the Liouville operator L

$$\Omega_{\nu\mu} = \sum_\lambda (G|G)^{-1}_{\nu\lambda}(G_\lambda|LG_\mu) \quad . \tag{2.7}$$

The main point is that the dynamics of the residual forces $f(t)$ are not governed by the Liouvillian, but by QLQ.

The normalized correlation matrix $\Xi(t)$

$$\Xi_{\nu\mu}(t) = \sum_{\lambda}(G|G)^{-1}_{\nu\lambda}(G_\lambda|G_\mu(t)) \tag{2.8}$$

obeys the matrix equation

$$\dot{\Xi}(t) = i\Xi(t)\Omega - \int_0^t \Xi(t-t')(G|G)^{-1}(f|f(t'))dt' \quad . \tag{2.9}$$

With help of the correlation matrix $\Xi(t)$, the Langevin equations (2.3) can formally be integrated to yield

$$G(t) = G\Xi(t) + \int_0^t f(t')\Xi(t-t')dt' \quad . \tag{2.10}$$

It is this form which we will use in our following treatment.

2.2 Expansion of $f(t)$ in terms of $\Xi(t)$ and static correlations

To find an expansion for the residual force we first establish an exact nonlinear system of equations for $f(t)$ in terms of the correlation functions (2.8). This will be achieved in two steps: We express $f(t)$ by the time derivatives $\dot{G}(t)$, insert Eq.(1.1) which leads to products of $G(t)$. Then the decomposition (2.10) of all $G_\nu(t)$ is used to get a closed system for $f(t)$.

Take the time derivative of Eq.(2.10), then using Eqs. (2.2) and (2.4) we find

$$f(t) = Q\,\dot{G}(t) - f(t)\otimes\dot{\Xi}(t) \quad , \tag{2.11}$$

where we abbreviate the convolution of two functions $a(t)$ and $b(t)$ by

$$\int_0^t a(t-t')b(t')dt' = a(t)\otimes b(t) \quad . \tag{2.12}$$

Substituting the derivatives (1.1) at time t

$$[\mathcal{H}, G_\mu(t)] = \sum_\nu V^{(1)}_{\mu,\nu} G_\nu(t) + \sum_{\nu,\lambda} V^{(2)}_{\mu,\nu\lambda} G_\nu(t) G_\lambda(t) + \cdots \tag{2.13}$$

abbreviated by

$$[\mathcal{H}, G(t)] = V^{(1)} G(t) + V^{(2)} \{G(t), G(t)\} + \cdots \tag{2.14}$$

into Eq.(2.11) we arrive at

$$f(t) = iQV^{(2)} \{G(t), G(t)\} - if(t) \otimes (G|G)^{-1}(G|V^{(2)} \{G(t), G(t)\}) + \cdots \quad ,(2.15)$$

where use has been made of the definition of $\dot{\Xi}(t)$ (2.8), and of the relation

$$V^{(1)} Q(G(t) - f(t) \otimes \Xi(t)) = V^{(1)} Q(G\Xi(t)) = 0 \tag{2.16}$$

which follows from Eqs.(2.10) and (2.2).

Finally we insert the decomposition (2.10) of $G(t)$ into Eq.(2.15). Then a closed set of equations arises which implicitely defines $f(t)$ in terms $\Xi(t)$ and static correlations. To make it clear we write down the result for the case, where $V^{(3)}, V^{(4)} \cdots$ vanish. One yields

$$\begin{aligned} f(t) = {} & iQV^{(2)} \{G\Xi(t) + f(t) \otimes \Xi(t), G\Xi(t) + f(t) \otimes \Xi(t)\} \\ & - if(t) \otimes (G|G)^{-1}(G|V^{(2)} \{G\Xi(t) + f(t) \otimes \Xi(t), G\Xi(t) + f(t) \otimes \Xi(t)\}) \quad . \end{aligned} \tag{2.17}$$

For simplicity we restrict to this case in the following.

The implicit system (2.17) for $f(t)$ is our basic result and will be the starting point for our approximations. To find an explicit expression for $f(t)$ we will iteratively solve Eq.(2.17). Let us illustrate this procedure for a simple case.

The expansion to be chosen depends on the magnitude of the matrix elements of $V^{(2)}$. Suppose that we can take all matrix elements of $V^{(2)}$ to be of the same order of magnitude of a smallness parameter ϵ,

$$V^{(2)} \sim \epsilon \quad . \tag{2.18}$$

Then we can write

$$f(t) = \epsilon f^{(1)}(t) + \epsilon^2 f^{(2)}(t) + \cdots \quad , \tag{2.19}$$

and comparing both sides of Eq.(2.17) we will find the explicit expressions for $f^{(n)}(t)$ in terms of correlation functions $\Xi(t)$ and products of operators G.

The lowest order contribution yields

$$f(t) = iQ\, V^{(2)} \{G\Xi(t), G\Xi(t)\} + \cdots \quad , \tag{2.20}$$

where $f(t)$ lies in the space spanned by G and the products GG, and the time–dependent coefficients are given by products of $\Xi(t)$.

From a physical point of view the result (2.20) can be interpreted as a sum of coupled modes, whose time dependency is given by $\Xi(t)$. In Eq.(2.20) the projector Q acting on the products GG projects out all contributions of the linear space spanned by the modes G_ν. Therefore the effect of the coupling of the $\Xi(t)$ can be very weak, although formally the bare interaction strength $V^{(2)}$ appears. This point will become more clear in our example in section 3, where we treat interacting spin waves. A further comment should be given as to the time scale for $f(t)$ appearing in Eq.(2.20). In a macroscopic interacting system the matrix $V^{(2)}$ implies a summation over a very large number of products $\Xi_{\nu\mu}(t)\,\Xi_{\lambda\sigma}(t)$. So the phase factors of these products can produce a correlation time for $f(t)$ which is entirely different from the relaxation times of $\Xi(t)$.

Iterating Eq.(2.17) one step further one obtains $f^{(2)}(t)$, which then results to be in the space spanned by G, GG, GGG. Although mathematically possible, we have found from the example discussed in section 3.1 that instead of calculating $f^{(2)}(t)$ it is more adequate to take a larger set of observables $\tilde{G}$ which comprises the products GG, and use the lowest order approximation (2.20) to this set. Then one obtains

$$\tilde{f}(t) = i\tilde{Q}\tilde{V}^{(2)} \left\{\tilde{G}\tilde{\Xi}(t), \tilde{G}\tilde{\Xi}(t)\right\} \quad , \tag{2.21}$$

where $\tilde{f}(t)$ is the column-vector of the residual forces arising for the set $\tilde{G}$. It includes the contribution of $f^{(2)}$ of the original set $\{G\}$. The relation between $\tilde{f}(t)$ and $f^{(2)}(t)$ is discussed in appendix A.

The simple expansion scheme starting with Eq.(2.18), or Eq.(2.20) respectively, will be illustrated in section 3.1, whereas an expansion of $f(t)$ with

$$V^{(2)} = V_0^{(2)} + \epsilon\, V_1^{(2)} \tag{2.22}$$

will be the basis for the treatment of our example in section 3.2.

2.3 Expansion of $G(t)$ in terms of $\Xi(t)$ and static correlations

Regarding the general decomposition (2.10) of $G(t)$ into $PG(t)$ and $QG(t)$ it is clear, that inserting approximations for $f(t)$ one obtains an expansion of $G(t)$ into powers of $\Xi(t)$ and static correlations. For the case (2.18) the lowest order contribution follows to be

$$G(t) = G\Xi(t) + iQV^{(2)}\{G\Xi(t), G\Xi(t)\} \otimes \Xi(t) + \cdots \quad . \tag{2.23}$$

The main point of this result is, that for an interacting system, $\Xi(t)$ exhibits damping, so that the Fourier transforms of $G(t)$ do not have divergent denominators. Furthermore the projector Q again weakens the effect of the given interaction $V^{(2)}\{G, G\}$, as the part $P(GG)$ is already contained in the dynamics of $\Xi(t)$. The structure of the result (2.23) is the same as it is known from an ordinary expansion of $G(t)$ with respect to $V^{(2)}$. For $[\mathcal{H}^{(0)}, G] = V^{(1)}G$, we would find Eq.(2.23) without Q, i.e. the full interaction, and $\Xi(t)$ being replaced by the transposal of exp $[i\,V^{(1)}t]$.

Once an approximation of $\Xi(t)$ is known, one can use Eq.(2.23) to calculate expectation values for relaxation processes or higher order response functions. If one wants to improve the result (2.23), one can again take the larger set of observables $\tilde{G}$ and use Eq.(2.23) for the corresponding quantities.

2.4 Nonlinear equations for $\Xi(t)$ in terms of static correlations

The correlation matrix $\Xi(t)$ is determined by Eq.(2.9), i.e. by the correlations $(f|f(t))$. Therefore use can be made of the expansion procedure for the residual force $f(t)$ of section 2.2 leading to closed nonlinear equations for $\Xi(t)$. Taking the case (2.18) and substituting the lowest order contribution of $f(t)$ (2.20) into Eq.(2.9) yields the following set of equations

$$\begin{aligned} \dot{\Xi}(t) = {} & i\Xi(t)\Omega \\ & - \int_0^t \Xi(t-t')(G|G)^{-1}(V^{(2)}\{G,G\}\,|QV^{(2)}\{G\Xi(t'), G\Xi(t')\})dt' \quad . \end{aligned} \tag{2.24}$$

It is clear that higher order equations can be obtained, if higher order terms of $f(t)$ are inserted into $(f|f(t))$. So we have found a systematic way to generate equations for correlation functions $\Xi(t)$.

But we need not write down these higher order equations for $\Xi(t)$, because – as already has been discussed in section 2.2 – the higher order approximations to $\Xi(t)$ are included in Eq.(2.24), if used for an extended set of observables $\tilde{G} = \{G, GG - \langle GG\rangle, GGG - \langle GGG\rangle, \cdots.\}$. with new parameters $\tilde{\Omega}$ and $\tilde{V}^{(2)}$ and the corresponding correlation matrix $\tilde{\Xi}(t)$.

Inspecting the result, (2.24) shows that it has the structure known from mode–mode coupling approximations. In our case we have obtained equations – as mentioned in the introduction – with bare interactions $V^{(2)}$ [5–7].

As a check of the validity of the approximation (2.24) one can take the time dependence $G(t)$ resulting from (2.23) with the approximate Ξ and calculate the correlation

$$\Delta(t) = (G|G)^{-1}\ (G(t)|G(t)) \tag{2.25}$$

which for the exact dynamics $G(t)$ is one. In the discussion of the example given in section 3.1 we have found that the deviation of Δ from 1 is directly related to the accuracy of the approximate Ξ.

2.5 Static correlations

The equations of motion for $\Xi(t)$ Eq.(2.24) contain static correlations. They can be viewed as given parameters and can be taken from any static theory which is available. In this section we want to point out that in many cases however, one can close the dynamic equations (2.24) by a set of equations for the static correlations which appear in $\Xi(t)$, so that all quantities – at least in principle – can be determined in a selfconsistent way. The key point is that the approximations obtained for the observables $G(t)$ in the Heisenberg picture are expressed in terms of c–number time functions and products of operators G at time $t = 0$. So the well known KMS–condition for the Heisenberg operators G at imaginary times $i\beta$

$$\langle G\,A\rangle_\beta = \langle AG(i\beta)\rangle_\beta \quad , \tag{2.26}$$

which can be cast into the relations

$$(A|G) = \int_{-\infty}^{\infty} \frac{d\omega}{\beta\omega} \langle [G(\omega), A^\dagger] \rangle_\beta \tag{2.27}$$

$$\langle A\, G \rangle_\beta = \int_{-\infty}^{\infty} d\omega (e^{\beta\omega} - 1)^{-1} \langle [G(\omega), A] \rangle_\beta \quad , \tag{2.28}$$

directly connects static and dynamic correlations. Here $G(\omega)$ denotes

$$G(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(t) e^{i\omega t} dt \quad , \tag{2.29}$$

and it has been assumed that the observables G are chosen to be orthogonal to 1 and no other constants of motion are to be projected out. Therefore we must only show that given an approximation for $G(t)$, or $f(t)$ respectively, Eq.(2.27) and Eq.(2.28) will provide us with a closed set of equations for the relevant static correlations appearing in $\Xi(t)$. To this end we will suppose that the operators G obey a Lie- algebra [2] [3]

$$[G, G] = \sum \cdots G + C1 \tag{2.30}$$

leading to

$$[G, GG] = \sum \cdots GG + \sum \ldots G \tag{2.31}$$

$$[GG, GG] = \sum \cdots GGG + \sum \ldots GG \quad . \tag{2.32}$$

For clarity in the presentation we refrain from writing down the structure constants explicitly, but focus on the observables. Let us first discuss the expansion scheme $V^{(2)} \sim \epsilon$ of section 2.2 with the lowest order approximation for $G(t)$ found to be

$$G(t) = G\Xi + iQV^{(2)} \{G\Xi, G\Xi\} \otimes \Xi \quad . \tag{2.33}$$

The corresponding equation for Ξ is given by (2.24). If we apply the Kubo identity

$$\beta (G|LA)_\beta = \langle [G^\dagger, A] \rangle_\beta \tag{2.34}$$

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[2] The matrix C can originate from the fact that the G have been chosen with the property $(1|G)_\beta = \langle G \rangle_\beta = 0$.

[3] If non–Hermitian operators G are used, the operators $G^\dagger$ are assumed to be elements of the space spanned by the set G.

to its frequency and memory matrices and carry out the commutators with help of Eqs.(2.30) and (2.31), and $\langle G\rangle_\beta = 0$, then we see that $\Xi(t)$ depends on the static correlations $(G|G)$, $\langle GG\rangle$, $(G|GG)$ only

$$\Xi = \Xi(t, (G|G), \langle GG\rangle, (G|GG)) \quad . \tag{2.35}$$

To connect these static quantities we start with two relations which are independent of the approximations. Regarding $LG = V^{(1)}G + V^{(2)}\{G, G\}$ and calculating $(G|LG)$ from the Kubo identity with Eq.(2.30) we arrive at

$$C = \beta(G|V^{(1)}G) + \beta(G|V^{(2)}\{G, G\}) \quad . \tag{2.36}$$

On the other hand we calculate $\langle G^\dagger G\rangle$ applying Eq.(2.28) to $A = G^\dagger$. Inserting (2.33) and the equation of motion for $\Xi(\omega)$ we arrive at

$$\langle G^\dagger G\rangle = (G|G) \int\limits_{-\infty}^{\infty} d\omega \frac{\beta\omega}{e^{\beta\omega} - 1} \Xi(\omega) \quad . \tag{2.37}$$

Two further relations are obtained, if we explicitly use the approximation (2.33) for $G(t)$ or $G(\omega)$ respectively. We regard Eq.(2.27) for $A = (GG)^\dagger$ and insert the Fouriertransform of (2.33)[4]. Then respecting the commutators (2.31) and (2.32) we find equations of the following structure

$$(G|GG) = \sum \cdots \langle GG\rangle + \sum \cdots \langle GGG\rangle + \sum \cdots \langle GG\rangle(G|G)^{-1}(G|GG) \quad , \tag{2.38}$$

where we have omitted the coefficients which are given by the structure constants of the Lie algebra and matrix elements of

$$\int \frac{d\omega}{\beta\omega}\Xi(\omega) \quad \text{and} \quad \int \frac{d\omega}{\beta\omega}(\Xi\Xi \otimes \Xi)(\omega) \quad . \tag{2.39}$$

To close this system of equations with $\langle GGG\rangle$ we regard Eq.(2.28) for $A = GG$ yielding

$$\langle GGG\rangle = \sum \cdots \langle GG\rangle + \sum \cdots \langle GGG\rangle + \sum \cdots \langle GG\rangle(G|G)^{-1}(G|GG) \tag{2.40}$$

[4] The correlations $(G|G)$ cannot be calculated from Eq.(2.27) with $A = G$, as in this case Eq.(2.27) identically holds, if the equation of motion for $\Xi(\omega)$ is inserted.

with coefficients analogous to the coefficients appearing in Eq.(2.38). The only difference is, that the denominators $\beta\omega$ in Eq.(2.39) are replaced by $(e^{\beta\omega}-1)$.

These four equations (2.36), (2.37), (2.38), (2.40) for $(G|G), \langle GG\rangle, (G|GG), \langle GGG\rangle$ now in principle allow for a determination of the static correlations in terms of functionals of the dynamic correlations $\Xi(\omega)$, where it is clear, that the solvability must be discussed in each application. Although these equations are extremely complicated, one can think of an iterative solution starting with suitable static values in the dynamics of Ξ. Another simplification occurs, if the temperature is high enough so that $\tanh\beta\omega$ can be replaced by $\beta\omega$. Then it holds

$$(G|G) = \frac{1}{2}\langle[G^\dagger, G]_+\rangle \tag{2.41}$$

$$(G|GG) = \frac{1}{2}\langle[G^\dagger, GG]_+\rangle \quad , \tag{2.42}$$

and the total system reduces to a set for the correlations $\langle GG\rangle$ and $\langle GGG\rangle$.

We emphasize that the basis for our discussions on the statics was the result (2.33) for the Heisenberg dynamics. If we now consider higher order contributions to $G(t)$, we have found two possibilities, as was pointed out in section 2.2 and 2.3. But as to the static correlations these two treatments are not equivalent. If we improve Eq.(2.33) by a residual force $f^{(2)}(t)$, so that $G(t)$ is an element of the space spanned by G, GG, GGG, then it is not difficult to see, that the static equations resulting from (2.27) and (2.28) are no longer closed. However, if we use the alternative and extend the set of observables to yield a set $\tilde{G}$ which includes the products GG, then the set of equations for the static correlations appearing in $\tilde{\Xi}(t)$ again can be closed (appendix A). This also indicates that the second way is more adequate.

So far we have discussed the equations for the static correlations which result from the expansion scheme for the residual forces with $V^{(2)} \sim \epsilon$. In general the static relations to be obtained will depend on the iteration procedure for $f(t)$ which will be chosen. In our example of section 3.2, where we treat the lowest order of a case $V^{(2)} = V_0^{(2)} + \epsilon V_1^{(2)}$, we will see that a closed set of equations can be derived again.

The considered approaches leading to closed sets for the static correlations have the common feature that they are valid to the same degree of accuracy as the dynamics in the Heisenberg picture is correct. In this sense dynamics and statics are treated at the same level of approximation.

3 Illustrations and discussion

In this section we will illustrate the general formalism of section 2 applying it to two examples. First we will study general features of the approximation scheme. To this end we choose a model as simple as possible: We take a spin system with long range interactions in the high temperature limit, so that we need not handle with the problem of the static correlations, and can obtain both, the exact solution to the dynamics and the approximations in analytic form. As a second example we will treat a Heisenberg ferromagnet at low temperatures. We will show that one can find an expansion of the residual forces in terms of spin operators which leads to meaningful results for the Heisenberg dynamics and the correlation functions, so that we can make contact to other approaches.

3.1 Exactly solvable model in the high temperature limit

Our model to be considered is a Heisenberg spin system with long range interactions in the high temperature limit, where we can carry through the general expansions of sections 2.2 and 2.3 to high order explicitly. We will find that the lowest order approximation to the residual forces leads to a coupling of two modes only, where one of them is a trivial constant of the motion. So the system might be a very special one, but we think that it correctly gives insight into the problems of time scales and convergence.

The Hamiltonian of our system reads

$$\mathcal{H} = -\frac{J}{\sqrt{N}} \sum_{ij} \vec{s}_i \cdot \vec{s}_j = -\frac{J}{\sqrt{N}} \vec{S}_0 \cdot \vec{S}_0, \tag{3.1}$$

where

$$\vec{S}_q = \sum_{i=1}^{N} e^{i\vec{q}\vec{R}_i} \vec{s}_i \tag{3.2}$$

$$\vec{S}_0 = \vec{S}_{q=0} \quad , \tag{3.3}$$

and the N spins ($s = \frac{1}{2}$) are located at lattice sites $\vec{R}_i$. In the high temperature limit the scalar product reduces to

$$(A|B) = (\mathrm{Tr}1)^{-1}\mathrm{Tr}(A^\dagger B), \tag{3.4}$$

so that static spin correlations can be evaluated.

In choosing a set of observables $\{G\}$ we take $\vec{S}_q$, but substract the components parallel to the constant of the motion $\vec{S}_0$, so that the dynamic correlation functions $\Xi(t)$ will decay to zero (c.f. appendix B). Therefore we take the set of observables to be

$$\begin{aligned} &\vec{G}_0 = \vec{S}_0 \\ &\vec{G}_q = \vec{S}_q - \frac{1}{2}(\vec{S}_0 \cdot \vec{S}_0)^{-1} \left((\vec{S}_0 \cdot \vec{S}_q)\vec{S}_0 + \vec{S}_0(\vec{S}_0 \cdot \vec{S}_q) \right) \quad q \neq 0 \end{aligned} \tag{3.5}$$

with $\vec{S}_0 \cdot \vec{S}_q = \sum_\alpha S_0^\alpha S_q^\alpha$. Then it holds

$$L\vec{G}_q = i\frac{J}{\sqrt{N}} \left(\vec{G}_q \times G_0 - G_0 \times \vec{G}_q \right) \quad q \neq 0 \quad , \tag{3.6}$$

which means, that the conditions of section 2.2

$$LG = V^{(1)}G + V^{(2)}\{G, G\} \tag{3.7}$$

are fulfilled, where $V^{(1)}$ vanishes and $V^{(2)}$ just couples $\vec{G}_q$ to $\vec{G}_0$. From the symmetry of the Hamiltonian it directly follows that the correlation matrix $\Xi(t)$ is diagonal with respect to $\vec{q}, \vec{q}'$ and cartesian components $\alpha, \alpha' = x, y, z$, so that the decompositions (2.10) specialize to

$$q = 0 : \vec{G}_0(t) = \vec{G}_0 \cdot 1 + 0 \tag{3.8}$$

$$q \neq 0 : \vec{G}_q(t) = \vec{G}_q \Xi(t) + \vec{f}_q(t) \otimes \Xi(t) \quad , \tag{3.9}$$

where

$$\Xi(t) = (G_q^\alpha | G_q^\alpha)^{-1} \left(G_q^\alpha | G_q^\alpha(t) \right) \tag{3.10}$$

for $q \neq 0$ does not depend on q and α. So we are ready to study the expansion of the residual forces $\vec{f}_q(t)$ with an expansion parameter $\epsilon \sim J$.

3.1.1 The first order approximation

We now take our model to carry through the expansions of section 2 for the case $V^{(1)} = 0$, $V^{(2)} \sim \epsilon \sim J$ iterating the Eq.(2.17) for $\vec{f}_q(t)$. Although J will be a formal expansion parameter the accuracy of the approximations will not be determined by the smallness of J but rather by a condition on time $Jt \ll \delta$, as for $V^{(1)} = 0$ we just have one time scale given by J^{-1}. Nevertheless in a high order approximation the bound δ may be so large that the "short time expansion" covers the whole range of physical interest. We will study this problem of time range in detail, calculating the correlation function $\Xi(t)$ to general order.

The lowest order approximation for the residual force $\vec{f}_q(t)$ follows from (2.20), (3.8) and (3.9) to yield [5]

$$\vec{f}_q(t) = \frac{J}{\sqrt{N}}(\vec{G}_0 \times \vec{G}_q - \vec{G}_q \times \vec{G}_0)\Xi = iL\vec{G}_q\Xi \quad , \tag{3.11}$$

where just two modes $\Xi_q = \Xi$ and $\Xi_{q=0} = 1$ couple, so that the force $\vec{f}_q(t)$ for all times is proportional to one fixed element in the space of the GG.

The dynamics of the Heisenberg operators $\vec{G}_q(t)$ corresponding to the approximation (3.11) are obtained from (2.23) to give

$$\begin{aligned}\vec{G}_q(t) &= \vec{G}_q\Xi(t) + \frac{J}{\sqrt{N}}(\vec{G}_0 \times \vec{G}_q - \vec{G}_q \times \vec{G}_0)\Xi(t) \otimes \Xi(t) \\ &= \vec{G}_q\Xi + iL\vec{G}_q\Xi \otimes \Xi \quad .\end{aligned} \tag{3.12}$$

In this expansion the coefficient $\Xi(t)$ of $\vec{G}_q$ is exact, whereas the coefficient $\Xi \otimes \Xi$ of $iL\vec{G}_q$ will be modified by higher order terms, if these are projected onto $L\vec{G}_q$. The equation of motion for the correlation function $\Xi(t)$ is given by Eq.(2.24) and simplifies to

$$\dot{\Xi} = -m_2\Xi \otimes \Xi \quad , \tag{3.13}$$

where

$$m_2 = \frac{(G_q^\alpha|L^2G_q^\alpha)}{(G_q^\alpha|G_q^\alpha)} \qquad (q \neq 0) \tag{3.14}$$

is independent of q and α. The solution of (3.13) for $\Xi(t)$ can be expressed by the

[5] As $(G_q|LG_q) = 0$ the projection operator Q can be ommitted.

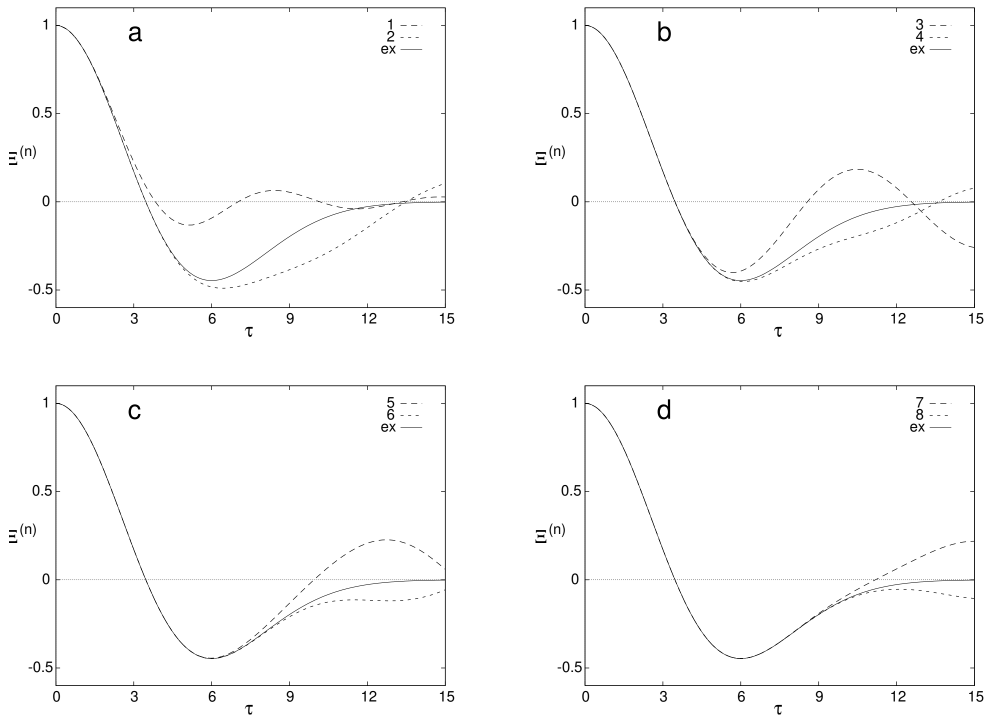

Fig. 1. Approximations $\Xi^{(n)}(\tau)$ compared to the exact correlation function $\Xi(\tau)$; a: $n = 1, 2$, exact; b: $n = 3, 4$, exact; c: $n = 5, 6$, exact; d: $n = 7, 8$, exact.

Bessel function J_1. Taking the Laplace transform of (3.13) one finds

$$\Xi^{(1)}(s) = 2\frac{-s + \sqrt{s^2 + 4m_2}}{4m_2} \quad , \tag{3.15}$$

or

$$\Xi^{(1)}(t) = 2\frac{J_1(\tau)}{\tau}, \quad \tau = 2\sqrt{m_2}t \tag{3.16}$$

respectively, where the index denotes the order of the approximation. This result for $\Xi^{(1)}(t)$ is compared to the exact solution in Fig.1. One sees that $\Xi^{(1)}(t)$ is close to the exact correlation function, as long as Jt is smaller than the zero of $\Xi(t)$, i.e. as long as it holds

$$Jt \leq 1 \quad . \tag{3.17}$$

At the end of section 3.1 we will show that the range of validity (3.17) for $\Xi^{(1)}(t)$ can be estimated from $\Xi^{(1)}(t)$ and (3.12) alone, without knowledge of the exact solution.

3.1.2 Higher order approximations

As there are more possibilities to derive higher approximations we will first study the second order approximation in some detail and then give the general results.

Iterating Eq. (2.17) for $\vec{f}_q(t)$ up to order J^2 we find for the residual force

$$\begin{aligned}\vec{f}_q(t) = & \frac{J}{\sqrt{N}} \left(\vec{G}_0 \times \vec{G}_q - \vec{G}_q \times \vec{G}_0\right) \Xi \\ & + \frac{J^2}{N} Q \left\{\vec{G}_0 \times \left(\vec{G}_0 \times \vec{G}_q - \vec{G}_q \times \vec{G}_0\right) - \left(\vec{G}_0 \times \vec{G}_q - \vec{G}_q \times \vec{G}_0\right) \times \vec{G}_0\right\} \Xi \otimes \Xi \\ = & \, iL\vec{G}_q \Xi + Q(iL)^2 \vec{G}_q \Xi \otimes \Xi \quad , \end{aligned} \tag{3.18}$$

and for the Heisenberg dynamics of $\vec{G}_q(t)$

$$\vec{G}_q(t) = \vec{G}_q \Xi + iL\vec{G}_q \Xi \otimes \Xi + Q(iL)^2 \vec{G}_q \Xi \otimes \Xi \otimes \Xi \quad . \tag{3.19}$$

The dynamics of $\Xi(t)$, however, keeps to be $\Xi^{(1)}(t)$, as the new added term in $\vec{f}_q(t)$ is orthogonal to $\vec{f}_q(0) = iL\vec{G}_q$,

$$(f_q^\alpha | Q(iL)^2 \, G_q^\alpha) = 0 \quad , \tag{3.20}$$

so that the memory function does not change. To improve $\Xi^{(1)}(t)$, at least third order terms in $f_q^\alpha(t)$ have to be considered which have a non–vanishing projection onto iLG_q^α.

An alternative approach to the second order result described above can be given, if we keep the basis we have obtained for $\vec{f}_q(t)$ and $\vec{G}_q(t)$ in (3.19), but use a formulation such that the factor of $iL\vec{G}_q$ will not be changed by higher order terms. This means that higher order terms must be constructed to be orthogonal to the products $iL\vec{G}_q = J/\sqrt{N}(\vec{G}_0 \times \vec{G}_q - \vec{G}_q \times \vec{G}_0)$ (c.f. appendix A).

For this alternative approach to the second order approximation we extend the set of observables G to the larger set $\{\tilde{G}\}$, which comprises the occuring basis vectors of products GG, i.e. $iL\vec{G}_q$:

$$\{\tilde{G}\} = \{\vec{G}_0, \vec{G}_{q,1} = \vec{G}_q, \vec{G}_{q,2} = iL\vec{G}_q\}. \tag{3.21}$$

The corresponding projection operator onto this space is denoted by $\tilde{P} = 1 - \tilde{Q}$. Then the general formalism of section 2 applies to the set $\{\tilde{G}\}$, as it holds

$$
\begin{aligned}
iL\vec{G}_{q,1} &= \vec{G}_{q,2} \\
iL\vec{G}_{q,2} &= \frac{J}{\sqrt{N}}\left(\vec{G}_0 \times \vec{G}_{q,2} - \vec{G}_{q,2} \times \vec{G}_0\right) \quad .
\end{aligned} \tag{3.22}
$$

Thus the condition (1.1) with $\tilde{V}^{(1)} \neq 0$ and $\tilde{V}^{(2)} \sim J$ again are fulfilled, and the lowest order approximation (2.20) for the residual forces $\left\{\tilde{f}\right\} = \left\{\vec{f}_{q,1}, \vec{f}_{q,2}\right\}$ reads

$$
\vec{f}_{q,1}(t) = 0 \tag{3.23}
$$

$$
\vec{f}_{q,2}(t) = \frac{J}{\sqrt{N}}\tilde{Q}\left(\vec{G}_0 \times \vec{G}_{q,2} - \vec{G}_{q,2} \times \vec{G}_0\right)\Xi_{22} \quad , \tag{3.24}
$$

where the matrix of the correlation functions $\Xi_{\nu\mu}(t)$ is defined by

$$
\Xi_{\nu\mu} = \frac{(G^\alpha_{q,\nu}|G^\alpha_{q,\mu}(t))}{(G^\alpha_{q,\nu}|G^\alpha_{q,\nu})} \quad \nu,\mu = 1,2 \quad . \tag{3.25}
$$

Hence the Heisenberg dynamics for $\vec{G}_q(t) = \vec{G}_{q,1}(t)$ follow to be

$$
\begin{aligned}
\vec{G}_q(t) = \vec{G}_{q,1}(t) &= \vec{G}_{q,1}\Xi_{11} + \vec{G}_{q,2}\Xi_{21} + \vec{f}_{q,2} \otimes \Xi_{21} \\
&= \vec{G}_q\Xi_{11} + iL\vec{G}_q\Xi_{21} + Q(iL)^2\vec{G}_q(\Xi_{22} \otimes \Xi_{21}) \quad .
\end{aligned} \tag{3.26}
$$

One sees that the result (3.26) for $\vec{G}_q(t)$ is spanned by the same basis vectors as it was in Eq.(3.19). Just the time–dependent coefficients have changed. [6]

In order to determine $\Xi(t)$, we now write down the equations of motion for the matrix $\Xi_{\nu\mu}(t)$ (c.f. Eq.(3.22)) which follow from the frequency matrix (2.7) and the memory matrix given by $(f^\alpha_{q,2}|f^\alpha_{q,2}(t))$. We obtain

$$
\dot{\Xi}_{11} = \Xi_{12}
$$

[6] If one extracts the residual force $\vec{f}_q(t)$ with respect to $\{G\}$ from the result (3.26), one finds that $\vec{f}_q(t)$ also has the same basis vectors as the approximation (3.18). It is not difficult to see, that the memory functions calculated from this $\vec{f}_q(t)$ just lead to the exact relation $\dot{\Xi} = -\frac{(f^\alpha_q|f^\alpha_q(t))}{(G^\alpha_q|G^\alpha_q)} \otimes \Xi$.

$$\dot{\Xi}_{12} = -c_2\Xi_{11} - c_3\Xi_{12} \otimes \Xi_{22} \tag{3.27}$$
$$\dot{\Xi}_{21} = \Xi_{22} \tag{3.28}$$
$$\dot{\Xi}_{22} = -c_2\Xi_{21} - c_3(\Xi_{22} \otimes \Xi_{22}), \tag{3.29}$$

where $c_2 = m_2$ and $c_3 = (m_4 - m_2^2)/m_2$, and m_4 denotes the fourth moment.

This system can be solved by Laplace transform to yield for $\Xi^{(2)} = \Xi_{11}$

$$\Xi^{(2)}(s) = \frac{-\frac{c_3}{c_2}s - 1/2\left(s + \frac{c_2}{s}\right) + \frac{1}{2}\sqrt{\left(s + \frac{c_2}{s}\right)^2 + 4c_3}}{-\frac{c_3}{c_2}s^2} \quad . \tag{3.30}$$

The corresponding result in time $\Xi^{(2)}(t)$ is shown in Fig.1. As compared to $\Xi^{(1)}(t)$ the range of validity of $\Xi^{(2)}(t)$ has obviously increased.

The alternative approach for the second order approximation can be extended to general order. Instead of iterating the Eq.(2.17) for $\vec{f}_q(t)$ and calculating $\vec{f}_q(t)$ up to order J^n, we choose a set $\{\tilde{G}\}$ given by $\vec{G}_q, iL\vec{G}_q, \cdots (iL)^n\vec{G}_q$, and take the lowest order approximation for the residual forces. The details are given in appendix B. Here we just list the results. To write them down, it is expedient to use an orthogonal basis $\vec{G}_{q,\nu}$ in the space $\left\{\tilde{G}\right\}$ introduced by

$$\begin{aligned} \vec{G}_{q,1} &= \vec{G}_q \\ \vec{G}_{q,2} &= iL\vec{G}_{q,1} \\ \vec{G}_{q,\nu} &= iL\vec{G}_{q,\nu-1} + \frac{(G^\alpha_{q,\nu-1}|G^\alpha_{q,\nu-1})}{(G^\alpha_{q,\nu-2}|G^\alpha_{q,\nu-2})}\vec{G}_{q,\nu-2} \qquad \nu = 3, \cdots, n \quad . \end{aligned} \tag{3.31}$$

Then the residual forces read

$$\begin{aligned} \vec{f}_{q,\nu}(t) &= 0 \qquad \nu = 1, \cdots n-1 \\ \vec{f}_{q,n}(t) &= \vec{G}_{q,n+1}\Xi_{nn} \quad , \end{aligned} \tag{3.32}$$

where $\vec{G}_{q,n+1}$ is defined by (3.31) with $\nu = n+1$. The Heisenberg dynamics result to be

$$\vec{G}_q(t) = \vec{G}_{q,1}(t) = \sum_{\nu=1}^{n} \vec{G}_{q,\nu}\,\Xi_{\nu 1} + \vec{G}_{q,n+1}\Xi_{nn} \otimes \Xi_{n1} \quad . \tag{3.33}$$

The equations for the correlation matrix

$$\Xi_{\nu\mu} = \frac{\left(G^{\alpha}_{q,\nu}|G^{\alpha}_{q,\mu}(t)\right)}{\left(G^{\alpha}_{q,\nu}|G^{\alpha}_{q,\nu}\right)} \tag{3.34}$$

are found from the frequency and memory matrix. The explicit solution for the Laplace transforms of $\Xi_{\nu 1}$ and Ξ_{nn} are

$$\Xi_{\nu 1}(s) = \frac{\Xi(s)B_{\nu-1}(s) - A_{\nu-1}(s)}{c_1 \cdots c_\nu}(-1)^{\nu-1} \qquad \nu = 2,\cdots,n \quad , \tag{3.35}$$

$$\Xi_{nn}(s) = B_{n-1}(s)\Xi_{n1}(s) \quad , \tag{3.36}$$

where $\Xi^{(n)} = \Xi_{11}$ is given by

$$\Xi^{(n)}(s) = \frac{A_{n-1}}{B_{n-1}} + \frac{-\frac{B_n}{B_{n-1}} + \sqrt{\left(\frac{B_n}{B_{n-1}}\right)^2 + 4c_{n+1}}}{2(-1)^{n-1}\frac{c_{n+1}}{c_1\cdots c_n}B^2_{n-1}} \quad , \tag{3.37}$$

and the $A_\nu(s), B_\nu(s)$ are polynominals in s defined by

$$\begin{aligned} A_\nu &= s\,A_{\nu-1} + C_\nu\,A_{\nu-2} \qquad A_0 = 0 \qquad A_1 = 1 \\ B_\nu &= s\,B_{\nu-1} + C_\nu\,B_{\nu-2} \qquad B_0 = 1 \qquad B_1 = s \qquad \nu = 2,\cdots,n \end{aligned} \tag{3.38}$$

with

$$\begin{aligned} c_1 &= 1 \\ c_\nu &= \frac{\left(G^{\alpha}_{q,\nu}|G^{\alpha}_{q,\nu}\right)}{\left(G^{\alpha}_{q,\nu-1}|G^{\alpha}_{q,\nu-1}\right)} \qquad \nu = 2,\cdots n, \quad \alpha = x,\ \text{or}\ y,z \quad . \end{aligned} \tag{3.39}$$

The functions $\Xi^{(n)}(s)$ for complex s are holomorphic for $\mathrm{Re}s > 0$ and have the correct property

$$\mathrm{Re}\Xi^{(n)}(s) \geq 0, \quad \mathrm{Re}s \geq 0 \quad . \tag{3.40}$$

The results for $\Xi^{(n)}(t)$ and the exact solution $\Xi(t)$ are plotted in Fig.1. One sees that the time region, where $\Xi^{(n)}(t)$ is a good approximation to $\Xi(t)$ increases with n. The

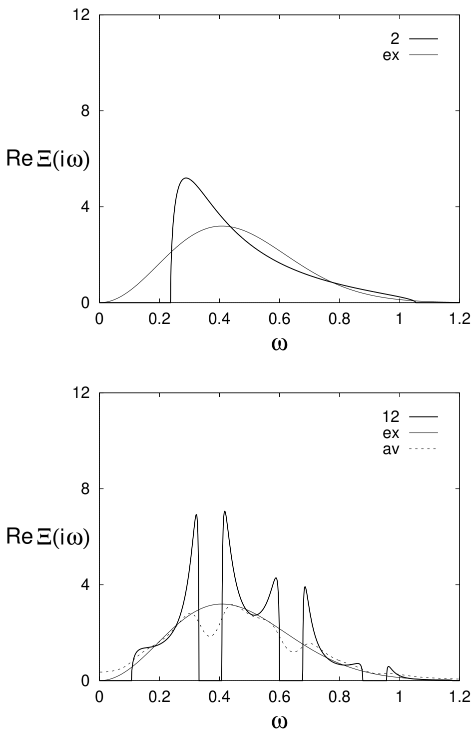

Fig. 2. Spectral densities of the approximations $\mathrm{Re}\Xi^{(n)}(i\omega)$, compared to the exact density for $n = 2, 3, 12, 13$. An averaged spectrum is shown for $n = 12$. Frequency and spectrum in units of $(4m_2)^{1/2}$ and $(4m_2)^{-1/2}$ respectively.

spectral densities $1/2\int_{-\infty}^{\infty} dt \Xi(t)e^{-i\omega t} = \mathrm{Re}\Xi^{(n)}(s = i\omega)$ are shown in Fig.2 [7]. The intervals where $\mathrm{Re}\Xi^{(n)}(i\omega)$ identically vanishes are due to the square root occuring in $\Xi^{(n)}(s)$ and are a consequence of the coupling of just two modes. Therefore in the case of many modes one can expect that the values $\mathrm{Re}\Xi^{(n)}(i\omega) \neq 0$ are no longer restricted to finite intervals which cause the asymptotic oscillations for long times in $\Xi^{(n)}(t)$.

At the end of this section we will discuss the validity of the approximations from a different point of view. Our approach does not only lead to equations for the correlation functions. The basis was the expansion of the residual force and the resulting Heisenberg dynamics $\vec{G}_q(t)$. From this we will be able to write down a necessary condition for the accuracy of the n–th order approximation for $\Xi(t)$ and $\vec{G}_q(t)$. Let us

[7] If one wants to get approximations which are valid for all times $0 \leq Jt \leq \infty$ one can average the spectral densities $\mathrm{Re}\Xi^{(n)}(i\omega)$ with a width δ which smoothens the intervals $\mathrm{Re}\Xi^{(n)}(i\omega) = 0$. An example for $n = 12$, $1/\pi \int d\omega' \mathrm{Re}\Xi^{(n)}(i\omega')\delta/[(\omega-\omega')^2+\delta^2] = \mathrm{Re}\Xi^{(n)}(\delta + i\omega)$ is given in Fig.2.

introduce the correlation at equal times

$$\Delta(t) = \frac{(G_q^\alpha(t)|G_q^\alpha(t))}{(G_q^\alpha|G_q^\alpha)} \tag{3.41}$$

which for the exact $\vec{G}_q(t)$ must be one. Inserting $\vec{G}_q(t)$ from (3.33) we find

$$\Delta^{(n)}(t) = \sum_{\nu=1}^{n} \Xi_{1\nu}(t)\Xi_{\nu 1}(t) + c_1 c_2 \cdots c_{n+1}(\Xi_{nn} \otimes \Xi_{n1})^2 \tag{3.42}$$

where the orthogonality of the $\vec{G}_{q,\nu}$ and the definitions (3.34) and (3.39) have been used. The expresion (3.42) for $\Delta^{(n)}$ can be simplified further with help of the equations of motion for $\Xi_{\nu\mu}(t)$, or the explicit solutions (3.35) and (3.36), e.g.

$$\Delta^{(1)}(t) = \left[\Xi^{(1)}(t)\right]^2 + \frac{1}{c_2}\left[\dot{\Xi}^{(1)}(t)\right]^2 \quad . \tag{3.43}$$

If the n–th order approximation is appropriate we must have

$$\Delta^{(n)}(t) \sim 1 \tag{3.44}$$

which gives a restriction to the region of time, as for $t = 0$ it holds $\Delta^{(n)}(t = 0) = 1$. The deviation of $\Delta^{(n)}(t)$ from 1 in Eq.(3.42) comes from the finite basis in Liouville space entering into $\vec{G}_q(t)$ and the approximation for the correlation functions, which is related to this subspace. Thus $\Delta^{(n)}(t) \sim 1$ requires that the restricted Liouville space in $\vec{G}_q(t)$ as well as the approximate $\Xi^{(n)}(t)$ are sufficient. In Fig.3 we have plotted $\Delta^{(n)}(t)$. Comparing the deviations $\Xi^{(n)}(t)$ from $\Xi(t)$ to $\Delta^{(n)}(t)$ one observes that $\Xi^{(n)}(t)$ is a good approximation to $\Xi(t)$

$$\Xi^{(n)}(t) \sim \Xi(t) \quad , \tag{3.45}$$

as long as it holds

$$\Delta^{(n)}(t) \gtrsim \frac{1}{2} \quad . \tag{3.46}$$

From this we conclude that one can take the condition (3.44) as a measure for the accuracy of the approximations without knowing the exact solution $\Xi(t)$.

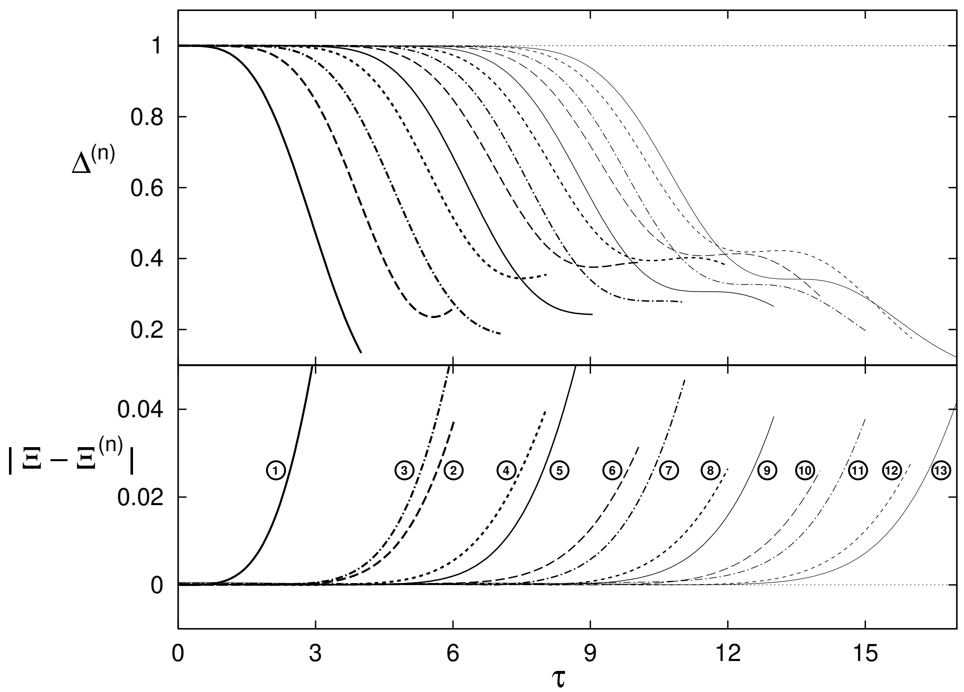

Fig. 3. Accuracy of the approximations; norm $\Delta^{(n)}(\tau)$ compared to the deviations of $\Xi^{(n)}(\tau)$ from the exact correlation function $\Xi(\tau)$ for several orders of the approximation $n = 1, 2, \ldots, 13$.

3.2 Heisenberg ferromagnet at low temperatures

Introducing the Heisenberg ferromagnet we want to show how our general method can be applied to a system where temperature dependent static correlations occur. We will not present more refined results, but rather want to study the selfconsistent method by comparing the results to those of other approaches. To this end we will simplify our equations for the dynamic and static correlation functions, so that we can recover standard results for temperature dependent spin wave frequencies and dampings. In applying our formalism we keep the spin operators and do not transform to Bose operators. Thus the Heisenberg dynamics of the spin operators are expressed in a basis of spin operators at $t = 0$ which may have some advantage for further use.

The Hamiltonian of our system is given by

$$\begin{aligned}\mathcal{H} &= -H \sum_i s_i^z - \sum_{i \neq j} J_{ij} \vec{s}_i \cdot \vec{s}_j \\ &= -H S_0^z - 1/N \sum_q J_q \vec{S}_q \cdot \vec{S}_{-q}, \quad H \to +0, \quad J_{ij} > 0 \end{aligned} \tag{3.47}$$

where N spins S are located at sites $\vec{R}_i$ in a lattice and $\vec{S}_q$ is given by Eq.(3.2). We want to treat this system for low temperatures. To this end we introduce a parameter ϵ to be the inverse of the spontaneous magnetization

$$\epsilon = \left(\frac{\langle S_0^z \rangle}{N} \right)^{-1} = \sigma^{-1}(T) \quad , \tag{3.48}$$

and scale the time to

$$\tau = \sigma t \quad , \tag{3.49}$$

and the spin operators according to

$$\hat{S}_q^{\pm} = \frac{S_q^{\pm}}{\sqrt{2\sigma}} \quad . \tag{3.50}$$

The operators $\delta S_q^z = S_q^z - \langle S_q^z \rangle$ will not be affected. Then the equations of motion for the scaled spins read

$$\frac{d}{d\tau} \delta S_1^z = - \frac{2i}{N} \sum_2 (J_{1-2} - J_2) \hat{S}_2^- \hat{S}_{1-2}^+ \tag{3.51}$$

$$\frac{d}{d\tau} \hat{S}_1^{\pm} = \mp 2i (J_0 - J_1) \hat{S}_1^{\pm} \pm \epsilon \frac{2i}{N} \sum_2 (J_{1-2} - J_2) \delta S_2^z \hat{S}_{1-2}^{\pm} \quad , \tag{3.52}$$

where we have used the shorthand notations $q_1 \to 1, q_1 - q_2 \to 1 - 2$. The parameter $\epsilon(T)$ will not approach zero, except for the case $S \to \infty$, but one can directly see from (3.51) and (3.52) that the zeroth order contribution in $\delta S_1^z(\tau)$ and $S_1^{\pm}(\tau)$ gives the correct spin wave approximation in lowest order [8] [8], so that introducing ϵ will allow for a low temperature approximation. This will be confirmed by the final results.

We want to apply the theory of section 2 to the dynamics with respect to τ, which means that we formally have a Liouvillian $\tilde{L} = L/\sigma$, or Hamiltonian $\tilde{\mathcal{H}} = \mathcal{H}/\sigma$, respectively. As a consequence we have a scaled temperature $\tilde{\beta}$ with $\tilde{\beta}\tilde{\mathcal{H}} = \beta\mathcal{H}$. Choosing the set of observables G to be all modes δS_q^z and $\hat{S}_q^{\pm}$

$$\{G\} = \{\delta S_q^z, \hat{S}_q^{\pm}\} \quad , \tag{3.53}$$

[8] As referred to time t we have the renormalized spin wave frequencies $\omega_1(T) = 2\sigma(T)(J_0 - J_1)$.

and inspecting the equations of motion (3.51) and (3.52) for G one sees that it holds

$$\tilde{L}G = V^{(1)}G + V^{(2)}GG \tag{3.54}$$

with

$$V^{(2)} = V_0^{(2)} + \epsilon V_1^{(2)} \quad , \tag{3.55}$$

so that our condition for an expansion of the residual forces is fulfilled. Furthermore the $G, 1$ form the Lie-algebra

$$\left[\hat{S}_1^+, \hat{S}_2^-\right] = N\delta_{1,-2} + \epsilon\delta S_{1+2}^z \tag{3.56}$$

$$\left[\delta S_1^z, \hat{S}_2^\pm\right] = \pm\hat{S}_{1+2}^\pm \quad , \tag{3.57}$$

which will be important for the statics.

3.2.1 Residual forces and Heisenberg dynamics

We start with the exact equations (2.17) for the residual forces which follow for our special dynamics. Regarding that the static and dynamic correlation matrices are diagonal with respect to wave numbers and components $\alpha = z, +, -$, and introducing

$$\Xi_1^z(\tau) = \frac{(\delta S_1^z|\delta S_1^z(\tau))}{(\delta S_1^z|\delta S_1^z)} \tag{3.58}$$

$$\Xi_1^\pm(\tau) = \frac{(\hat{S}_1^\pm|\hat{S}_1^\pm(\tau))}{(\hat{S}_1^\pm|\hat{S}_1^\pm)} = \frac{(S_1^\pm|S_1^\pm(\tau))}{(S_1^\pm|S_1^\pm)} \tag{3.59}$$

we have [9]

$$\begin{aligned} f_1^z(\tau) = & -\frac{2i}{N}\sum_2 (J_{1-2} - J_2)Q\left(\hat{S}_2^-\Xi_2^- + \hat{f}_2^- \otimes \Xi_2^-\right)\left(\hat{S}_{1-2}^+\Xi_{1-2}^+ + \hat{f}_{1-2}^+ \otimes \Xi_{1-2}^+\right) \\ & + f_1^z \otimes \frac{2i}{N}\sum_2 \frac{(J_{1-2} - J_2)}{(\delta S_1^z|\delta S_1^z)} \\ & \cdot \left(\delta S_1^z\right| \left(\hat{S}_2^-\Xi_2^- + \hat{f}_2^- \otimes \Xi_2^-\right)\left(\hat{S}_{1-2}^+\Xi_{1-2}^+ + \hat{f}_{1-2}^+ \otimes \Xi_{1-2}^+\right)\Big) \quad , \end{aligned} \tag{3.60}$$

[9] The convolutions refer to τ.

and

$$
\begin{aligned}
\hat{f}_1^{\pm}(\tau) = &\pm\epsilon\frac{2i}{N}\sum_2 (J_{1-2}-J_2)Q\left(\delta S_2^z\Xi_2^z + f_2^z\otimes\Xi_2^z\right)\left(\hat{S}_{1-2}^{\pm}\Xi_{1-2}^{\pm} + \hat{f}_{1-2}^{\pm}\otimes\Xi_{1-2}^{\pm}\right)\\
&\mp\epsilon\hat{f}_1^{\pm}(\tau)\otimes\frac{2i}{N}\sum_2\frac{(J_{1-2}-J_2)}{(\hat{S}_1^{\pm}|\hat{S}_1^{\pm})}\\
&\cdot\left(S_1^{\pm}|\left(\delta S_2^z\Xi_2^z + f_2^z\otimes\Xi_2^z\right)\left(\hat{S}_{1-2}^{\pm}\Xi_{1-2}^{\pm} + \hat{f}_{1-2}^{\pm}\otimes\Xi_{1-2}^{\pm}\right)\right) \quad . \qquad (3.61)
\end{aligned}
$$

One directly sees that the transversal forces $\hat{f}_1^{\pm}(\tau)$ start with a first order contribution in ϵ whereas the longitudinal forces $f_1^z(\tau)$ have a term of zeroth order. This structure of Eqs.(3.60) and (3.61) allows for a solution in powers of ϵ. Restricting to the non–vanishing lowest order approximation[10] we find

$$
f_1^z(\tau) = -\frac{2i}{N}\sum_2 Q\hat{S}_2^- \; \hat{S}_{1-2}^+(J_{1-2}-J_2)\phi_{12}(\Xi^+,\Xi^-) \qquad (3.62)
$$

$$
\begin{aligned}
\hat{f}_1^{\pm}(\tau) = &\pm\epsilon\frac{2i}{N}\sum_2(J_{1-2}-J_2)Q\left\{\delta S_2^z\hat{S}_{1-2}^{\pm}\Xi_2^z\Xi_{1-2}^{\pm}\right.\\
&\left. -\frac{2i}{N}\sum_3 Q\left(\hat{S}_3^-\hat{S}_{2-3}^+\right)\hat{S}_{1-2}^{\pm}(J_{2-3}-J_3)\left(\phi_{23}\otimes\Xi_2^z\right)\Xi_{1-2}^{\pm}\right\} \quad , \qquad (3.63)
\end{aligned}
$$

where ϕ_{12} is a functional of the correlations Ξ^+, Ξ^- and can be expressed by Laplace transform to yield

$$
\phi_{12}(s) = \frac{\left(\Xi_2^-\Xi_{1-2}^+\right)(s)}{1-\frac{2i}{N}\sum_3\frac{\left(\delta S_1^z|\hat{S}_3^-\hat{S}_{1-3}^+\right)}{(\delta S_1^z|\delta S_1^z)}(J_{1-3}-J_3)(\Xi_3^-\Xi_{1-3}^+)(s)} \quad . \qquad (3.64)
$$

The Heisenberg dynamics of the spins follow from the general relations (2.10). Regarding the symmetry of the correlation matrices we find

$$
\delta S_1^z(\tau) = \delta S_1^z\Xi_1^z(\tau) + f_1^z(\tau)\otimes\Xi_1^z(\tau) \qquad (3.65)
$$

$$
\hat{S}_1^{\pm}(\tau) = \hat{S}_1^{\pm}\;\Xi_1^{\pm}(\tau) + \hat{f}_1^{\pm}(\tau)\otimes\Xi_1^{\pm}(\tau) \quad . \qquad (3.66)
$$

Inserting the approximations for the residual forces (3.62) and (3.63) into (3.65) and (3.66) respectively, yields the corresponding approximations for the Heisenberg dy-

[10] For $f_1^{\pm}(\tau)$ the first order contribution is necessary as to obtain spin wave damping, whereas the first order correction to $f_1^z(\tau)$ would just modify $\Xi_1^z(\tau)$ quantitatively.

namics. One sees that the longitudinal components $\delta S_1^z(\tau)$ move in a subspace spanned by δS_1^z and all products $\hat{S}_2^- \hat{S}_{1-2}^+$, whereas the transverse components are restricted to a space spanned by $\hat{S}_1^\pm$ and all the products $\delta S_2^z \hat{S}_{1-2}^\pm$ and $\hat{S}_3^- \hat{S}_{2-3}^+ \hat{S}_{1-2}^+$ respectively

$$\delta S_1^z(\tau) = \cdots \delta S_1^z + \sum_2 \cdots \hat{S}_2^- \hat{S}_{1-2}^+ \tag{3.67}$$

$$\hat{S}_1^\pm(\tau) = \cdots \hat{S}_1^\pm + \epsilon \sum_2 \cdots \delta S_2^z \hat{S}_{1-2}^\pm + \epsilon \sum_{2,3} \cdots \hat{S}_3^- \hat{S}_{2-3}^+ \hat{S}_{1-2}^\pm \quad . \tag{3.68}$$

The time dependent coefficients are given by functionals of the dynamic correlations $\Xi^z(\tau), \Xi^\pm(\tau)$, and the exchange parameters, and static correlations. It should be noted that the results for $\delta S^z(\tau)$ and $\hat{S}^\pm(\tau)$ have the same subspaces as would have been obtained by a simple perturbational expansion of the dynamic equations (3.51) and (3.52). The essential difference of (3.67) and (3.68) to such an expansion is, that the coefficients of δS_1^z and $\hat{S}_1^\pm$ in (3.67) and (3.68) comprise all contributions of the simple perturbational series which have a projection onto δS^z, $\hat{S}^\pm$. As compared to a Holstein Primakoff approach [11] , $\hat{S}^\pm(\tau)$ corresponds to a perturbational treatment of the four magnon interaction, if in addition, the Bose operators are summed up to give the spin operators, and the coefficients will be renormalized.

3.2.2 Dynamic and static correlations

The dynamics of the correlation matrix Ξ is governed by the Mori equations (2.9). Regarding the symmetry of the Hamiltonian we get

$$\frac{d}{d\tau}\Xi_1^z = -\gamma_1^{||} \otimes \Xi_1^z \tag{3.69}$$

$$\frac{d}{d\tau}\Xi_1^\pm = \mp i\omega_1 \Xi_1^\pm - \gamma_1^\perp \otimes \Xi_1^\pm \quad , \tag{3.70}$$

where we have introduced the memory functions

$$\gamma_1^{||}(\tau) = \frac{(f_1^z | f_1^z(\tau))}{(\delta S_1^z | \delta S_1^z)} = \frac{-i}{\tilde{\beta}(\delta S_1^z | \delta S_1^z)} \langle [S_{-1}^z, f_1^z(\tau)] \rangle \tag{3.71}$$

[11] Expanding the coefficients in (3.68) into powers of ϵ with $\epsilon(T=0) = 1/S$ and inserting the expansions of $\hat{S}^\pm$ into Bose operators $a, a^\dagger$ into (3.68), then up to order S^{-1} the result for $\hat{S}_1^+(\tau)$ coincides with the dynamics of $a(\tau)$ calculated with the four magnon interaction as a perturbation.

$$\gamma_1^{\perp}(\tau) = \frac{(\hat{f}_1^+|\hat{f}_1^+(\tau))}{(\hat{S}_1^+|\hat{S}_1^+)} = \frac{-i}{\tilde{\beta}(\hat{S}_1^+|\hat{S}_1^+)}\langle[\hat{S}_{-1}^-, \hat{f}_1^+(\tau)]\rangle \quad , \tag{3.72}$$

and the frequency

$$\omega_1(T) = N\left(\tilde{\beta}(\hat{S}_1^+|\hat{S}_1^+)\right)^{-1} . \tag{3.73}$$

In the following we will use the commutator forms for $\gamma^{\|}$ and $\gamma^{\perp}$ [12]. Inserting the approximations for $f_1^z(\tau)$ and $f_1^{\pm}(\tau)$ (3.62), (3.63) into (3.71) and (3.72), we obtain the following expressions for the memory functions:

$$\gamma_1^{\|}(\tau) = \frac{2}{N}\sum_2 (J_{1-2} - J_2) A_{12}(T)\phi_{12}[\Xi^+, \Xi^-] \tag{3.74}$$

$$\begin{aligned} \gamma_1^{\perp}(\tau) = {} & \epsilon\frac{2}{N}\sum_2 (J_{1-2} - J_2) B_{12}(T)\Xi_2^z\Xi_{1-2}^+ \\ & + \epsilon\left(\frac{2}{N}\right)^2 \sum_{2,3}(J_{1-2} - J_2)(J_{2-3} - J_3) C_{12,3}(T)\left(\phi_{23}\otimes\Xi_2^z\right)\Xi_{1-2}^+ \quad , \end{aligned} \tag{3.75}$$

where the temperature dependent coefficients are given by

$$A_{12}(T) = \frac{1}{\tilde{\beta}(\delta S_1^z|\delta S_1^z)}\left(\langle \hat{S}_{2-1}^- \hat{S}_{1-2}^+\rangle - \langle \hat{S}_2^- \hat{S}_{-2}^+\rangle\right) \tag{3.76}$$

$$B_{12}(T) = \frac{1}{\tilde{\beta}(\hat{S}_1^+|\hat{S}_1^+)}\left(\langle \hat{S}_{2-1}^- \hat{S}_{1-2}^+\rangle - \epsilon\langle \delta S_2^z \delta S_{-2}^z\rangle - \frac{(\hat{S}_1^+|\delta S_2^z \hat{S}_{1-2}^+)}{(\hat{S}_1^+|\hat{S}_1^+)}\right) \tag{3.77}$$

$$\begin{aligned} C_{12,3}(T) = {} & \frac{(\delta S_2^z|\hat{S}_3^- \hat{S}_{2-3}^+)}{(\delta S_2^z|\delta S_2^z)} B_{12}(T) \\ & + \frac{1}{\tilde{\beta}(\hat{S}_1^+|\hat{S}_1^+)}\Bigg((\delta_{3,2-1} + \delta_{2,0}) N\langle \hat{S}_3^- \hat{S}_{-3}^+\rangle - \frac{(\hat{S}_1^+|\hat{S}_3^- \hat{S}_{2-3}^+ \hat{S}_{1-2}^+)}{(\hat{S}_1^+|\hat{S}_1^+)} \\ & + \epsilon\langle \hat{S}_3^- \delta S_{2-3}^z \hat{S}_{1-2}^+\rangle + \epsilon\langle \hat{S}_3^- \hat{S}_{2-3}^+ \delta S_2^z\rangle\Bigg) \quad . \end{aligned} \tag{3.78}$$

Inspecting the time dependence of the memory function, one sees that $\gamma^{\|}$ and $\gamma^{\perp}$ are determined by Ξ^+, Ξ^-, or Ξ^+, Ξ^-, Ξ^z, respectively. Thus we have a nonlinear coupled set of equations for Ξ^z, Ξ^+, Ξ^-. This set of equations is very complicated, as it is nonlinear and contains static correlations which must be known, or determined from

[12] We avoid Mori products of the form $(GG|A)$.

the dynamic equations. For this reason we first state, how the static correlations in principle can be obtained in a selfconsistent way. Then we calculate their leading terms for $T \to 0$ and show, how the equations for Ξ^z and Ξ^+ reduce to the standard forms.

The static correlations entering into Ξ^z and $\Xi^\pm$ are found from Eqs. (3.76)–(3.78) to read

$$\begin{array}{cccc} (\delta S^z|\delta S^z), & \langle \delta S^z \delta S^z \rangle, & (\hat{S}^+|\hat{S}^+), & \langle \hat{S}^- \hat{S}^+ \rangle, \\ (\delta S^z|\hat{S}^-\hat{S}^+), & (\hat{S}^+|\delta S^z \hat{S}^+), & (\hat{S}^+|\hat{S}^-\hat{S}^+\hat{S}^+), & \langle \hat{S}^-\hat{S}^+\delta\hat{S}^z \rangle \end{array} . \tag{3.79}$$

If additionally one takes into account the correlations

$$\langle \delta\hat{S}^z \delta\hat{S}^z \rangle, \quad \langle \hat{S}^-\hat{S}^-\hat{S}^+\hat{S}^+ \rangle, \quad \langle \hat{S}^-\hat{S}^+\delta\hat{S}^z\delta\hat{S}^z \rangle, \quad \langle \hat{S}^-\hat{S}^-\hat{S}^+\hat{S}^+\delta\hat{S}^z \rangle \quad , \tag{3.80}$$

then one can find a closed set of equations for this extended set (3.79), (3.80). The procedure is similar to the considerations in section 2.5. The difference is, that our iteration with $V_0^{(2)} + \epsilon V_1^{(2)}$ has lead to residual forces which also have contributions of the form GGG, so that the commutators are modified. The details are given in appendix C.

For our purpose, however, it is sufficient to have the static correlations for $T \to 0$. To this end we iterate the system of static equations with respect to ϵ, as the first order contributions result to be smaller than those of zeroth order. In zeroth order the coupled system of dynamic and static correlations for $\Xi_1^z, \Xi_1^\pm$ and the correlations (3.79) can be solved exactly. Then the expressions of first order follow in a straight forward manner. As those terms we need are exact, they can also be obtained in a different way. Introducing

$$\tilde{\omega}_1 = 2(J_0 - J_1) \tag{3.81}$$

$$n_1 = \frac{1}{e^{\tilde{\beta}\tilde{\omega}_1} - 1} \tag{3.82}$$

we explicitly find for the transverse correlations [13]

$$\langle \hat{S}_{-1}^- \hat{S}_1^+ \rangle = N n_1 + \epsilon n_1 (1 + n_1) \tilde{\beta} \sum_2 (\tilde{\omega}_2 - \tilde{\omega}_{1-2}) n_2 + \mathcal{O}(\epsilon^2) \tag{3.83}$$

[13] The results are given in zeroth order, and up to first order, where they will be needed.

$$
\begin{aligned}
\frac{(\hat{S}_1^+|\delta S_2^z \hat{S}_{1-2}^+)}{(\hat{S}_1^+|\hat{S}_1^+)} = &-n_{1-2} \\
&- \epsilon \left\{ n_{1-2}(1+n_{1-2}) \frac{\tilde{\beta}}{N} \sum_3 (\tilde{\omega}_3 - \tilde{\omega}_{1-3}) n_3 - \frac{1}{N} \sum_3 n_3 (1+n_{2-3}) \right. \\
&+ \frac{1}{N} \sum_3 [n_3(1+n_{1-2}+n_{2-3}) - n_{1-2} n_{2-3}] \\
&\left. \cdot \frac{\tilde{\omega}_2 - \tilde{\omega}_{1-2} + \tilde{\omega}_{1+3-2} - \tilde{\omega}_{2-3}}{\tilde{\omega}_3 - \tilde{\omega}_{1-2} - \tilde{\omega}_{2-3}} \right\} + \mathcal{O}(\epsilon^2)
\end{aligned} \tag{3.84}
$$

$$
\begin{aligned}
\frac{(\hat{S}_1^+|\hat{S}_3^- \hat{S}_{2-3}^+ \hat{S}_{1-2}^+)}{(\hat{S}_1^+|\hat{S}_1^+)} = &N(\delta_{3,2-1} + \delta_{2,0}) n_3 \\
&+ \epsilon \left\{ (\delta_{3,2-1} + \delta_{2,0}) n_3 (1+n_3) \tilde{\beta} \right. \\
&\cdot \sum_4 (\tilde{\omega}_4 - \tilde{\omega}_{3-4}) n_4 - n_3(1+n_{1-2}+n_{2-3}) \\
&+ [n_3(1+n_{1-2}+n_{2-3}) - n_{1-2} n_{2-3}] \\
&\left. \cdot \frac{\tilde{\omega}_2 - \tilde{\omega}_{1-2} + \tilde{\omega}_{1+3-2} - \tilde{\omega}_{2-3}}{\tilde{\omega}_3 - \tilde{\omega}_{1-2} - \tilde{\omega}_{2-3}} \right\} + \mathcal{O}(\epsilon^2),
\end{aligned} \tag{3.85}
$$

whereas the longitudinal correlations are calculated to yield

$$
\langle \delta S_{-1}^z \delta S_1^z \rangle = \sum_2 n_2 (1+n_{1-2}) + \mathcal{O}(\epsilon) \tag{3.86}
$$

$$
\langle \hat{S}_{-2}^- \hat{S}_{2-1}^+ \delta S_1^z \rangle = -N n_2 (1+n_{1-2}) + \mathcal{O}(\epsilon) \tag{3.87}
$$

$$
(\delta S_1^z | \delta S_1^z) = \sum_2 \frac{n_2 - n_{1-2}}{\tilde{\beta}(\tilde{\omega}_{1-2} - \tilde{\omega}_2)} + \mathcal{O}(\epsilon) \tag{3.88}
$$

$$
(\hat{S}_{1-2}^- \hat{S}_2^+ | \delta S_1^z) = -N \frac{n_2 - n_{1-2}}{\tilde{\beta}(\tilde{\omega}_{1-2} - \tilde{\omega}_2)} + \mathcal{O}(\epsilon) \quad . \tag{3.89}
$$

All the static correlations (3.83)–(3.89) listed above still depend on the spontaneous magnetization $\sigma(T) = \epsilon^{-1}$. This can be determined from the condition $\sum_i \vec{s}_i \cdot \vec{s}_i = NS(S+1)$ which can be cast into the form

$$
\begin{aligned}
0 = &(\sigma - S) + (\sigma - S) \left(\frac{2}{N^2} \sum_1 \langle \hat{S}_{-1}^- \hat{S}_1^+ \rangle(\sigma) + 2S + 1 \right) \\
&+ \frac{1}{N^2} \sum_1 \left(\langle \delta S_{-1}^z \delta S_1^z \rangle(\sigma) + 2S \langle \hat{S}_{-1}^- \hat{S}_1^+ \rangle(\sigma) \right)
\end{aligned} \tag{3.90}
$$

and leads to the magnon result

$$\sigma = S - \frac{1}{N}\sum_1 n_1 + \cdots \quad . \tag{3.91}$$

Once the statics are known we now can go back to the dynamics of Ξ^z and $\Xi^\pm$, calculating the lowest order contribution to the memory functions (3.74) and (3.75). For $\gamma_1^{\|}(s)$ we find the zeroth order result

$$\begin{aligned}\gamma_1^{\|}(s) = &\frac{1}{s}\left(\sum_2 \frac{n_{1-2}-n_2}{(\tilde\omega_2-\tilde\omega_{1-2})\,(s-i(\tilde\omega_2-\tilde\omega_{1-2}))}\right)^{-1}\\ &\cdot\sum_2 \frac{(\tilde\omega_2-\tilde\omega_{1-2})(n_{1-2}-n_2)}{s-i(\tilde\omega_2-\tilde\omega_{1-2})}\end{aligned} \tag{3.92}$$

which leads to

$$\Xi_1^z(\tau) = \left(\sum_2 \frac{n_{1-2}-n_2}{\tilde\omega_2-\tilde\omega_{1-2}}\right)^{-1}\sum_2 \frac{n_{1-2}-n_2}{\tilde\omega_2-\tilde\omega_{1-2}}e^{i(\tilde\omega_2-\tilde\omega_{1-2})\tau} \quad , \tag{3.93}$$

whereas the memory function $\gamma_\perp(\tau)$ is of second order and reads

$$\begin{aligned}\gamma_1^{\perp}(\tau) = &(\frac{\epsilon}{N})^2\tilde\beta\tilde\omega_1\sum_{2,3}(\tilde\omega_2-\tilde\omega_{1-2})\frac{\tilde\omega_2-\tilde\omega_{1-2}+\tilde\omega_{1+3-2}-\tilde\omega_3}{\tilde\omega_3-\tilde\omega_{2-3}-\tilde\omega_{1-2}}\\ &\cdot[n_{1-2}n_{2-3}(1+n_3)-(1+n_{1-2})(1+n_{2-3})n_3]\mathrm{e}^{i(\tilde\omega_3-\tilde\omega_{2-3}-\tilde\omega_{1-2})\tau} \quad .\end{aligned} \tag{3.94}$$

The spin wave frequency (3.73) up to second order yields

$$\begin{aligned}\omega_1(T) = &\tilde\omega_1 - \frac{\epsilon}{N}\sum_2(\tilde\omega_2-\tilde\omega_{1-2})n_2\\ &-(\frac{\epsilon}{N})^2\sum_2(\tilde\omega_2-\tilde\omega_{1-2})\sum_3 n_3[n_{2-3}+n_2(1+n_2)\tilde\beta(\tilde\omega_3-\tilde\omega_{1-3})]\\ &-\frac{\gamma_1^{\perp}(\tau=0)}{\tilde\beta\tilde\omega_1} \quad .\end{aligned} \tag{3.95}$$

Comparing our results for $T\to 0$ to those of spin wave theory and regarding

$$\tau\tilde\omega_1 = t\cdot 2\sigma(T)(J_0-J_1) \tag{3.96}$$
$$\tilde\beta\tilde\omega_1 = \beta\cdot 2\sigma(T)(J_0-J_1) \tag{3.97}$$

we see that $\Xi^z(t)$ coincides with the correlation function obtained by Lovesey [8], provided we take our temperature dependent spin wave frequency $2\sigma(T)(J_0 - J_1)$ at $T = 0$. The memory function $\gamma_1^\perp(t) = \gamma_1^\perp(\tau)(d\tau/dt)^2$ (3.94) agrees with the Holstein Primakoff result for the four magnon interaction [5], if again $\sigma(T) \to S$ is used.

It is clear that the presented procedure for the Heisenberg ferromagnet is rather complicated. Just for calculating spin wave frequencies and dampings one would choose the usual way. But we think it is important to have shown that one is not forced to expand spin operators into Bose operators, as to obtain the correlation functions at low temperatures. In this context our main result is, that the Heisenberg operators $\vec{s}_i(t)$ (c.f. Eqs.(3.65) and (3.66)) can be expressed in terms of correlation functions and spin operators at $t = 0$. This point will be useful, if one wants to derive equations of motion for expectation values of spins which go beyond linear response, as in such a case the expectation value of $\langle S_q^+\rangle(t)$ cannot simply be replaced by the expectation value of one Bose operator $\langle a_q\rangle(t)$

4 Conclusion

It has been shown, that incorporating the time evolution of products of observables $(GG)(t) = G(t)G(t)$ into the frame work of Mori's theory, one can give selfconsistent approximations for the residual forces. These can be expressed in terms of time–dependent correlation functions and operators at $t = 0$. In this way it is possible to deduce approximations for the Heisenberg dynamics of the observables as well as for the dynamic and static correlation functions. We have tested this approach comparing the approximations to the exact solution of a model and to the theory of interacting spin waves. From this comparison we conclude that the selfconsistent approximations in Mori's theory can be successfully used to attack the dynamics of correlation functions and Heisenberg operators of interacting systems.

The dynamic equations for the correlation functions we have found, are of the type of mode–mode coupling equations, but the coefficients involved are given by bare interactions. In addition, our approach allows for a quantitative estimation of the validity of the presented mode–mode coupling approximation. A point of further investigation would be, how the expansion scheme can be generalized to give mode–mode coupling equations with the bare interactions replaced by matrix elements of the Liouville operator.

In our illustrations we have been concerned with spin systems. But the given formalism also applies to Fermi or Bose systems, if for the statics of Fermion systems the fluctuation–dissipation theorems are used in an adequate way. Thus, the possibility arises to relate expansions in Mori's theory to other many-body treatments, and especially find a link between projection–operator expansions and those in Green's function theories.

Summarizing we think that the main advantage of the presented expansions is, that they lead to approximations for the Heisenberg dynamics. These can be used to derive equations of motion for expectation values which go beyond linear response.

A Second order approximations to the residual forces

A.1 Expansion into powers of $\epsilon \sim V^{(2)}$ with fixed correlations $\Xi(t)$

The expansion of the residual forces in powers of ϵ, with fixed dynamic and static correlations, is obtained from (2.17). The first order result was given in (2.20). Up to second order one finds

$$\begin{aligned} f(t) = {} & iQV^{(2)}\{G\Xi, G\Xi\} \\ & + iQV^{(2)}\{iQV^{(2)}\{G\Xi, G\Xi\} \otimes \Xi, G\Xi\} + iQV^{(2)}\{G\Xi, iQV^{(2)}\{G\Xi, G\Xi\} \otimes \Xi\} \\ & - iQV^{(2)}\{G\Xi, G\Xi\} \otimes (G|G)^{-1}(G|iV^{(2)}\{G\Xi, G\Xi\}) + \mathcal{O}(\epsilon^3) \quad . \end{aligned} \tag{A.1}$$

The approximate $f(t)$ now is an element of a linear space spanned by the products QGG and $QGGG$. The selfconsistent equations for the dynamic correlations $\Xi(t)$ are given by Eq.(2.9) with the force correlation functions $(f|f(t))$ calculated from (A.1). A general feature of the expansion (A.1) of $f(t)$ is that terms of second, and higher order, will contribute to the projections onto the forces at $t = 0$

$$f = iQV^{(2)}\{G, G\} \quad . \tag{A.2}$$

That means they will contribute to the force correlation functions. In the sense of an orthogonal decomposition of $f(t)$, the coefficients of QGG are changed by each order of the iteration. This is, why it seems to be reasonable, to sum up all contributions of higher order terms which are parallel to the products QGG. To make this reasoning explicit, we introduce a basis F_ν for the QGG by

$$F_\nu = Q \sum_{\mu,\lambda} \alpha_{\nu,\mu\lambda}(G_\mu G_\lambda - \langle G_\mu G_\lambda \rangle) \tag{A.3}$$

which is abbreviated by

$$F = Q\alpha\{G,G\} - \langle\alpha\{G,G\}\rangle \quad . \tag{A.4}$$

Then $f(t)$ can be decomposed as

$$f(t) = F(F|F)^{-1}(F|f(t)) + \tilde{Q}f(t) \quad , \tag{A.5}$$

where

$$\tilde{Q} = \{(1 - |F)(F|F)^{-1}(F|\}Q \quad , \tag{A.6}$$

and $(F|f(t))$ is no longer affected by the approximations of $\tilde{Q}f(t)$ which are orthogonal to (A.3). In the next section A.2 we will calculate $f(t)$ to second order with fixed $\Xi(t)$ and fixed components $(F|f(t))$.

A.2 Expansion into powers of $\epsilon \sim V^{(2)}$ with fixed correlations $\Xi(t)$ and $\Gamma(t)$

For a treatment of $f(t)$ according to (A.5) it is expedient to decompose $f(t)$ into a sum

$$f(t) = e^{iQLQt} iQLG = K(t) i\Omega^{(r)} \quad , \tag{A.7}$$

where

$$K(t) = e^{iQLQt}F \quad , \tag{A.8}$$

and the matrix $\Omega^{(r)}$ is defined by

$$\Omega^{(r)} = (F|F)^{-1}(F|LG) = (F|F)^{-1}(F|V^{(2)}\{G,G\}) \quad . \tag{A.9}$$

Here use had been made of the fact that [14]

$$QLG = Q\left(V^{(1)}G + V^{(2)}\{G,G\}\right) = F\Omega^{(r)} \quad . \tag{A.10}$$

[14] From $(1|LG) = 0$ and $(1|G) = 0$ it follows $(1|V^{(2)}\{G,G\}) = 0$.

Then corresponding to (A.5) we can write

$$K(t) = F\Gamma(t) + \tilde{Q}K(t) \tag{A.11}$$

with

$$\Gamma(t) = (F|F)^{-1}(F|K(t)) = (F|F)^{-1}(F|e^{iQLQt}F) \quad . \tag{A.12}$$

In the sequel we will focus on the expansion of the quantity $K(t)$, which is of course equivalent to the expansion of the residual force $f(t)$.

For $K(t)$ we will set up an exact equation with fixed $\Xi(t)$ and $\Gamma(t)$ which can be iterated. As a first step we cast $K(t)$ into the form

$$K(t) = F\Gamma(t) + \tilde{Q}e^{iLt}QiLF \otimes \Gamma(t) - i\tilde{Q}e^{iLt}F \otimes (F|F)^{-1}(LF|K(t)) \tag{A.13}$$

which can be verified by Laplace transform and the completeness relation

$$F(F|F)^{-1}(F|QGG) = QGG - \langle GG\rangle \quad . \tag{A.14}$$

Next we take the Heisenberg dynamics of G and F, which can be expressed as

$$G(t) = G\Xi(t) + K(t)i\Omega^{(r)} \otimes \Xi(t) \tag{A.15}$$

$$F(t) = G\Xi(t) \otimes i\Omega^{(l)}\Gamma(t) + K(t)\left(1 - \otimes\Omega^{(r)}\Xi(t)\Omega^{(l)} \otimes \Gamma(t)\right) \quad . \tag{A.16}$$

Here $\Omega^{(l)}$ denotes the matrix

$$\Omega^{(l)} = (G|G)^{-1}(G|LF) = (G|G)^{-1}(V^{(2)}\{G,G\}|F) \quad , \tag{A.17}$$

and use has been made of Eqs.(2.9) and (A.7), and

$$\dot{G} = F(t)i\Omega^{(r)} + G(t)i\Omega = G\dot{\Xi}(t) + f(t) + f(t) \otimes \dot{\Xi}(t) \quad . \tag{A.18}$$

Calculating LF from the definition (A.3) and inserting Eqs.(A.15) and (A.16) into the right hand side of Eq.(A.13) one arrives at an exact system of nonlinear equations for $K(t)$

$$
\begin{aligned}
K(t) = {} & F\Gamma(t) \\
& + \tilde{Q}\alpha_s \Big\{ -G\Xi(t) \otimes \Omega^{(l)}\Gamma(t)\Omega^{(r)} + K(t)i\Omega^{(r)} \left(1 - \otimes\Xi(t) \otimes \Omega^{(l)}\Gamma(t)\Omega^{(r)}\right), \\
& \quad G\Xi(t) + K(t)i\Omega^{(r)} \otimes \Xi(t) \Big\} \otimes \Gamma(t) \\
& - \tilde{Q}K(t)i\Omega^{(r)} \otimes \Xi(t)(G|G)^{-1}(G|\alpha_s\{Fi\Omega^{(r)}, G\}) \otimes \Gamma(t) \\
& + \tilde{Q}K(t)\left(1 - \otimes\Omega^{(r)}\Xi(t)\Omega^{(l)} \otimes \Gamma(t)\right) \otimes (F|F)^{-1}\left(\alpha_s\{Fi\Omega^{(r)}, G\}|K(t)\right)
\end{aligned}
\tag{A.19}
$$

where the abbreviation

$$
\alpha_s\{A, B\} := \alpha\{A, B\} + \alpha\{B, A\} \tag{A.20}
$$

has been introduced. This system corresponds to Eq.(2.17) for $f(t)$. The difference is that in Eq.(A.19) the correlation functions $\Xi(t)$ of the observables *and* the correlations $\Gamma(t)$ (A.12) of the residual forces (A.8) appear.

The system (A.19) now can be iterated. Remembering that according to (A.9) and (A.17) $\Omega^{(r)}$ and $\Omega^{(l)}$ are of first order in $V^{(2)}$, we find from (A.19) for fixed $\Xi(t), \Gamma(t)$ (in treating $\Gamma(t)$ fixed the summation of higher order contributions is performed):

$$
K(t) = F\Gamma(t) + \tilde{Q}\alpha_s\left\{F\Gamma(t)i\Omega^{(r)}, G\Xi(t)\right\} \otimes \Gamma(t) + \mathcal{O}(\epsilon^2) \quad . \tag{A.21}
$$

According to Eq.(A.7) it is a second order result for $f(t)$. The main point is, that the approximation (A.21) conserves the exact relation

$$
\begin{aligned}
(G|G)^{-1}(f|f(t)) &= (G|G)^{-1}(iQLG|F)(F|F)^{-1}(F|K(t))i\Omega^{(r)} \\
&= \Omega^{(l)}\Gamma(t)\Omega^{(r)} \quad .
\end{aligned}
\tag{A.22}
$$

The matrix $\Gamma(t)$ can be calculated from the differential equation

$$
\dot{\Gamma}(t) = i(F|F)^{-1}(F|LF)\Gamma(t) - (F|F)^{-1}(iLF|\tilde{Q}K(t)) \tag{A.23}
$$

which follows from Eqs.(A.11) and (A.12). Inserting the approximation (A.21) for $\tilde{Q}K(t)$ and using the definition (A.4) we find

$$
\begin{aligned}
\dot{\Gamma}(t) = {} & i(F|F)^{-1}(F|LF)\Gamma(t) \\
& - (F|F)^{-1}\left(\alpha_s\left\{Fi\Omega^{(r)}, G\right\}\middle|\, \tilde{Q}\left(\alpha_s\left\{F\Gamma(t)i\Omega^{(r)}, G\Xi(t)\right\}\right)\right) \otimes \Gamma(t) \quad .
\end{aligned}
\tag{A.24}
$$

Together with the dynamic equation for $\Xi(t)$

$$\dot{\Xi}(t) = \Xi(t)i\Omega - \Xi(t) \otimes \Omega^{(l)}\Gamma(t)\Omega^{(r)} \tag{A.25}$$

we have a coupled system for the correlations $\Gamma(t)$ and $\Xi(t)$. As Eq.(A.25) can be solved by Laplace transform in terms of $\Gamma(s)$, Eq.(A.24) can be viewed as a nonlinear integral equation for the Laplace transforms $\Gamma(s)$. It should be noted that the approximations (A.24), (A.25) have the exact second order moment of $\Gamma(t)$ or the exact forth moment for $\Xi(t)$ respectively. For later use we note the Heisenberg dynamics for $G(t)$ which result from the approximation (A.21). One obtains

$$\begin{aligned} G(t) &= G\Xi(t) + f(t) \otimes \Xi(t) = G\Xi(t) + F\Gamma(t)i\Omega^{(r)} \otimes \Xi(t) \\ &\quad + \tilde{Q}\alpha_s \left\{ F\Gamma(t)i\Omega^{(r)}, G\Xi(t) \right\} \otimes \Gamma(t)i\Omega^{(r)} \otimes \Xi(t) \quad . \end{aligned} \tag{A.26}$$

A.3 Expansion of the residual forces $\tilde{f}(t)$

We want to show that the results of section A.2 can be obtained in a simple way by extending the set of observables G to $\tilde{G}$ and applying the procedure of section 2.2 to $\tilde{f}$. Let us choose a set $\tilde{G}$ by

$$\tilde{G} = \{G_\nu, F_\mu\} \tag{A.27}$$

where F_ν is defined by (A.3). Then we have a projection operator (A.6)

$$\tilde{Q} = 1 - \tilde{P} = 1 - |G)(G|G)^{-1}(G| - |F)(F|F)^{-1}(F| \quad . \tag{A.28}$$

The matrix $\tilde{\Xi}(t)$ can be written in block matrices as

$$\tilde{\Xi} = \begin{pmatrix} \Xi_{GG} & \Xi_{GF} \\ \Xi_{FG} & \Xi_{FF} \end{pmatrix} \quad . \tag{A.29}$$

Similar the frequency matrix $\tilde{\Omega}$ reads

$$\tilde{\Omega} = \begin{pmatrix} \Omega_{GG} & \Omega_{GF} \\ \Omega_{FG} & \Omega_{FF} \end{pmatrix} \tag{A.30}$$

where $\Omega_{GG} = \Omega$, and Ω_{GF} and Ω_{FG} coincide with the definitions (A.17) and (A.9) for $\Omega^{(l)}$ and $\Omega^{(r)}$.

First we study the derivatives $L\tilde{G}$ and prove that the conditions (2.14) of section 2.2 apply. The derivative

$$LG = V^{(1)}G + V^{(2)}\{G, G\} \tag{A.31}$$

is a linear combination of G_ν and F_ν. Hence in abbreviated notation we have

$$LG = G\Omega_{GG} + F\Omega_{FG} \quad . \tag{A.32}$$

The derivatives LF are found from (A.4). Together with (A.32) one yields[15]

$$\begin{aligned} LF = & \, G\left[(G|G)^{-1}(G|\alpha_s\{G\Omega_{GG}, G\}) - \Omega_{GG}(G|G)^{-1}(G|\alpha\{G,G\})\right] \\ & + F\left[(F|F)^{-1}(F|\alpha_s\{G\Omega_{GG}, G\}) - \Omega_{GG}(G|G)^{-1}(G|\alpha\{G,G\})\right] \\ & + \alpha_s\{F\Omega_{FG}, G\} \quad . \end{aligned} \tag{A.33}$$

Eqs.(A.32) and (A.33) together show that $L\tilde{G}$ has the desired structure

$$L\tilde{G} = \tilde{V}^{(1)}\tilde{G} + \tilde{V}^{(2)}\{\tilde{G}, \tilde{G}\} \quad , \tag{A.34}$$

where the matrix elements of $\tilde{V}^{(1)}$ and $\tilde{V}^{(2)}$ can be taken from (A.32) and (A.33). A special feature of $\tilde{V}^{(2)}$ is, that it just couples F and G, but no couplings FF occur.

Having shown that the condition (1.1) holds, we use Eq.(2.17) to expand the residual forces $\tilde{f}$. As

$$\tilde{V}^{(2)} \sim \Omega_{FG} \sim V^{(2)} \sim \epsilon \quad , \tag{A.35}$$

the interaction $\tilde{V}^{(2)}$ still is of first order in ϵ. Expanding $\tilde{f}$ we want to keep fixed $\Xi(t)$ and $\Gamma(t)$ in the sense of section A.2. Therefore we must express the correlations $\tilde{\Xi}(t)$ in terms of $\Xi(t)$ and $\Gamma(t)$. From the definitions of $\tilde{\Xi}$ and (A.15) and (A.16) one obtains

$$\Xi_{GG}(t) = \Xi(t)$$

[15] We take the case that for symmetry reasons the constant term in (A.33) vanishes. If it does not vanish it can be handled without difficulty.

$$
\begin{aligned}
\Xi_{FG}(t) &= \Gamma(t) i\Omega^{(r)} \otimes \Xi(t) \\
\Xi_{GF}(t) &= \Xi(t) \otimes i\Omega^{(l)}\Gamma(t) \\
\Xi_{FF}(t) &= \Gamma(t)\left(1 - \otimes\Omega^{(r)}\Xi(t)\Omega^{(l)} \otimes \Gamma(t)\right) \quad .
\end{aligned} \tag{A.36}
$$

This means that fixing $\Xi(t)$ and $\Gamma(t)$ is equivalent to fixing the matrices $\Xi_{GG}, \Xi_{GF}, \Xi_{FG}$, but due to $\Omega^{(r)}, \Omega^{(l)}$ in (A.36), the submatrices Ξ_{FG} and Ξ_{GF} are to be treated as first order terms, whereas Ξ_{FF} has a zeroth and a second order contribution. Hence expanding $\tilde{f}$ in Eq.(2.21) up to first order yields

$$
\tilde{f} = \tilde{Q}\tilde{V}^{(2)}\{(\tilde{G}\tilde{\Xi})^0, (\tilde{G}\tilde{\Xi})^0\} + \mathcal{O}(\epsilon^2) \tag{A.37}
$$

where

$$
(\tilde{G}\tilde{\Xi})^0_G = G\Xi_{GG}, \qquad (\tilde{G}\tilde{\Xi})^0_F = F\Gamma(t) \quad . \tag{A.38}
$$

Explicitly the residual forces (A.37) read

$$
\tilde{f} = \begin{pmatrix} f_G \\ f_F \end{pmatrix} = \begin{pmatrix} 0 \\ \tilde{Q}\alpha_s\{F\Gamma(t)i\Omega_{FG}, G\Xi_{GG}(t)\} \end{pmatrix} \quad . \tag{A.39}
$$

The selfconsistent equations for $\tilde{\Xi}(t)$ are found from $\tilde{\Omega}$ and $(\tilde{f}|\tilde{f}(t))$ to be

$$
\begin{aligned}
\dot{\Xi}_{GG} &= \Xi_{GG} i\Omega_{GG} + \Xi_{GF} i\Omega_{FG} \\
\dot{\Xi}_{GF} &= \Xi_{GG} i\Omega_{GF} + \Xi_{GF} i\Omega_{FF} - \Xi_{GF} \otimes \gamma_{FF} \\
\dot{\Xi}_{FG} &= \Xi_{FG} i\Omega_{GG} + \Xi_{FF} i\Omega_{FG} \\
\dot{\Xi}_{FF} &= \Xi_{FG} i\Omega_{GF} + \Xi_{FF} i\Omega_{FF} - \Xi_{FF} \otimes \gamma_{FF}
\end{aligned} \tag{A.40}
$$

where

$$
\gamma_{FF}(t) = (F|F)^{-1}\left(iLF|\tilde{Q}\alpha_s\{F\Gamma(t)i\Omega_{FG}, G\Xi_{GG}(t)\}\right) \otimes \Gamma(t) \quad . \tag{A.41}
$$

The approximation for the Heisenberg dynamics for $G(t)$ are obtained from

$$
\tilde{G}(t) = \tilde{G}\tilde{\Xi}(t) + \tilde{f}(t) \otimes \tilde{\Xi}(t) \tag{A.42}
$$

to yield

$$
G(t) = G\Xi_{GG}(t) + F\Xi_{FG}(t) + \tilde{Q}\alpha_s\{F\Gamma(t)i\Omega_{FG}, G\Xi_{GG}(t)\} \otimes \Xi_{FG}(t) \quad . \tag{A.43}
$$

Now the results of sections A.2 and A.3 can be compared. One sees that the Heisenberg dynamics (A.26) of section A.2 agree with (A.43) of section A.3: Inserting the relations (A.36) into (A.26) one obtains the results (A.43). Furthermore, using the relations (A.36) as a definition for the left hand sides, one can convert the equations of motion (A.24) and (A.25) into the Eqs.(A.40) for $\tilde{\Xi}$. Thus we have demonstrated that the approaches of sections A.2 and A.3 are equivalent. It is clear, however, that one can also expand $\tilde{f}$ with $\tilde{\Xi}(t)$ being fixed and taking Ξ_{GF}, Ξ_{FG} of first order, which replaces $\Gamma(t)$ in (A.38) by Ξ_{FF}. Alternatively, one can directly use the expansion of section 2.2 leading to $\tilde{f} = \tilde{Q}V^{(2)}(\tilde{G}\tilde{\Xi}, \tilde{G}\tilde{\Xi})$, c.f. Eq.(A.37). Such expansions sum up further higher order contributions and would include the results of section A.2. The spin model of section 3.1 is treated in this way.

We conclude this section making some remarks upon the static correlations which occur in the treatment with the extended set $\tilde{G}$. Let the approximate $\tilde{f}$ be a linear combination of $\tilde{Q}(GF)$ (e.g. Eq.(A.39)), and take the commutator forms for $\tilde{\Omega}$ and $(\tilde{f}|\tilde{f}(t))$, then the correlation functions $\tilde{\Xi}(t)$ depend on $(\tilde{G}|\tilde{G})$ and $\langle\tilde{G}\tilde{G}\rangle$, and $(\tilde{G}|\tilde{G}\tilde{G})$, similar to the case of Eq.(2.35). The essential point however is, that owing to the commutators $[\tilde{G},\tilde{G}]$, $(\tilde{G}|\tilde{G}\tilde{G})$ only enter as combinations $(G|GF)$ and $(F|GF)$. Treating the correlations along the lines of section 2., with exact equations relating $(\tilde{G}|\tilde{G}), \langle\tilde{G}\tilde{G}\rangle$ to $(G|GG), (G|GF), (F|GF)$, and using the approximations for $(G|GG), (G|GF), (F|GF)$, one sees that the system is closed, if $\langle FGF\rangle$ is included.

B n–th order approximation and exact solution for the spin model of section 3.1

B.1 Selfconsistent equations for $\Xi^{(n)}$

Take the orthogonal set $\tilde{G} = \{\vec{G}_0, \vec{G}_{q,1}, \ldots, \vec{G}_{q,n}; q \neq 0\}$ defined by (3.31), then the time derivatives of $\vec{G}_{q,\nu}$ read

$$
\begin{aligned}
iL\vec{G}_0 &= 0 \\
iL\vec{G}_{q,1} &= \vec{G}_{q,2} \\
&\vdots \\
iL\vec{G}_{q,\nu} &= -c_\nu \vec{G}_{q,\nu-1} + \vec{G}_{q,\nu+1} \qquad \nu = 2, \ldots, n-1 \\
&\vdots
\end{aligned}
$$

$$iL\vec{G}_{q,n} = -c_n \ \vec{G}_{q,n-1} + \frac{J}{\sqrt{N}}\left(\vec{G}_0 \times \vec{G}_{q,n} - \vec{G}_{q,n} \times \vec{G}_0\right) \tag{B.1}$$

with c_ν defined by Eq.(3.39). This means that in the interaction

$$L\tilde{G} = \tilde{V}^{(1)}\tilde{G} + \tilde{V}^{(2)}\{\tilde{G}, \tilde{G}\} \tag{B.2}$$

just matrix elements $\tilde{V}^{(2)}_{n,0n}$ and $\tilde{V}^{(2)}_{n,n0}$ are different from zero. Therefore the approximation (2.20) with $\epsilon = J$ for the residual forces yields

$$\begin{aligned} f^{\alpha}_{q,\nu}(t) &= 0 \qquad \nu = 1, \ldots, n-1 \\ f^{\alpha}_{q,n}(t) &= \tilde{Q}\frac{J}{\sqrt{N}}(\vec{G}_0 \times \vec{G}_{q,n} - \vec{G}_{q,n} \times \vec{G}_0)^{\alpha}\Xi_{nn}(t) + \mathcal{O}(\epsilon^2) \\ &= G^{\alpha}_{q,n+1}\Xi_{nn}(t) + \mathcal{O}(\epsilon^2), \qquad \alpha = x \text{ or } y, z \end{aligned} \tag{B.3}$$

leading to the memory matrix

$$\gamma_{\nu\mu}(t) = \frac{(f^{\alpha}_{q,\nu}|f^{\alpha}_{q,\mu}(t))}{(G^{\alpha}_{q,\nu}|G^{\alpha}_{q,\nu})} = \delta_{\nu n}\delta_{\mu n}c_{n+1}\Xi_{nn}(t) + \mathcal{O}(\epsilon^3) \quad . \tag{B.4}$$

The equations of motion of the matrix $\Xi_{\nu\mu}(t)$ (2.9) follow from (2.7) with

$$i\Omega_{\nu\mu} = -c_\mu\delta_{\nu,\mu-1} + \delta_{\nu,\mu+1} \tag{B.5}$$

and (B.4) for $\gamma_{\nu\mu}(t)$. In the approximation for the Heisenberg dynamics (2.23) the matrix elements $\Xi_{\nu 1}, \nu = 1, \ldots, n$ and Ξ_{nn} enter. We therefore regard the Laplace transforms of $\Xi_{\nu 1}$ and $\Xi_{n\mu}$ which can be written as

$$\begin{array}{llll} s\Xi_{11} + c_2\Xi_{21} & & = 1 & \\ s\Xi_{21} + c_3\Xi_{31} & - \Xi_{11} & = 0 & \\ \vdots & & & \\ s\Xi_{\nu 1} + c_{\nu+1}\Xi_{\nu+1,1} & - \Xi_{\nu-1,1} & = 0 & \qquad \nu = 2, \ldots, n-1 \end{array} \tag{B.6}$$

and

$$\begin{array}{llll} s\Xi_{n1} - \Xi_{n2} & & = 0 & \\ s\Xi_{n2} - \Xi_{n3} & + c_2\Xi_{n1} & = 0 & \\ \vdots & & & \\ s\Xi_{n\nu} - \Xi_{n\nu+1} & + c_\nu\Xi_{n\nu-1} & = 0 & \nu = 2,\ldots,n-1 \\ s\Xi_{nn} + c_{n+1}(\Xi_{nn})^2 & + c_n\Xi_{nn-1} & = 1 & \end{array} \quad . \tag{B.7}$$

Eqs.(B.6) and (B.7) provide the selfconsistent solutions. The coefficients c_ν can be found from the orthogonality of the $G_{q,\nu}$ to yield

$$\begin{aligned} c_1 &= 1 \\ c_\nu &= -\frac{\varphi_\nu\varphi_{\nu-2}}{\varphi_{\nu-1}^2}, \qquad \nu > 1 \\ \varphi_0 &= 1, \quad \varphi_\nu = \begin{vmatrix} \alpha_1 & \alpha_2 & \ldots & \alpha_\nu \\ \alpha_2 & \alpha_3 & \ldots & \alpha_{\nu+1} \\ \vdots & & & \\ \alpha_\nu & \alpha_{\nu+1} & \ldots & \alpha_{2\nu-1} \end{vmatrix} \quad \begin{array}{r} \alpha_{2\nu} = 0 \\ \alpha_{2\nu+1} = (-1)^\nu m_{2\nu} \\ \nu \geq 0, \end{array} \end{aligned} \tag{B.8}$$

where $m_{2\nu}$ denotes the exact 2ν-th moment

$$m_{2\nu} = \frac{(G_q^\alpha|(L)^{2\nu}G_q^\alpha)}{(G_q^\alpha|G_q^\alpha)} \quad , \tag{B.9}$$

which can be expressed in the thermodynamic limit $N \to \infty$ by the second moment (see (B.29))

$$m_{2\nu} = (m_2)^\nu \frac{2\nu+1}{6^\nu}\frac{(2\nu)!}{\nu!} \quad . \tag{B.10}$$

B.2 Explicit Solution of $\Xi^{(n)}(s)$

The system (B.6) can be solved in terms of $\Xi_{11} = \Xi^{(n)}$. With help of the polynominals $A_\nu(s)$ and $B_\nu(s)$ defined by Eq.(3.38) one directly finds the result (3.35). For the solution of the system (B.7) we first take the equations for $\nu = 1,\ldots,n-1$ expressing $\Xi_{n\nu+1}$ by Ξ_{n1} which gives

$$\Xi_{n\nu+1} = B_\nu\Xi_{n1} \quad \nu = 1,\ldots,n-1 \quad . \tag{B.11}$$

With help of (B.11) and (3.38) and

$$\Xi_{nn-1} = \frac{B_{n-2}}{B_{n-1}} \Xi_{nn} \tag{B.12}$$

the last equation of (B.7) can be converted into a quadratic equation for Ξ_{nn}

$$c_{n+1}(\Xi_{nn})^2 + \frac{B_n}{B_{n-1}} \Xi_{nn} - 1 = 0 \quad , \tag{B.13}$$

which has the solution

$$\Xi_{nn} = \frac{-\frac{B_n}{B_{n-1}} + \sqrt{\left(\frac{B_n}{B_{n-1}}\right)^2 + 4c_{n+1}}}{2c_{n+1}} \quad . \tag{B.14}$$

The other solution is not a Laplace transform of a function $\Xi_{nn}(t)$ regular at $t = 0$. Combining Eq.(3.35) for $\nu = n$ with (B.11) for $\nu = n-1$ gives the solution (3.37) of section 3.1 for $\Xi^{(n)}(s)$ which can also be written in terms of Ξ_{nn} as

$$\Xi^{(n)}(s) = \frac{A_n + c_{n+1}\Xi_{nn}A_{n-1}}{B_n + c_{n+1}\Xi_{nn}B_{n-1}} \tag{B.15}$$

if, following from Eq.(3.38), the relation

$$A_n B_{n-1} - A_{n-1} B_n = (-1)^{n+1} c_1 \cdots c_n \tag{B.16}$$

is used.

The analytic properties of $\Xi^{(n)}(s)$ follow from $\Xi_{nn}(s)$ and the representation (B.15). First one proves that $\Xi_{nn}(s)$ is holomorphic for Re$s > 0$, and it holds

$$\mathrm{Re}\Xi_{nn}(s) > 0 \quad \text{for} \quad \mathrm{Re}s > 0 \quad . \tag{B.17}$$

To see this, we take the definitions of the polynominals $B_\nu(s)$ writing

$$\frac{B_\nu}{B_{\nu-1}} = s + \frac{c_\nu}{\frac{B_{\nu-1}}{B_{\nu-2}}}, \quad c_\nu > 0 \tag{B.18}$$

which by induction leads to the result

$$\mathrm{Re}\frac{B_\nu}{B_{\nu-1}} > 0, \quad \mathrm{Re}s > 0 \quad . \tag{B.19}$$

Together with the property, that the $B_\nu(s)$ have no zeros for $\mathrm{Re}s > 0$ [9], the mapping (B.14) of B_n/B_{n-1} onto Ξ_{nn} completes the proof. For $\Xi^{(n)}(s)$ in Eq.(B.15) we use the recurrence relations (3.38) writing

$$\frac{A_n + c_{n+1}\Xi_{nn}A_{n-1}}{B_n + c_{n+1}\Xi_{nn}B_{n-1}} = \frac{A_{n-1} + \frac{c_n}{s+c_{n+1}\Xi_{nn}}A_{n-2}}{B_{n-1} + \frac{c_n}{s+c_{n+1}\Xi_{nn}}B_{n-2}} \tag{B.20}$$

where from (B.17) it follows that

$$\mathrm{Re}\frac{1}{s + c_{n+1}\Xi_{nn}(s)} > 0 \quad \text{for} \quad \mathrm{Re}s > 0 \quad . \tag{B.21}$$

Iterating this procedure one sees that (B.17) induces $\Xi^{(n)}(s)$ to be holomorphic for $\mathrm{Re}s > 0$ and to have the property

$$\mathrm{Re}\Xi^{(n)}(s) > 0 \quad \text{for} \quad \mathrm{Re}s > 0 \quad . \tag{B.22}$$

As a last point it is not difficult to see that for s approaching the imaginary axis, $\mathrm{Re}s \to +0$, the function $\Xi(s)$ keeps to be finite.

B.3 Exact solution $\Xi(t)$

To derive the exact solution for the dynamic correlation function

$$\Xi(t) = \frac{\mathrm{Tr}G^\alpha_{-q}G^\alpha_q(t)}{\mathrm{Tr}G^\alpha_{-q}G^\alpha_q} \tag{B.23}$$

we start with an exact differential equation of second order for the Heisenberg dynamics of $G_q(t)$

$$\frac{d^2\vec{G}_q}{dt^2} + 2i\frac{J}{\sqrt{N}}\frac{d\vec{G}_q}{dt} + 4\left(\frac{J}{\sqrt{N}}\right)^2(\vec{S}_0\cdot\vec{S}_0)\vec{G}_q(t) = 0, \quad q \neq 0 \quad . \tag{B.24}$$

In the Hilbertspace of our model (N spins 1/2) we use now a partition of the identity operator into operators P_S projecting onto the eigenspaces of $\vec{S}_0 \cdot \vec{S}_0$ leading immediately to

$$\frac{d^2}{dt^2}\mathrm{Tr}G^\alpha_{-q}P_S G^\alpha_q(t) + 2i\frac{J}{\sqrt{N}}\frac{d}{dt}\mathrm{Tr}G^\alpha_{-q}P_S G^\alpha_q(t) + 4\left(\frac{J}{\sqrt{N}}\right)^2 S(S+1)\mathrm{Tr}G^\alpha_{-q}P_S G^\alpha_q(t) = 0 \tag{B.25}$$

with the solution

$$\begin{aligned}&\mathrm{Tr}G^\alpha_{-q}P_S G^\alpha_q(t)\\ &= \left(\frac{S+1}{2S+1}\mathrm{Tr}G^\alpha_{-q}P_S G^\alpha_q - \frac{i/2}{2S+1}\frac{\sqrt{N}}{J}\mathrm{Tr}G^\alpha_{-q}P_S \dot{G}^\alpha_q(0)\right) e^{2iStJ/\sqrt{N}}\\ &+ \left(\frac{S}{2S+1}\mathrm{Tr}G^\alpha_{-q}P_S G^\alpha_q + \frac{i/2}{2S+1}\frac{\sqrt{N}}{J}\mathrm{Tr}G^\alpha_{-q}P_S \dot{G}^\alpha_q(0)\right) e^{-2i(S+1)tJ/\sqrt{N}} \quad .\end{aligned} \tag{B.26}$$

By calculating the traces which are independent of q and $\alpha = x$ or y, z, with

$$\mathrm{Tr}P_S = \frac{(2S+1)^2}{N/2+S+1}\begin{pmatrix} N \\ N/2+S \end{pmatrix} \quad , \tag{B.27}$$

and evaluating the sums we arrive at

$$\Xi_{(N)}(t) = N\left(\cos\frac{J}{\sqrt{N}}t\right)^{N-2}\left(\frac{N+1}{N}\cos^2\left(\frac{J}{\sqrt{N}}t\right) - 1\right) \tag{B.28}$$

or, taking the thermodynamic limit $N \to \infty$

$$\Xi(t) = \lim_{N\to\infty}\Xi_{(N)}(t) = e^{-J^2t^2/2}(1 - J^2t^2) \quad . \tag{B.29}$$

C Dynamic and static correlations of a Heisenberg ferromagnet

C.1 Selfconsistent equations in lowest order

By the approximation discussed in section 3.2 the dynamic correlation functions $\Xi^z(t)$ and $\Xi^\pm(t)$ of a Heisenberg ferromagnet depend on the following static correlations $(\delta S^z|\delta S^z)$, $\langle\delta S^z\delta S^z\rangle$, $(\hat S^\pm|\hat S^\pm)$, $\langle\hat S^-\hat S^z\rangle$, $(\delta S^z|\hat S^-\hat S^+)$, $(\hat S^\pm|\delta S^z\hat S^\pm)$, $\langle\hat S^-\hat S^+|\delta S^z\rangle$, $(\hat S^\pm|\hat S^-\hat S^+\hat S^\pm)$ (see Eqs. (3.69)–(3.78)).

In this appendix we want to point out now, that one can close the dynamic equations (3.69)–(3.75) of section 3.2 by a set of relations determining the static correlations in terms of the dynamic ones. The procedure is analogous to the the general scheme discussed in section 2.5, the only difference is, that the iteration with $V_0^{(2)}+\epsilon V_1^{(2)}$ has led to residual forces, which have contributions of the form GGG. Therefore there appear higher–product static correlations, e.g. $(\hat S^\pm|\hat S^-\hat S^+\hat S^\pm)$, and the set of static quantities has to be extended in order to find a closed system of equations.

Again we start with exact relations between $(G|G)$ and $(G|GG)$ on the one hand, and between $(G|G)$ and $\langle G^\dagger G\rangle$ on the other hand (compare Eqs.(2.36) and (2.37) of section 2.5) [16]

$$(\delta S^z_1|\delta S^z_1) = -\frac{2}{(2+\epsilon)N}\sum_2(\delta S^z_1|\hat S^-_2\hat S^+_{1-2}) - \frac{\epsilon}{(2+\epsilon)N}\sum_2(\delta S^z_1|\delta S^z_2\delta S^z_{1-2}) \qquad (C.2)$$

$$N = 2\tilde\beta(J_0-J_1)(\hat S^\pm_1|\hat S^\pm_1) - \epsilon\frac{2\tilde\beta}{N}\sum_2(J_{1-2}-J_2)(\hat S^\pm_1|\delta S^z_2\hat S^\pm_{1-2}) \qquad (C.3)$$

$$\langle\delta S^z_{-1}\delta S^z_1\rangle = (\delta S^z_1|\delta S^z_1)\int d\omega\frac{\tilde\beta\omega}{e^{\tilde\beta\omega}-1}\Xi^z_1(\omega) \qquad (C.4)$$

[16] For the longitudinal case the relation analogous to Eq. (C.3) would read

$$0 = \sum_2(J_{1-2}-J_2)(\delta S^z_1|\hat S^-_2\hat S^+_{1-2}) \qquad (C.1)$$

and would not supply any further information, because by symmetry Eq.(C.1) is identically fulfilled. We therefore have replaced Eq.(C.1) by (C.2), following from

$$\sum_2(\delta S^z_1|\vec S_2\cdot\vec S_{1-2}) = 0$$

$$\langle \hat{S}^-_{-1}\hat{S}^+_1\rangle = (\hat{S}^+_1|\hat{S}^+_1)\int d\omega \frac{\tilde{\beta}\omega}{e^{\tilde{\beta}\omega}-1}\Xi^+_1(\omega) \quad . \tag{C.5}$$

Using now the approximation (3.62) and (3.63) in Eqs.(3.65) and (3.66) of section 3.2 for the Heisenberg dynamics of $\delta S^z(\omega)$ and $\hat{S}^+(\omega)$

$$\delta S^z_1(\omega) = \delta S^z_1\Xi^z_1(\omega) - \frac{2i}{N}\sum_2 Q\hat{S}^-_2\hat{S}^+_{1-2}(J_{1-2}-J_2)(\phi_{12}\otimes\Xi^z_1)(\omega) \tag{C.6}$$

$$\begin{aligned}\hat{S}^+_1(\omega) = \hat{S}^+_1\Xi^+_1(\omega) + \epsilon\frac{2i}{N}\sum_2(J_{1-2}-J_2)Q\Big\{\delta S^z_2\hat{S}^+_{1-2}\left((\Xi^z_2\Xi^+_{1-2})\otimes\Xi^+_1\right)(\omega)-\\ -\frac{2i}{N}\sum_3 Q(\hat{S}^-_3\hat{S}^+_{2-3})\hat{S}^+_{1-2}(J_{2-3}-J_3)\left[\left((\phi_{23}\otimes\Xi^z_2)\,\Xi^+_{1-2}\right)\otimes\Xi^+_1\right](\omega)\Big\}\end{aligned} \tag{C.7}$$

the equations analogous to Eqs.(2.28) and (2.29) of section 2.5 explicitly read

$$(A|\delta S^z_1) = a_1\langle[S^z_1, A^\dagger]\rangle + \sum_2 b_{12}\langle[\hat{S}^-_2\hat{S}^+_{1-2}, A^\dagger]\rangle \tag{C.8}$$

$$\begin{aligned}(A|\hat{S}^+_1) = c_1\langle[\hat{S}^+_1, A^\dagger]\rangle\\ +\epsilon\sum_2 d_{12}\langle[\delta S^z_2\hat{S}^+_{1-2}, A^\dagger]\rangle + \epsilon\sum_{2,3} e_{123}\langle[\hat{S}^-_3\hat{S}^+_{2-3}\hat{S}^+_{1-2}, A]\rangle\end{aligned} \tag{C.9}$$

$$\langle A\delta S^z_1\rangle = \hat{a}_1\langle[S^z_1, A]\rangle + \sum_2 \hat{b}_{12}\langle[\hat{S}^-_2\hat{S}^+_{1-2}, A]\rangle \tag{C.10}$$

$$\begin{aligned}\langle A\hat{S}^+_1\rangle = \hat{c}_1\langle[S^z_1, A]\rangle\\ +\epsilon\sum_2 \hat{d}_{12}\langle[\delta S^z_2\hat{S}^+_{1-2}, A]\rangle + \epsilon\sum_{2,3}\hat{e}_{123}\langle[\hat{S}^-_3\hat{S}^+_{2-3}\hat{S}^+_{1-2}, A]\rangle\end{aligned} \tag{C.11}$$

with coefficients

$$a_1 = \int\frac{d\omega}{\tilde{\beta}\omega}\Xi^z_1(\omega) - \sum_2\frac{(\delta S^z_1|\hat{S}^-_2\hat{S}^+_{1-2})}{(\delta S^z_1|\delta S^z_1)}b_{12} \tag{C.12}$$

$$b_{12} = -\frac{2i}{N}(J_{1-2}-J_2)\int\frac{d\omega}{\tilde{\beta}\omega}(\phi_{12}\otimes\Xi^z_1)(\omega) \tag{C.13}$$

$$c_1 = \int\frac{d\omega}{\tilde{\beta}\omega}\Xi^+_1(\omega) - \epsilon\sum_2\frac{(\hat{S}^+_1|\delta S^z_2\hat{S}^+_{1-2})}{(\hat{S}^+_1|\hat{S}^+_1)}d_{12} + \epsilon\sum_{2,3}\frac{(\hat{S}^+_1|\hat{S}^-_3\hat{S}^+_{2-3}\hat{S}^+_{1-2})}{(\hat{S}^+_1|\hat{S}^+_1)}e_{123} \tag{C.14}$$

$$d_{12} = \frac{2i}{N}(J_{1-2}-J_2)\int\frac{d\omega}{\tilde{\beta}\omega}\left\{(\Xi^z_2\otimes\Xi^+_{1-2})\otimes\Xi^+_1\right\}(\omega) - \sum_3\frac{(\delta S^z_2|\hat{S}^-_3\hat{S}^+_{2-3})}{(\delta S^z_2|\delta S^z_2)}e_{123} \tag{C.15}$$

$$e_{123} = -\left(\frac{2i}{N}\right)^2 (J_{1-2} - J_2)(J_{2-3} - J_3) \int \frac{d\omega}{\tilde{\beta}\omega} \left\{ \left((\phi_{23} \otimes \Xi^z_2)\Xi^+_{1-2} \right) \otimes \Xi^+_1 \right\} (\omega) \quad (C.16)$$

and analogous expressions for the coefficients $\hat{a}_1, \hat{b}_{12}, \hat{c}_1, \hat{d}_{12}$ and $\hat{e}_{123}$. The only difference is, that the denominators $\tilde{\beta}\omega$ in Eqs.(C.12)–(C.16) are replaced by $(e^{\tilde{\beta}\omega} - 1)$.

We now use[17] Eq. (C.8) for

$$A = \hat{S}^-_{1-2}\hat{S}^+_2 \quad , \qquad (C.17)$$

Eq. (C.9) for

$$A = \begin{cases} \hat{S}^+_{1-2}\delta S^z_2 \\ \hat{S}^+_{1-2}\hat{S}^-_{2-3}\hat{S}^+_3 \end{cases} \quad , \qquad (C.18)$$

Eq. (C.10) for

$$A = \begin{cases} \hat{S}^-_{-2}\hat{S}^+_{2-1} \\ \delta S^z_{-2}\delta S^z_{2-1} \\ \hat{S}^-_{-3}\hat{S}^+_{3-2}\delta S^z_{2-1} \\ \hat{S}^-_{-4}\hat{S}^+_{4-3}\hat{S}^-_{3-2}\hat{S}^+_{2-1} \end{cases} \quad , \qquad (C.19)$$

and last not least Eq. (C.11) for

$$A = \hat{S}^-_{-3}\hat{S}^+_{3-2}\hat{S}^-_{2-1} \quad , \qquad (C.20)$$

and evaluate the commutators on the right hand side with help of

$$\left[\hat{S}^+_1, \hat{S}^-_2\right] = N\delta_{1,-2} + \epsilon\delta S^z_{1+2} \qquad (C.21)$$

$$\left[\delta S^z_1, \hat{S}^\pm_2\right] = \pm\hat{S}^\pm_{1+2} \quad . \qquad (C.22)$$

Then it is easy to see, that Eqs.(C.2)–(C.5) together with Eqs.(C.17)–(C.20) constitute a system of 12 equations determing the 12 static correlations $(\delta S^z|\delta S^z)$, $\langle\delta S^z\delta S^z\rangle$, $(\hat{S}^-|\hat{S}^-)$, $\langle\hat{S}^-\hat{S}^+\rangle$, $(\delta S^z|\hat{S}^-\hat{S}^+)$, $(\hat{S}^-|\delta S^z\hat{S}^-)$, $\langle\hat{S}^-\hat{S}^+\delta S^z\rangle$, $(\hat{S}^-|\hat{S}^-\hat{S}^+\hat{S}^-)$,

[17] For the transverse case it suffices to regard correlations like $(\hat{S}^-_1|\ldots\hat{S}^-_1)$. The correlations $(\hat{S}^+_1|\ldots\hat{S}^+_1)$ follow from symmetry arguments, e.g. $(\hat{S}^+_1|\hat{S}^+_1) = (\hat{S}^-_1|\hat{S}^-_1)$.

$\langle \delta S^z \delta S^z \delta S^z \rangle$, $\langle \hat{S}^- \hat{S}^+ \hat{S}^- \hat{S}^+ \rangle$, $\langle \hat{S}^+ \hat{S}^+ \delta S^z \delta S^z \rangle$, $\langle \hat{S}^- \hat{S}^+ \hat{S}^- \hat{S}^+ \delta S^z \rangle$ in terms of the dynamic correlation functions $\Xi^z(t)$ and $\Xi^\pm(t)$. Thus together with the equations of motion (see Eqs.(3.69) and (3.70) of section 3.2)

$$\frac{d}{d\tau}\Xi_1^z = -\gamma_1^{||} \otimes \Xi_1^z \tag{C.23}$$

$$\frac{d}{d\tau}\Xi_1^\pm = \mp i\omega_1 \Xi_1^\pm - \gamma_1^\perp \otimes \Xi_1^\pm \tag{C.24}$$

with $\gamma_1^{||}$ and $\gamma_1^\perp$ given by Eqs.(3.74) and (3.75) of section 3.2, we have found the desired closed system of equations coupling static and dynamic correlations.

C.2 Zeroth order solution

The easiest way to find the zeroth order contributions in ϵ to the dynamic– and static correlations of a Heisenberg ferromagnet is to use perturbation theory to the Heisenberg equation of motion (3.58) and (3.59) of section 3.2 for $\delta S^z(\tau)$ and $\hat{S}^\pm(\tau)$. For demonstration purposes we want to sketch, how these simplest approximations to the correlations can be found from the zeroth order solution of the rather complicated coupled system of equations constructed in appendix C.1

First the zeroth order of the frequency $\omega_1^{(0)}$ (see Eq.(3.73) of section 3.2) can be found from Eq.(C.3) to yield

$$\omega_1^{(0)} = \frac{N}{\tilde{\beta}(\hat{S}_1^+|\hat{S}_1^+)^{(0)}} = 2(J_0 - J_1) =: \tilde{\omega}_1 \quad . \tag{C.25}$$

Since the correlation function $\gamma^\perp(\tau)$ of the transverse residual force is of second order $\gamma^\perp(\tau) \sim \epsilon^2$, Eq.(3.75) can easily be integrated

$$\Xi_1^{\pm(0)}(\tau) = e^{\mp i\tilde{\omega}_1 \tau} \tag{C.26}$$

by Eq.(C.5) immediately leading to

$$\frac{1}{N}\langle \hat{S}_{-1}^- \hat{S}_1^+ \rangle^{(0)} = \left(e^{\tilde{\beta}\tilde{\omega}_1} - 1\right)^{-1} =: n_1 \quad . \tag{C.27}$$

To find the zeroth order of the longitudinal correlations, we first notice, that (C.2) leads to

$$(\delta S_1^z|\delta S_1^z)^{(0)} = -\frac{1}{N}\sum_2 \left(\delta S_1^z|\hat{S}_2^- \hat{S}_{1-2}^{\pm}\right)^{(0)} \tag{C.28}$$

and (C.17) to

$$\left(\delta S_1^z|S_2^- S_{1-2}^+\right)^{(0)} = N\left(a_1^{(0)} - b_{11-2}^{(0)}\right)(n_2 - n_{1-2}) \tag{C.29}$$

with

$$a_1^{(0)} = \mathrm{Pr}\!\int \frac{d\omega}{\tilde{\beta}\omega}\Xi_1^{z(0)}(\omega) - \sum_2 \frac{(\delta S_1^z|\hat{S}_2^- \hat{S}_{1-2}^+)^{(0)}}{(\delta S_1^z|\delta S_1^z)^{(0)}} b_{12}^{(0)} \tag{C.30}$$

$$b_{12}^{(0)} = -\frac{i}{N}(\tilde{\omega}_2 - \tilde{\omega}_{1-2})\,\mathrm{Pr}\!\int \frac{d\omega}{\tilde{\beta}\omega}\left(\phi_{12}\otimes\Xi_1^z\right)^{(0)}(\omega) \quad . \tag{C.31}$$

To evaluate the principal value integrals they are expressed by

$$\mathrm{Pr}\!\int \frac{d\omega}{\omega}\Psi(\omega) = \frac{i}{2}\left(\Psi_>(\eta) - \Psi_<(-\eta)\right), \quad \eta \to +0 \tag{C.32}$$

with the abbreviation

$$\Psi_{\gtrless}(s) := \int_0^\infty d\tau e^{\mp s\tau}\Psi(\pm\tau) \quad . \tag{C.33}$$

The expressions $\Xi_{\gtrless}^{z(0)}(s)$ and $(\phi_{12}\otimes\Xi_1^z)_{\gtrless}^{(0)}(s)$ can be found from the defining Eq.(3.69) together with (3.74) of section 3.2 using the zeroth order result (C.26) of $\Xi_1^{\pm}(\tau)$. They depend on the static correlations $(\delta S_1^z|\hat{S}_2^- \hat{S}_{1-2}^+)^{(0)}$ and $(\delta S_1^z|\delta S_1^z)^{(0)}$. Thus Eqs.(C.28) and (C.29) together with the definitions (C.30) and (C.31) lead to a coupled system of equations, which can be solved by using Eq.(C.32) to yield

$$(\delta S_1^z|\hat{S}_2^- \hat{S}_{1-2}^+)^{(0)} = N\frac{n_2 - n_{1-2}}{\tilde{\beta}(\tilde{\omega}_2 - \tilde{\omega}_{1-2})} \tag{C.34}$$

$$(\delta S_1^z|\delta S_1^z)^{(0)} = -\sum_2 \frac{n_2 - n_{1-2}}{\tilde{\beta}(\tilde{\omega}_2 - \tilde{\omega}_{1-2})} \quad . \tag{C.35}$$

This implies

$$\Xi_1^{z(0)}(\tau) = \left(\sum_2 \frac{n_2 - n_{1-2}}{\tilde{\beta}(\tilde{\omega}_2 - \tilde{\omega}_{1-2})} \right)^{-1} \sum_2 \frac{n_2 - n_{1-2}}{\tilde{\beta}(\tilde{\omega}_2 - \tilde{\omega}_{1-2})} e^{i(\tilde{\omega}_2 - \tilde{\omega}_{1-2})\tau} \quad . \tag{C.36}$$

The results for the expectation values

$$\langle \delta S^z_{-1} \delta S^z_1 \rangle^{(0)} = \sum_2 n_2 (1 + n_{1-2}) \tag{C.37}$$

$$\langle \hat{S}^-_{-2} \hat{S}^+_{2-1} \delta S^z_1 \rangle^{(0)} = -N n_2 (1 + n_{1-2}) \tag{C.38}$$

follow from Eqs.(C.4) and (C.19) with Eq.(C.36).

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