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The memory function formalism in the study of the dynamics of a many body system

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Abstract. In this paper we present a review of applications of the memory function formalism proposed by Mori. Particular attention is paid to the techniques available in the literature for the termination of the continued fraction expansion. Some examples are given to illustrate those techniques.

1. Introduction

Time-dependent correlation functions afford a powerful theoretical tool for investigating nonequilibrium behavior, providing a rigorous connection between the macroscopic transport coefficients of phenomenological theories and the microscopic molecular properties. A wide variety of nonequilibrium phenomena are described by thermodynamically averaged expectation values of products of pairs of densities at different space-time points. In particular these correlation functions completely describe the nonequilibrium behavior of a system in which the deviation from equilibrium is small [1]. Several general techniques, having the necessary feature of treating the many-body dynamical calculation as an initial-value problem, have been devised for the calculation of correlation functions [2]. One of the most useful and fundamental progress towards the study of the time evolution of those functions was devised by Zwanzig [3], using many-body projection operators to select out only the "relevant" information contained in the full dynamical expressions. Later, Mori [4] generalized the projection-operator technique and obtained an expression for the Laplace transform of an autocorrelation function in the form of a continued fraction. Mori's method is physically appealing, because it shows how two time scales, one fast and another slow, could possibly arise from Hamiltonian systems and how transport coefficients could be related to the interaction energy. One difficult with this method is how to terminate the continued fraction expansion, and several approaches have been used in the literature [5–16]. Recently, we have shown that the incorrect use of truncation schemes leads to incorrect results for the relaxation function [17]. In this paper, which is largely pedagogical, we shall be primarily concêrned with the techniques to evaluate the memory function used to

terminate the expansion. The article is presented as follows. In Section 2 we present briefly the Mori's method. In Section 3 we consider the cases where certain assumption may be made on the behavior of the frequency moments $\langle \omega^{2n} \rangle$ appearing in the expansion, as $n \to \infty$, thus making the continued fraction tractable without truncation. In Section 4 we study the correct use of the N-pole approximation and finally in Section 5 we discuss a technique that can be used at low temperature.

2. The memory-function method

If A denotes a Hermitian dynamical variable, e.g., the spin component S_q^α in a magnetic system ($\alpha = x, y, z$), its time evolution is formally given as

$$A(t) = e^{iHt} A e^{-iHt} \tag{2.1}$$

which leads to the equation of motion

$$\frac{dA(t)}{dt} = iLA(t) \tag{2.2}$$

where H is the Hamiltonian of the system and $L = i[H, .]$ the Liouville Operator. We assume that $A(t)$ denotes the deviation from its invariant part. The knowledge of $A(t)$ permits us to obtain the relaxation function $F(\omega)$ which is of paramount importance since it can be directly related to scattering cross sections by Van Hove's relation [18]. The Fourier transform of the relaxation function is defined by

$$F(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-i\omega t} \frac{(A(t), A^*(0))}{(A(0), A^*(0))} \tag{2.3}$$

where $(A(t), B)$ given by [19]

$$(A(t), B) = \frac{1}{\beta} \int_0^\beta \langle e^{\lambda H} A(t) e^{-\lambda H} B \rangle d\lambda \tag{2.4}$$

defines an inner product of two variables A and B belonging to the Hilbert space of dynamical variables. In (2.4) $\beta = 1/kT$ where T is the temperature.

The starting point of Mori is to separate the time derivative (2.2) into a function $F_1[A(s), t \geq s \geq \text{initial time } t_0]$ depending upon the past history of $A(t)$, and an additional term $F_2(t, t_0)$ depending explicitly upon the other degrees of freedom; then, expanding the function F_1 in terms of $A(s)$ and extracting the linear term, Mori defines the first random force $f_1(t)$ as the sum of $F_2(t, t_0)$ and the non-linear terms. Now the same procedure can be applied to $f_1(t)$ to define a second random force $f_2(t)$, then to $f_2(t)$ to define a third random force $f_3(t)$ and so on. In this way a hierarchy of random forces $f_j(t)$ is generated, the values of which at initial time $t_0 = 0$, which we denote by f_j obey the recurrence equations

$$f_j = \left(1 - \sum_{l=0}^{j-1} P_l\right) iLf_{j-1}, \qquad f_0 \equiv [A(t)]_{t=0} = A, \tag{2.5}$$

where P_l, the projection operator onto the vector f_l, is given by

$$P_l B \equiv (B, f_l)(f_l, f_l)^{-1} f_l. \tag{2.6}$$

These vectors f_j form an orthogonal set,

$$(f_j, f_k) = 0 \qquad j \neq k, \tag{2.7}$$

and evolve in time according to the equations

$$f_j(t) = \exp(iL_j t) iL_j f_{j-1} \qquad (j \geq 1), \qquad f_0(t) = A(t) \tag{2.8}$$

where

$$L_j = (1 - P_{j-1}) L_{j-1}, \qquad L_0 = L. \tag{2.9}$$

The initial time derivatives $\dot{f}_j = [df_j(t)/dt]_{t=0}$ satisfy the recurrence equations

$$\dot{f}_j = \left(1 - \sum_{l=0}^{j-1} P_l\right) iL f_j. \tag{2.10}$$

For Hermitian operators we have

$$\dot{f}_j = f_{j+1}. \tag{2.11}$$

Introducing the quantities

$$\delta_j = (f_j, f_j)/(f_{j-1}, f_{j-1}), \tag{2.12}$$

the Laplace transform of the relaxation function $\Xi(t) = (A(t), A)/(A, A)$ can be written

$$\Xi(z) = \int_0^\infty \Xi(t) e^{-zt}\, dt = \cfrac{1}{z + \cfrac{\delta_1}{z + \cfrac{\delta_2}{z + \cdots}}}. \tag{2.13}$$

This expansion is Mori's infinite continued fraction representation for the Laplace transform of time auto-correlation functions. Equation (2.13) is sometimes written in the form

$$\Xi(z) = \frac{1}{z + \delta_1 \Xi_1(z)}, \qquad \Xi_l(z) = \frac{1}{z + \delta_{l+1} \Xi_{l+1}(z)}, \tag{2.14}$$

where $\Xi_j(z)$ is the Laplace transform of $\Xi_j(t) = (f_j(t), f_j)(f_j, f_j)^{-1}$. The knowledge of singularities of the function represented by (2.13) is essential, since they determine the relaxation of $A(t)$. If one is going to describe the approach of $A(t)$ toward an equilibrium value, these singularities are expected to be located in the half-plane $\mathrm{Re}\, z < 0$.

After the work of Mori, Dupuis [20] investigated the mathematical structure associated to Mori's generalized random forces showing that these random forces could be obtained by a Schmidt orthogonalization of the sequence of initial time derivatives of the dynamical variable considered. He also established the relation

between the continued fraction representation (2.13) and the moment expansion

$$\Xi(t) = 1 + \frac{s_2}{2!}t^2 + \frac{s_4 t^4}{4!} + \cdots + \frac{s_{2n}}{(2n)!}t^{2n} + \cdots \tag{2.15}$$

where

$$s_{2n} = \frac{(A^{2n}, A)}{(A, A)} = (-1)^n \frac{(A^n, A^n)}{(A, A)}, \tag{2.16}$$

and $A^n = [d^n A(t)/dt^n]_{t=0}$. The coefficients s_{2n} are related to the moments $\langle \omega^{2n} \rangle$ of $F(\omega)$, the frequency distribution of $\Xi(t)$ (equation 2.3), by the equation

$$s_{2n} = \left[\frac{d^{2n}\Xi(t)}{dt^{2n}}\right]_{t=0} = \int_{-\infty}^{\infty} (i\omega)^{2n} F(\omega)\, d\omega = (-1)^n \langle \omega^{2n} \rangle. \tag{2.17}$$

Applying Mori's recurrence formula (2.5) Dupuis was able to express the coefficients δ_j in terms of the moments $\langle \omega^{2k} \rangle$ and vice-versa. For the first δ's we have

$$\begin{aligned}
\delta_1 &= \langle \omega^2 \rangle \\
\delta_2 &= \langle \omega^4 \rangle / \langle \omega^2 \rangle - \langle \omega^2 \rangle \\
\delta_3 &= (\langle \omega^6 \rangle / \langle \omega^2 \rangle - \langle \omega^4 \rangle^2 / \langle \omega^2 \rangle^2)/\delta_2 \\
\delta_4 &= (\langle \omega^8 \rangle / \langle \omega^2 \rangle - 2\langle \omega^6 \rangle \langle \omega^4 \rangle / \langle \omega^2 \rangle^2 + \langle \omega^4 \rangle^3 / \langle \omega^2 \rangle^3)/\delta_2\delta_3 - \delta_3.
\end{aligned} \tag{2.18}$$

Dupuis also examined the convergence criteria for the continued fraction representation. Introducing the number k_n defined by the recurrence law

$$k_1 = 1 \qquad k_n k_{n+1} = 1/\delta_n$$

he found that if the series $\sum_p k_p$ is divergent, then the continued fraction expansion converges to $\Xi(z)$ for every z such that $\mathrm{Re}\, z > 0$. For the question of convergence see also Ref. [21].

As pointed out by Lee and Dekeyser [22], for nontrivial Hamiltonians, it is not a simple matter to obtain $\langle \omega^{2n} \rangle$ even for n relatively small. Thus, one does not have explicit forms of δ_n except for possibly the first few of them. It is, nevertheless evident that all correlation functions δ_n exist as $n \to \infty$. This implies that the continued fraction (2.13) does not in general terminate, i.e., it is an infinite series. So another problem is the nature of the approximation which is used to terminate the continued fraction. As we can see from equation (2.8), the time evolution of the first memory function $\Xi_1(t)$ is determined by QLQ, where $Q = 1 - P$, higher order memory functions having more complicated expressions. The order of truncation of the continued fraction is decisive in determining the form of the relaxation function in the frequency region of interest, and as has been shown by Oitmaa et al [23] there appears to be no way of assessing the validity of the approximations which are used to terminate the continued fraction and, as it is often the case there is no systematic convergence of the approximants as more and more moments are used. In the following sections we give some examples of situations where Mori's method can be correctly used.

3. Exact results

For certain physical models as has been extensively discussed by Lee et al [24, 40], the continued fraction expansion can be terminated exactly. Below we present some examples.

3.1. *Finite dimensional Hilbert spaces*

If owing to some symmetry of the system all basis vectors f_j for $j \geqslant N$ vanish the Hilbert space of the dynamical variables shrinks to N dimensions [41]. It follows then from (2.12) that $\delta_N = 0$. From (2.14) we have

$$\Xi_{N-1}(z) = 1/z, \qquad \Xi_{N-2}(z) = z(z^2 + \delta_{N-1})^{-1}, \tag{3.1}$$

and for the time dependent memory function

$$\Xi_{N-2}(t) = \cos \sqrt{\delta}_{N-1} t. \tag{3.2}$$

From (2.13) and knowing that

$$F(\omega) = \frac{1}{\pi} \operatorname{Re} \Xi(z = i\omega) \tag{3.3}$$

we see that $F(\omega)$ is a sun of pure oscillatory functions. The same conclusion can also be reached directly from (2.13) putting $\delta_N = 0$. The denominator is a polynomial of order N and the poles can be calculated easily. We find that all roots are imaginary and therefore ω is real. For instance if $\delta_3 = 0$ we find for the poles

$$\omega = 0, \qquad \omega = \pm(\delta_1 + \delta_2)^{1/2}, \tag{3.4}$$

if $\delta_4 = 0$ we find

$$\omega^2 = \tfrac{1}{2}\{(\delta_1 + \delta_2 + \delta_3) \mp [(\delta_1 + \delta_2 + \delta_3)^2 - 4\delta_1\delta_3]^{1/2}\} \tag{3.5}$$

In all cases the dynamical variable A can precess in the N-dimensional Hilbert space. The frequency of the precession corresponding to the energy of the collective excitational modes arising from many particles interacting coherently.

This case $\delta_N = 0$ is a special case of the N-pole approximation (in fact if $\delta_N = 0$ the approximation is exact) to be discussed in Section 4, where a more general study will be presented. The classical harmonic oscillator chain with the number of oscillators finite is a trivial example of the case discussed here. Other physical systems belonging to this dynamical class are: the XY model in the high frequency limit, the one-dimensional homogeneous electron gas at zero temperature, the spin van der Waals model in the Ising regime below the critical temperature. These systems will be discussed in more general form in the next two subsections.

3.2. *Convergente sequence of the coefficients* δ

The second important case occurs when the coefficients δ_n converges to a value δ, i.e.

$$\lim_{n\to\infty} \delta_n = \delta.$$

For example, for a square function defined by

$$F(\omega) = \begin{cases} 1/2a; & -a < \omega < a \\ 0; & |\omega| > a, \end{cases} \tag{3.6}$$

where a is the width of the curve and $\int F(\omega)\, d\omega = 1$, we obtain $\delta_1 = a^2/3$, $\delta_2 = (4/5)\delta_1$, $\delta_3 = (27/28)\delta_2$, $\delta_4 = (80/81)\delta_3, \ldots$

We can choose a N and do the approximation

$$\delta_N = \delta_{N+1} = \delta_{N+2} = \cdots = \delta \tag{3.7}$$

Taking (3.7) into (2.14) we find

$$\Xi_N(z) = \frac{1}{z + \delta\Xi_N(z)}, \tag{3.8}$$

which give for the Nth order memory function

$$\Xi_n(z) = [-z + (z^2 + 4\delta)^{1/2}]/2\delta. \tag{3.9}$$

The time dependent memory function is easily calculated

$$\Xi_N(t) = \frac{1}{\sqrt{\delta t}} J_1(\sqrt{\delta} t), \tag{3.10}$$

where J_1 is the Bessel function of order 1.

In this case we have a systematic convergence of the approximation as more and more moments are used, this is, the accuracy of the approximation increases when we use higher values of N. As a test we have used the memory function (3.9) in (2.13) as an approximation to calculate $F(\omega)$ defined by (3.6). We have found an excellent fit even at the second stage. This approximation was used by Engelsberg and Chao [42] to calculate NMR line shapes in paramagnetic systems, obtaining an excellent agreement with experimental data. See also Ref. [12].

If the condition (3.7) holds true the memory function is exactly given by (3.9). One example of this case is the homogeneous electron gas at $T = 0$ in two dimensions [28].

The electron gas may be defined by the following model:

$$H = \sum_k \varepsilon_k a_k^+ a_k + \sum_k v_k \rho_k \rho_{-k} \tag{3.11}$$

where $\varepsilon_k = K^2/2m$, m is the electron mass, v_k is the two body interaction ($k \neq 0$), a_k^+ and a_k are the fermion creation and annihilation operators, and $\rho_k = \sum_p a_p^+ a_{p-k}$. We choose $A = \rho_k$, such that (ρ_k, ρ_k) is the static susceptibility.

In two dimensions at $T=0$ and $k \ll K_F$ (K_F is the Fermi wave vector) Lee and Hong [28] have found that

$$\delta_1 = 2\Delta + \Gamma \quad \text{and} \quad \delta_n = \Delta, \qquad n \geq 2 \tag{3.12}$$

where $\Delta = (k\varepsilon_F)^2$, $\Gamma = 2\pi\ \rho e^2 k/m$ (ε_F is the Fermi energy, ρ number density, e charge). The relaxation function is then given by

$$\Xi(t) = s\sum_{n=0}^{\infty} (-\alpha u^{-2})^n (\partial/\partial t)^{2n} J_1(ut)/ut + P\cos\Gamma t \tag{3.13}$$

where

$$s = 1-(1-\alpha)^{1/2}, \quad \cdot \quad p = [(1-\alpha)^{1/2} - (1-\alpha)]/(\alpha/2)$$

and

$$\alpha = 4\Delta(1-\Delta/\delta_1)/\delta_1, \qquad u = 2\Delta^{1/2}, \qquad \Gamma = \alpha^{-1/2}u,$$

J_1 is the Bessel function of order 1. For the ideal degenerate electron gas at zero temperature we have $\Gamma = 0$ and the relaxation function reduces to

$$\Xi(t) = J_0(ut), \tag{3.14}$$

where J_0 is the Bessel function of order zero. The solution (3.13) satisfies the moment sum rules to all orders.

3.3. *Gaussian function*

For convenience let us write the nth order memory function as [14]

$$\Xi_n(z = i\omega) = a_n(\omega) - ib_n(\omega) \tag{3.15}$$

with

$$\begin{aligned} a_n(\omega) &= \int_0^{\infty} \Xi_n(t)\cos\omega t\, dt, \\ b_n(\omega) &= \int_0^{\infty} \Xi_n(t)\sin\omega t\, dt, \end{aligned} \tag{3.16}$$

the spectral shape is found to be

$$F(\omega) = \frac{1}{\pi}\frac{\delta_1 a_1(\omega)}{[\omega - \delta_1 b_1(\omega)]^2 + [\delta_1 a_1(\omega)]^2}, \tag{3.17}$$

or

$$F(\omega) = \frac{1}{\pi}\frac{\delta_1\delta_2 a_2(\omega)}{\{\omega[\omega - \delta_2 b_2(\omega)] - \delta_1\}^2 + \{\omega\delta_2 a_2(\omega)\}^2}, \tag{3.18}$$

according to whether the continued fraction is stopped at the first ($n=1$) or the second ($n=2$) stage, respectively. A Gaussian form for the memory function

$\Xi_n(t)(n=1, 2)$

$$\Xi_n(t) = \exp(-\tfrac{1}{2}\delta_{n+1}t^2) \tag{3.19}$$

has been used by several authors [7, 12, 14, 43–51]. Such a memory function has the correct expansion in the $t \to 0$ limit and all the integrals $\int_0^\infty t^n \Xi_j(t)\,dt$ exist, moreover, it has been exactly derived as a limiting case in an approach to the line-shape theory [52] which complements the continued fraction theory. With the choice (3.19) the spectral function automatically conserve the first $n+2$ even-frequency moments. For (3.19) the quantities $a_j(\omega)$ and $b_j(\omega)$ are found to be

$$a_j(\omega) = \left(\frac{\pi}{2\delta_{j+1}}\right)^{1/2} \exp(-\omega^2/2\delta_{j+1}), \tag{3.20}$$

$$b_j(\omega) = \frac{\exp(-\omega^2/2\delta_{j+1})}{(\delta_{j+1}/2)^{1/2}} \int_0^s e^{x^2}\,dx, \tag{3.21}$$

where $s = \omega/(2\delta_{j+1})^{1/2}$. Now using (3.19) we obtain the successive δ according to the relation

$$\delta_{n+1+m} = (m+1)\delta_{n+1} \tag{3.22}$$

and this restricts severely the cases where the Gaussian memory function can be employed, this is, the coefficients δ's should satisfy (3.22) at least approximately, in order that we could use the Gaussian as a termination function.

It is not easy to trace the position of poles of $\Xi(z)$ in general when $\Xi_n(t)$ is a Gaussian. However, when it is possible, it is of some help in understanding the characteristic behaviour of the spectrum as a whole. For the case $n=1$ see Ref. [53].

As example we mention the quantum one-dimensional XY model described by the Hamiltonian

$$H = 2J\sum_i (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y) \tag{3.23}$$

where s_i^α are spin-$\frac{1}{2}$ operator ($\alpha = x, y, z$). We choose $A = s_j^x$. At $T = \infty$ Florencio and Lee [39] have found that $\delta_n = n\Delta$, $n \geq 1$ where $\Delta = 2J^2$.

Other example is the spin van der Waals model. This model refers to a system of spins arranged in a regular lattice, each of which is coupled to all other spins with equal strength. The model may be defined by the following Hamiltonian [26, 34]:

$$H = -\frac{1}{N}\sum_{i\neq j}^{N} [J(s_i^x s_j^x + s_i^y s_j^y) + J_z s_i^z s_j^z] \tag{3.24}$$

where N is the total number of spins, the coupling constants J and J_z are both taken to be non-negative and $s_i^\alpha = 1/2 (\alpha = x, y, z)$. The system will be referred to as XY-like if $J > J_z$ and as Ising-like if $J < J_z$. If we take $A = S_x = \sum_i s_i^x$, for $T > T_c = J/2K_B$, we find that in the XY regime $\delta_n = n\Delta$, $n \geq 1$, where $\Delta = 4\omega^2\langle S_z^2\rangle$, where $\omega = (J - J_z)/N$ and $\langle S_z^2\rangle = N/2(2 - \beta J_z)$. The same result holds

for $T < T_c$ only that now $\langle S_z^2 \rangle = N/2\beta(J - J_z)$. In the Ising regime and $T > T_c = J_z/2k_B$ one also has $\delta_n = n\Delta$. For $T < T_c$, the ordered state is now characterized by $\langle S_z \rangle$ and we find that $\delta_1 = 4\omega^2\langle S_z^2 \rangle$ and $\delta_n = 0$ if $n \geq 2$. The time evolution properties for the low temperature Ising regime are exactly as given in subsection 3.1.

4. N-pole approximation

A standard procedure to truncate the continued fraction, first considered by Mori on physical grounds and often found in the literature [5, 6, 11, 54] is to replace $\Xi_n(z)$ by a constant z_0. This is equivalent to a "short-memory" approximation $\Xi_n(t) = \tau_N \delta(t)$, and is a N-pole approximation to a function with an infinite number of poles. This approximation is equivalent to take

$$\Xi_{N-1}(t) = \delta_{N-1} e^{-t/\tau_N} \tag{4.1}$$

which gives

$$\Xi_{N-1}(z) = \delta_{N-1}(z + 1/\tau_N)^{-1}. \tag{4.2}$$

This type of truncation may be justified in some problems, but in others it is an ad hoc assumption. A further disadvantage of such closures is the introduction of adjustable parameters such as τ_N. However if the approximation is justified it has the advantage that the poles can easily be calculated (at least for small N) since the denominator of equation (2.13) is a polynomial of order N. This is $\Xi(z)$ can be written as a ratio of two polynomials

$$\Xi(z) = \sum_{n=0}^{N-1} \alpha_n z^n \Big/ \sum_{n=0}^{N} \beta_n z^n \tag{4.3}$$

which for convenience can be rewritten as [55]

$$i\Xi(is) = \sum_{n=0}^{N-1} a_n s^n \Big/ \sum_{n=0}^{N} b_n s^n. \tag{4.4}$$

The coefficients a_n and b_n are completely determined by the δ's and τ_N. The inverse Laplace transform of equation (4.4) is given by

$$\Xi(t) = \sum_{j=1}^{N} C_j e^{-x_j t} \tag{4.5}$$

where

$$C_j = \sum_{n=0}^{N-1} a_n x_j^n \Big/ \sum_{n=0}^{N-1} (n+1) b_n x_j^n, \tag{4.6}$$

and x_j, $j = 1, \ldots, N$ denote the roots of the equation

$$\sum_{n=0}^{N} b_n s^n = 0. \tag{4.7}$$

We now discuss the circumstances in which it becomes possible to introduce the N-pole approximation. The condition that $\Xi_n(t)$ decays rapidly corresponds to the description of $\Xi(t)$ in the time scale Δt distinctly larger than the decay time τ_{N+1} of $\Xi_n(t)$, $\Delta t \gg \tau_{N+1}$. This is $\Xi(t)$ is a slowly-varying function of time in the time scale Δt. The region of interest in the z plane is given by $|z| = 1/\Delta t$ so we should have $|z| \ll \tau_{N+1}^{-1}$ in order that $\Xi_N(z)$ could be approximated by a constant. This condition means that the n poles of $\Xi(z)$ should be located in the neighborhood of the center of the semi-circle the radius equal to $1/\tau_{N+1}$ in the left-half z plane. These poles represent slow processes and therefore we have a long-time approximation. In taking this approximation we have neglected the higher order frequency components, which correspond to the singularities of $\Xi(z)$ associated to $\Xi_N(z)$, i.e. rapid process. If only m ($<N$) poles locate near the center and the others are distributed away from them, then the m poles correctly represent m singularities of $\Xi(z)$ near the center, whereas the other $(N-m)$ poles are not insured to represent any singularities of $\Xi(z)$. Thus the N-pole approximation is convenient if there is a clear distinction between slow and fast processes. A typical example is a particle undergoing Brownian motion: the time scales of the fluctuating forces are much smaller than the time scales of the collective coordinates for the particle. Other example is the long-lived hydrodynamic modes in many-body systems [56].

We can reach the same conclusions quantitatively starting from the inverse Laplace transform of (2.14)

$$\frac{d\Xi_N}{dt}(t) = -\int_0^t \Xi_{N+1}(t')\Xi_N(t-t')\,dt'. \tag{4.8}$$

Assuming that $\Xi_{N+1}(t)$ decays much faster than $\Xi_N(t)$ (and this means [57] $\delta_{N+1} \gg \delta_N$) we obtain

$$\frac{d\Xi}{dt}(t) = -\left[\int_0^\infty \Xi_{N+1}(t')\,dt'\right]\Xi_N(t), \tag{4.9}$$

which gives

$$\Xi_N(t) = e^{-t/\tau}N + 1, \tag{4.10}$$

where

$$\tau_{N+1}^{-1} = \int_0^\infty \Xi_{N+1}(t')\,dt'. \tag{4.11}$$

In order to calculate τ_{N+1} we have to approximate $\Xi_{N+1}(t)$ by a known function to calculate the integral, or then step it down, using the relation between successive memory functions, and use some $\Xi_m(t)$ of lower order [57]. For example in the three pole approximation proposed by Lovesey and Meserve [5, 6] where $N=3$, they have used for $\Xi_1(t)$ a Gaussian function. There are other approximations to τ_N in the literature [54] but all of them reduce to the Lovesey and Meserve expression in the limit $\delta_N \ll \delta_{N+1}$, where the approximation of

N-poles should work. An alternative procedure is to choose τ_N to fix $F(\omega = 0)$ but in most problems of interest we do not know $F(0)$.

Here we present what we think is the correct way to choose τ_N. Writing $\gamma_N = \tau_N^{-1}$ in Eq. (4.2) and calling the Fourier transform of $\Xi_N(t)$ by $F_N(\omega)$ we have

$$F_{N-1}(\omega) \equiv \frac{1}{\pi} \operatorname{Re} \Xi_{N-1}(i\omega) = \frac{\delta_{n-1}\gamma_N/\pi}{\omega^2 + \gamma_N^2}. \tag{4.12}$$

As it is well known, the problem with a Lorentzian is that all moments are infinite. To overcome this difficulty we use a truncated Lorentzian

$$F_{N-1}(\omega) = \begin{cases} \dfrac{\delta_{N-1}\gamma_N/\pi}{\omega^2 + \gamma_N^2}; & |\omega| \leq \omega_c \\ 0; & |\omega| > \omega_c \end{cases} \tag{4.13}$$

where ω_c is a cut off to be determined. We obtain for the moments $\langle \omega_{N-1}^m \rangle$ of $F_{N-1}(\omega)$

$$\langle \omega_{N-1}^2 \rangle = 2\omega_c \frac{\gamma_N}{\pi}, \qquad \langle \omega_{N-1}^4 \rangle = \frac{2\omega_c^3 \gamma_N}{3\pi} \tag{4.14}$$

which gives

$$\gamma_N = \frac{\pi}{\sqrt{12}} \left[\frac{\langle \omega_{N-1}^2 \rangle^3}{\langle \omega_{N-1}^4 \rangle} \right]^{1/2} \tag{4.15}$$

$$\omega_c = \sqrt{3} \left[\frac{\langle \omega_{N-1}^4 \rangle}{\langle \omega_{N-1}^2 \rangle} \right]^{1/2}. \tag{4.16}$$

Expressing $\langle \omega_{N-1}^m \rangle$ in terms of the coefficients δ_N we obtain

$$\gamma_N = \frac{\pi}{\sqrt{12}} \frac{\delta_N}{\sqrt{\delta_{N+1}}}, \qquad \omega_c = \sqrt{3\delta_{N+2}}. \tag{4.17}$$

The validity of approximation (4.13) requires $\gamma_N \ll \omega_c$, which means $\langle \omega_{N-1}^4 \rangle / \langle \omega_{N-1}^2 \rangle^2 \gg 1$, or

$$\delta_N \ll \delta_{N+1}. \tag{4.18}$$

If we step down in order to calculate τ_N we will not get the value given by (4.17) for γ_N. Thus to use the N-pole approximation first we should have $\delta_N \ll \delta_{N+1}$ and this shows that we can use this kind of cut off only at the Nth stage. The method is not convergent in the sense that if we use a $N+1$ pole approximation in general δ_{N+2} is not large compared to δ_{N+1} and the approximation fails. It has already been noted in the literature that results obtained by progressively terminating the continued fraction by an exponential have not lead to a progressively improved shape [55, 58]. Second, we should use the correct τ_N, as given by (4.17), to be consistent with our boundary conditions: $\langle \omega_{N-1}^4 \rangle / \langle \omega_{N-1}^2 \rangle^2 \gg 1$. Therefore if $\delta_{j+2} \gg \delta_{j+1}$ we can use a Lorentzian form for

$\Xi_j(z)$. This will be a good approximation for small ω. However if $F(\omega)$ has a side peak at $\omega = \omega_p$, the region of validity of the approximation should be sufficiently large to include this peak, this is, from (4.17) we obtain $\omega_p < \sqrt{3\delta_{j+2}}$. This condition is equivalent to the condition already mentioned that the N-poles of $\Xi(z)$ should lie, in the complex plane, within a semi-circle of radius τ_{j+1}^{-1}.

With regard to higher order δ's we see that equation (4.13) is equivalent to

$$F_N(\omega) = \begin{cases} \gamma_N; & |z| \leq \omega_c \\ 0; & |z| > \omega_c. \end{cases} \tag{4.19}$$

But (4.19) is the square function defined in (3.6) for which $\delta_{N+2} \simeq \delta_{N+1}$ so that the $N+1$ pole approximation to $\Xi(z)$ would fail because the condition $\delta_{N+2} \gg \delta_{N+1}$ is not satisfied.

In conclusion, the validity of the N-pole approximation requires not only that $\delta_N \ll \delta_{N+1}$ but also that δ_{N+1} be of the same order as δ_{N+2}. If these conditions are met we can use the cut-off $\Xi_N(z) = \gamma_N$, at the nth stage, with γ_N given by (4.17).

Pires and Franco [59] have applied the theory discussed in this section to calculate the neutron scattering cross section in the magnetic compound $(CH_3)_4NM_nCl_3$, obtaining a good agreement with experimental data.

5. Low temperature approximation

The inverse Laplace transform of (2.14) is given by

$$\frac{d}{dt}\Xi(t) = -\int_0^t \phi(\tau)\Xi(t-\tau)\,d\tau, \tag{5.1}$$

where

$$\phi(\tau) = \delta_1\Xi_1(\tau) = \frac{(f_1(\tau), f_1)}{(A, A)}, \tag{5.2}$$

and

$$f_1(t) = e^{it(1-P)L}i(1-P)LA. \tag{5.3}$$

As we have seen (5.1) is exact, and hence only a formal identity with the equation of motion for the many body system. The memory function $\phi(t)$ contains the modified propagator $\exp[it(1-P)L]$ and its study would involve solving the many body problem directly. To obtain useful results we then have to introduce approximations, as we have already seen.

In this section we discuss an approximation that can be used when the Hamiltonian of a many-body system can be written as

$$H = H_0 + V, \tag{5.4}$$

as is frequently the case at low temperatures. In (5.4) H_0 is an approximation to

H, for instance the Random Phase Approximation (RPA) Hamiltonian, and V is the part of H not contained in H_0.

To approximate $\phi(t)$ a systematic approach would be to apply standard perturbative methods. This provides a consistent evaluation of $\phi(t)$ to a given order of perturbation of the Hamiltonian V. For instance, in the weak-coupling approximation, the modified propagator $\exp[it(1-P)L]$ is replaced by the free propagator $\exp[it(1-P)L_0] = \exp[itL_0]$ where $L_0 = i[H_0, .]$. Let $D = (1-P)LA$, then

$$\phi(t) = (D(t), D)(A, A)^{-1} \tag{5.5}$$

where now $D(t) = \exp[itL_0]D$. This gives for the Fourier transform $\phi(\omega)$

$$\phi(\omega) = \frac{1-e^{-\beta\omega}}{\omega} \sum_{i,j} |D_{ij}|^2 \, \delta(\omega - E_{ji}^0) \frac{e^{-\beta E_i^0}}{Z} (A, A)^{-1}. \tag{5.6}$$

where $E_{ji}^0 = E_j^0 - E_i^0$, $D_{ij} = \langle i | D | j \rangle$ is the matrix element between RPA modes and Z is the partition function. Note that we suppose that we can solve H_0 exactly. The above formalism leads rather naturally to an extension of the zero-temperature RPA for finite temperatures, and it provides a prescription for the calculation of the damping width of the RPA modes. An approximation of this kind was used by Ayik [60] to study relaxation process in nuclear collisions at finite temperatures.

We can also go one step further and approximate the modified propagator in the calculation of the second order memory function

$$\Xi_2(t) = -(QL^2A, e^{-iQLQt}QL^2A)(LA, LA)^{-1} \tag{5.7}$$

where $Q = 1 - P$. Higher order approximations becomes increasingly difficult to perform. We show this kind of approximation with an example.

Let us consider the classical one dimensional antiferromagnet described by the Hamiltonian

$$H = \tfrac{1}{2} \sum_q J(q) \vec{S}_q \cdot \vec{S}_{-q}, \tag{5.8}$$

where $J(q) = 2J \cos q$, and q is in units of the lattice parameter. The spins in the spherical coordinates are given by

$$\begin{aligned} S_n^x &= (-1)^n S \sin\theta_n \cos\tau_n \\ S_n^y &= (-1)^n S \sin\theta_n \sin\tau_n \\ S_n^z &= (-1)^n S \cos\theta_n \end{aligned} \tag{5.9}$$

The $(-1)^n$ factor is present because, at low temperatures, the spins are almost antiferromagnetically aligned. At low temperatures, the spins are ordered antiferromagnetically for distances less than a correlation length. Although strictly speaking spin-wave theory is applicable to systems which are almost completely polarized we can use an extension of the method for one dimensional systems in which there is a well developed local order. Following Reiter [61], and

De Raedt et al [62], we can calculate correlation functions of operators that are combined in rotationally invariant quantities involving spins located within a distance much less than a coherence length. To get the correct isotropic result in the spin wave formalism we could then choose an arbitrary direction for the magnetization but we should calculate, for instance, $\langle S_q^\alpha S_{-q}^\alpha \rangle$ $(\alpha = x, y, z)$, add the three correlation functions and divide by 3, since $\sum_\alpha \langle S_q^\alpha S_{-q}^\alpha \rangle$ is rotationally invariant. Having this in mind we introduce the coordinates

$$\Psi_n = \pi/2 - \theta_n, \qquad \phi_n = \tau_n - \tau \tag{5.10}$$

where τ is arbitrarily chosen and Ψ_n is taken in a way so that the ground state corresponds to the spin in the XY plane. Substituting (5.9) and (5.10) into Hamiltonian (5.8), and expanding in Ψ_n and ϕ_n we obtain, after performing a Fourier transformation of Ψ_n and ϕ_n,

$$H_0 = \frac{S}{2} \sum_q [b(q)\phi_q \phi_{-q} + d(q)\Psi_{\pi-q}\Psi_{-\pi+q}] \tag{5.11}$$

where

$$\begin{aligned} b(q) &= 2JS(1 - \cos q) \\ d(q) &= 2JS(1 + \cos q). \end{aligned} \tag{5.12}$$

In this approximation the one-dimensional system (5.8) is analogous to the anharmonic magnon system. Performing the canonical transformation

$$\begin{aligned} \phi_q &= \alpha(q)(a_q^+ + a_{-q}) \\ \Psi_{\pi-q} &= i\beta(q)(a_q^+ - a_{-q}), \end{aligned} \tag{5.13}$$

where

$$\alpha(q) = \frac{1}{\sqrt{2S}} \left(\frac{d(q)}{b(q)}\right)^{1/4}, \qquad \beta(q) = \frac{1}{\sqrt{2S}} \left(\frac{b(q)}{d(q)}\right)^{1/4}, \tag{5.14}$$

and a_q and a_{-q}^+ are the magnon creation and annihilation operators, we find the harmonic Hamiltonian

$$H_0 = \sum_q \omega(q)(n_q + \tfrac{1}{2}), \tag{5.15}$$

where

$$\omega^2(q) = b(q)d(q) = 4J^2S^2(1 - \cos^2 q), \tag{5.16}$$

is the characteristic frequency and $n_q = a_q^+ a_q$ is the usual occupation number. Using the comutation relation $[a_q, a_{-q'}^+] = \delta_{qq'}$ and inserting the Hamiltonian (5.15) into the equation of motion for operators a_q and a_q^+ we easily obtain

$$\begin{aligned} \phi_q(t) &= \alpha(q)[e^{i\omega(q)t}a_q^+(0) + e^{-i\omega(q)t}a_{-q}(0)], \\ \Psi_{\pi-q}(t) &= i\beta(q)[e^{i\omega(q)t}a_q^+(0) - e^{-i\omega(q)t}a_{-q}(0)]. \end{aligned} \tag{5.17}$$

To proceed we write the second order memory function (5.7) as

$$\Xi_2(t) = -M_q(t)(LS_q^x, LS_q^x)^{-1} \tag{5.18}$$

$$M_q(t) = (QL^2S_q^x, e^{-iQLQt}QL^2S_q^x), \tag{5.19}$$

whose expansion in powers of t is

$$M_q(t) = \sum_{n=0}^{\infty} \frac{(-it)^{2n}}{(2n)!}(QL^2S_q^x, (QLQ)^{2n}QL^2S_q^x). \tag{5.20}$$

Considering each coefficient separately we can expand each of them in a temperature series. Reiter and Sjölander [63] have shown that all but the first terms in this temperature series contribute to order T^3 in (5.20) and that keeping only the lowest-order contribution is equivalent to omitting the Q operators in the time evolution. With this simplication we have

$$M_q(t) = (QL^2S_q^x, e^{-iLt}QL^2S_q^x) + 0(T^3) \tag{5.21}$$

where $M_q(t)$ needs to be evaluated to lowest non vanishing order in temperature. The essential gain obtained with this approximation is that we can use H_0 to calculate (5.21). To calculate $QL^2S_q^x$ we use Hamiltonian (5.8) finding

$$QL^2S_q^x = L^2S_q^x - \langle\omega^2\rangle_q S_q^x \tag{5.22}$$

where the second moment $\langle\omega^2\rangle$ is equal to $\omega^2(q)$ at the lowest order in temperature and

$$L^2S_q^x = -\sum_{q_1,q_2,q_3} \delta_{q_1+q_2+q_3,q} \frac{\Gamma(q_1, q_2, q_3)}{2}[S_{q_1}^x S_{q_2}^z S_{q_3}^z - S_{q_1}^x S_{q_2}^y S_{q_3}^z], \tag{5.23}$$

where

$$\begin{aligned}\Gamma(q_1, q_2, q_3) = {} & [J(q - q_2) - J(q_2)][J(q_3) - J(q_1)] \\ & + [J(q - q_3) - J(q_3)][J(q_2) - J(q_1)].\end{aligned} \tag{5.24}$$

An expansion in the normal coordinates ϕ_q and Ψ_q gives

$$QL^2S_q^x = S\sum_k \left[f(k)\Psi_{(q^*/2)+k}\Psi_{(q^*/2)-k} + g(k)\phi_{(q^*/2)+k}\phi_{(q^*/2)-k}\right], \tag{5.25}$$

where

$$f(k) = 8J^2S^2\left\{\cos^2\frac{q}{2}\left(1 - \cos^2\frac{q}{2}\right) + \sin\frac{q}{2}\cos k\left(1 + \sin\frac{q}{2}\cos k\right)\right\}, \tag{5.26}$$

$$g(k) = 4J^2S^2\left\{\cos^2\frac{q}{2}(1 - \cos q) + 2\sin\frac{q}{2}\cos k\left(1 + \sin\frac{q}{2}\cos k\right)\right\}, \tag{5.27}$$

and

$$q^* = \pi - q.$$

The evaluation of $\Xi_2(t)$ is straightforward. The time evolution e^{-iLt} is replaced by the harmonic time evolution specified by (5.17) and the expectation values are taken using the harmonic Hamiltonian (45). The final expression is

$$M_{q^*}(t) = -\frac{(2JST)^2}{N}\sum_q \{[s(q,k)-t(q,k)]^2\cos(\Omega_+ t) + [s(q,k)+t(q,k)]^2\cos(\Omega_- t)\} \tag{5.28}$$

where

$$s(q,k) = \left\{\sin^2\frac{q}{2}(1+\cos q) + 2\cos k\cos\frac{q}{2}\left(1+\cos k\cos\frac{q}{2}\right)\right\} \times\left[1+\cos\left(k+\frac{q}{2}\right)\right]^{1/2}\left[1+\cos\left(k-\frac{q}{2}\right)\right]^{1/2}, \tag{5.29}$$

$$t(q,k) = \left\{\sin^2\frac{q}{2}(1+\cos q) - 2\cos k\cos\frac{q}{2}\left(1-\cos k\cos\frac{q}{2}\right)\right\} \times[1-\cos(k+q/2)]^{-1/2}[1-\cos(k-q/2)]^{1/2}, \tag{5.30}$$

$$\Omega\pm = 2\sqrt{2}JS\left\{\sin\left(\frac{k}{2}+\frac{q}{4}\right)\left[1+\cos\left(k+\frac{q}{2}\right)\right]^{1/2} \pm\sin\left(\frac{k}{2}-\frac{q}{4}\right)\left[1+\cos\left(k-\frac{q}{2}\right)\right]^{1/2}\right\}. \tag{5.31}$$

Equation (5.28) is a sum of N oscillatory terms. In the limit $N\to\infty$ the sum can be replaced by an integral and we find

$$\Xi_2(t) = -8JST\left\{\sin^2\frac{q}{2}\frac{J_1(\Omega_1 t)}{\Omega_1 t} + \cos^4\frac{q}{2}J_0(\Omega_2 t)\right\} \tag{5.32}$$

$$\Omega_1 = 4JS\left|\sin\frac{q}{2}\right|; \qquad \Omega_2 = 4JS\left|\cos\frac{q}{2}\right|. \tag{5.33}$$

A system with a finite number of particles may have only a finite-dimensional Hilbert space, and there will therefore be a δ_N such that $\delta_N = 0$, but the dimensionality may grow with the number of particles, that is infinite in the thermodynamic limit.

Equation (5.32) was obtained by Reiter and Sjölander [63] without resorting to a spin wave expansion, as we did here, and since these authors have discussed extensively these results we add just one comment. For $q = 0$, equation (5.32) becomes

$$\Xi(t) = -8JSTJ_0(\Omega t), \tag{5.34}$$

which gives

$$\Xi(z) = \frac{-8JS}{\sqrt{z^2+\Omega^2}} \tag{5.35}$$

and for $q = \pi$ one has

$$\Xi_\pi(t) = -8JST\frac{J_1(\Omega t)}{\Omega t} \tag{5.36}$$

and then

$$\Xi_\pi(z) = -\frac{8JST}{\Omega^2}(\sqrt{z^2+\Omega^2} - z), \tag{5.37}$$

where $\Omega = 4JS$.

On account of the discussion of Section 3 we see that we have $\delta_4 = \delta_5 = \cdots = \Omega$ for $q = 0$ and $\delta_3 = \delta_4 = \delta_5 = \cdots = \Omega$ for $q = \pi$. This is in agreement with the low temperature calculations [12] of the parameters δ for the Hamiltonian (5.8).

We have chosen this example for its simplicity and because it has been already studied in detail by Reiter and Sjölander [63] using a different approach. However the method can also be applied to other models, such as anisotropic Hamiltonians, magnetic chains in the presence of external fields, quantum models, etc., where Reiter and Sjölander's approach is not appropriate.

6. Conclusion

The problem of expanding the correlation function into continued fraction was considered in the light of the Mori formalism. We have examined some of the techniques available in the literature for terminating the continued fraction expansion and shown how to use correctly each of them. We hope our paper can be used as a guide to the reader interested in applying Mori's method to study the dynamics of physical problems.

The use of the memory function formalism for coupled operators can be found, for instance in Ref. [64]. Extension of the method to treat non-Hermitian case is found in Ref. [65].

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