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Calculation of relaxation functions: A new development within the Mori formalism

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The problem of expanding the correlation functions into continued fractions is considered in the light of a Mori-type formalism. First, we examine the techniques available in the literature for extracting the parameters of the Mori chain from the moments; then, on the basis of physical considerations, we provide a new surprisingly simple and efficient technique and discuss its significance. Some examples are given to illustrate the elegance and the convenience of our procedure.

I. INTRODUCTION

In the past few years there has been a growing interest in the foundations of the methods for calculating correlation functions and spectra.[1] It would be impossible to mention here all possible ways to approach the actual physical problems in that they come from very different areas of research, which are often of an interdisciplinary nature. However, among the leading formalisms in the literature, a particular importance is recognized to the Mori theory,[2] the Padé approximants,[3] the Lanczos method,[4] the recurrence method,[5] and the generalized method of recurrence relations.[6]

At first sight it would seem that each approach involves completely different theoretical backgrounds; but to a less superficial examination it is apparent, though sometimes not yet explored in depth, that these approaches are closely related to each other. For example, a connection can be established between the Lanczos method and the Padé approximants,[3,4,7] and furthermore, the latter method can be related[8] to those inspired to the Mori theory. The recurrence method of Haydock, Heine, and Kelly,[5] which has assumed so much importance in the calculation of electronic states in disordered systems[9] as well as of phonons,[10] and the generalized method of recurrence relations[6] have significant overlaps, whose ultimate consequences are still to be explored; on the other hand, the generalized method of recurrence relations,[6] although it is an alternative to the Mori formalism, borrows from the latter important concepts such as that of random forces and their dynamics.

From the above considerations it is evident that the Mori formalism plays a central role in the problem of the calculation of relaxation functions. In our opinion, this is so because the methods based on a Mori-type theory enjoy the extra bonuses which come from a foundation mainly physical in nature rather than mathematical. This provides, for example, a firm theoretical basis on which new approaches for dealing with many-body problems, such as the reduced model theory[11] for phonon thermal baths[12] and the "doorway method"[13] in spectroscopic problems, may be constructed. But an even more important bonus of the Mori theory is its extension[1,11] to the case of a non-Hermitian Liouvillian, which allows a new set of problems to be faced, and which includes nonequilibrium properties besides standard equilibrium ones.

Although the generalized Mori theory is such a powerful theoretical tool to provide a continued-fraction expansion of correlation functions, the situation is not yet satisfactory under the technical, but rather subtle, aspect of an explicit evaluation of the parameters of the Mori chain. It is unpleasant that so important a theoretical tool encounters in several situations serious difficulties under this aspect.

In this paper we first examine the technique adopted in the literature for obtaining the parameters of the Mori chain. Except for particular though relevant models (for instance, the tight-binding Hamiltonian of Haydock, Heine, and Kelly[5] or the Kubo stochastic oscillator[14,15]), the standard way for obtaining the parameters of the Mori chain exploits the knowledge of the spectral moments, with tech-

niques essentially based on the mathematical results of Dupuis.[16] Then we provide a new, simple, and efficient technique, exploiting only the physical foundation of the Mori theory. A couple of examples are given to illustrate the convenience of the new procedure.

II. THE GENERALIZED VERSION OF THE MORI THEORY

A. Survey of the generalized Mori theory

The Mori theory is having an increasing success in the interpretation of a number of relaxation phenomena; its recent and appealing generalized version[15] has further attracted the attention of researchers in the field of correlation functions. To make this paper reasonably self-contained, we shall concisely survey some relevant points, referring the reader for a complete account to Refs. 1 and 15.

Consider a dynamical variable A, whose time evolution $A(t)$ is given by

$$\frac{d}{dt}A = iLA \ . \tag{1}$$

Notice that the dynamical operator L does not necessarily coincide with the rigorous Liouvillian operator of the many-body system under study. As shown in Ref. 12, the Mori theory itself can be used to replace the rigorous operator iL with an "equivalent" Fokker-Planck–type operator.[17] The advantage of this approach is to significantly reduce the amount of degrees of freedom, since the frictional and diffusional terms of the Fokker-Planck–type operator simulate indeed an infinite number of them. Basically, the same ideas are behind the works of other authors.[18] This explains why it is important to extend the Mori theory to situations without a definite symmetry (dynamical operator L neither Hermitian nor anti-Hermitian).

The generalization of the Mori theory can be arrived at as follows. First of all, as in the standard Mori approach, a suitable scalar product concerning variables is defined in the form

$$\langle A \mid B \rangle = \int A^{\dagger}(\Gamma) B(\Gamma) W(\Gamma) d\Gamma \ , \tag{2}$$

where $W(\Gamma)$ is an appropriate weighting function so as to perform averaging operations, A and B are two generic variables of the coordinates Γ of the physical space under study. We are interested in evaluating the correlation function

$$\Phi_0(t) = \frac{\langle A \mid A(t) \rangle}{\langle A \mid A \rangle} = \frac{\langle A \mid e^{iLt} \mid A \rangle}{\langle A \mid A \rangle} \ . \tag{3}$$

Notice that also nonequilibrium properties such as $\langle A(t) \rangle$ can be expressed under the form of a correlation function. In such a case $W(\Gamma)$ is not an equilibrium distribution, thereby destroying the eventual Hermitian property of L with respect to the scalar product of Eq. (2).

It is convenient to construct a biorthogonal set of vectors and the corresponding projection operators

$$\begin{aligned}
&|f_0\rangle = A, \quad P_0 = \frac{|f_0\rangle\langle f_0|}{\langle f_0 | f_0\rangle} \ , \\
&|f_1\rangle = (1-P_0)iL\,|f_0\rangle, \quad \langle \tilde{f}_1| = \langle f_0 | iL(1-P_0), \quad P_1 = \frac{|f_1\rangle\langle \tilde{f}_1|}{\langle \tilde{f}_1 | f_1\rangle} \ , \\
&|f_2\rangle = (1-P_1)(1-P_0)iL\,|f_1\rangle, \quad \langle \tilde{f}_2| = \langle \tilde{f}_1 | iL(1-P_0)(1-P_1), \quad P_2 = \frac{|f_2\rangle\langle \tilde{f}_2|}{\langle \tilde{f}_2 | f_2\rangle} \ ,
\end{aligned} \tag{4}$$

etc. By a suitable extension of the standard Mori approach, we obtain for the motion of the variables $|f_i(t)\rangle$ the interdependent integral equations:

$$\frac{d}{dt}|f_i(t)\rangle = \lambda_i |f_i(t)\rangle - \Delta_{i+1}^2 \int_0^t \Phi_{i+1}(t-\tau)\,|f_i(\tau)\rangle d\tau + |f_{i+1}(t)\rangle \ , \tag{5}$$

where

$$\lambda_i = \frac{\langle \tilde{f}_i \mid iL \mid f_i\rangle}{\langle \tilde{f}_i \mid f_i\rangle} \ , \tag{6}$$

$$\Delta_{i+1}^2 = -\frac{\langle \tilde{f}_{i+1} | f_{i+1}\rangle}{\langle \tilde{f}_i | f_i\rangle} \ , \tag{7}$$

$$\Phi_{i+1}(t) = \frac{\langle \tilde{f}_{i+1} | f_{i+1}(t)\rangle}{\langle \tilde{f}_{i+1} | f_{i+1}\rangle} \ , \tag{8}$$

and $|f_{i+1}(t)\rangle$ is driven by the projected Liouvillian

$$iL_{i+1} = \left[\prod_{j=0}^{i}(1-P_{i-j})\right] iL \ .$$

The physical meaning of Eq. (5) is quite appealing. Equation (5) is a generalized Langevin equation. The motion of $|f_{i+1}(t)\rangle$ depends on the interaction with the following infinite states of the Mori chain, thereby making often its explicit evaluation practically inacessible. The variable $|f_{i+1}(t)\rangle$ can therefore be regarded as being a stochastic force related to the memory kernel Φ_{i+1} by the fluctuation-dissipation relationship embodied in Eq. (5) and (8); we will exploit these physical aspects later in the paper.

It is convenient to multiply Eq. (5) by $\langle \tilde{f}_i |$ on the left. Using Eq. (8), we then obtain the hierarchy of equations for the memory functions:

$$\frac{d}{dt}\Phi_0(t)=\lambda_0\Phi_0(t)-\Delta_1^2\int_0^t\Phi_1(t-\tau)\Phi_0(\tau)d\tau\ ,$$
$$\cdots\ , \tag{9}$$
$$\frac{d}{dt}\Phi_i(t)=\lambda_i\Phi_i(t)-\Delta_{i+1}^2\int_0^t\Phi_{i+1}(t-\tau)\Phi_i(\tau)d\tau\ ,$$
$$\cdots\ .$$

By Laplace-transforming Eqs. (9) we finally arrive at the continued-fraction expansion

$$\hat{\Phi}_0(z)=\cfrac{1}{z-\lambda_0+\cfrac{\Delta_1^2}{z-\lambda_1+\cfrac{\Delta_2^2}{z-\lambda_2+\cdots}}}\ . \tag{10}$$

B. Mathematical procedures for the evaluation of the continued-fraction parameters

The direct evaluation of the Mori chain parameters λ_i and Δ_i^2, expressed formally by Eqs. (6) and (7), becomes so tedious in most practical situations that one seeks to limit the direct evaluation to the first few steps only. The best way to cope with the problem at this time is to proceed through the introduction of a set of orthogonal polynomials and exploit the properties of the Hankel determinants. We call this mathematical procedure the Dupuis algorithm[16] from the author who first gave a detailed account of it, although several papers[19–21] have given important contributions in this field.

The Dupuis algorithm for extracting the parameters of the Mori chain from the knowledge of the spectral moments

$$s_n=\frac{\langle f_0|(iL)^n|f_0\rangle}{\langle f_0|f_0\rangle} \tag{11}$$

can be outlined as follows.

One introduces the Hankel determinants ($D_{-1}\equiv 1$)

$$D_n=\begin{vmatrix} s_0 & s_1 & \cdots & s_n \\ s_1 & s_2 & \cdots & s_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ s_n & s_{n+1} & \cdots & s_{2n} \end{vmatrix} \quad (n\geq 0)\ . \tag{12}$$

One then defines the orthogonal set of polynomials $P_n(\lambda)$ given by $[P_0(\lambda)\equiv 1]$:

$$P_n(\lambda)=\frac{1}{D_{n-1}}\begin{vmatrix} s_0 & s_1 & \cdots & s_n \\ s_1 & s_2 & \cdots & s_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ s_{n-1} & s_n & \cdots & s_{2n-1} \\ 1 & \lambda & \cdots & \lambda^n \end{vmatrix} \quad (n\geq 1)\ . \tag{13}$$

A scalar product for polynomials is defined as

$$\mathcal{F}(c_0+c_1\lambda+c_2\lambda^2+\cdots)$$
$$\equiv c_0s_0+c_1s_1+c_2s_2+\cdots\ .$$

After some lengthy algebra it can be shown[16] that

$$\lambda_i=\frac{D_{i-1}}{D_i}\mathcal{F}[\lambda P_i(\lambda)P_i(\lambda)]\ , \tag{14}$$

$$\Delta_i^2=-D_iD_{i-2}/D_{i-1}^2\ . \tag{15}$$

The Dupuis expression (15) for Δ_i^2 is much more convenient from a computational point of view than the corresponding Mori expression (7); but the Dupuis expression (14) for the λ_i is still of limited help.

However, one can further simplify Eq. (14) by introducing the modified Hankel determinants

$$R_n=\begin{vmatrix} s_0 & s_1 & \cdots & s_n \\ s_1 & s_2 & \cdots & s_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ s_{n-1} & s_n & \cdots & s_{2n-1} \\ s_{n+1} & s_{n+1} & \cdots & s_{2n+1} \end{vmatrix} \quad (n\geq 1)\ .$$

Manipulating Eq. (14), it is possible[20] to arrive at the expression

$$\lambda_i=\frac{R_i}{D_i}-\frac{R_{i-1}}{D_{i-1}} \quad (i\geq 1)\ , \tag{14'}$$

with $\lambda_0\equiv s_1$. It is interesting to note that the same result (14') can be arrived at in a completely independent way[21] through the construction of a Jacobi matrix.

Equation (14') and (15) constitute the most convenient expressions presently available for actual

calculations. But, despite the elegant simplicity of expressions (14′) and (15), this difficult problem is not yet at its final stage, and rather it offers a new challenge. In fact, a solution which proceeds through the evaluation of Hankel determinants becomes rapidly ill conditioned[22] as the order n increases. For instance, if one applies the Hankel-determinant procedure to the moments of a Gaussian spectrum, one gets unreliable parameters as n approaches ten, or so. Neither the use of double or more extended precision arithmetic, nor the introduction of an optimized time scale[20] can avoid this difficulty.

C. A new physical procedure for the evaluation of the continued-fraction parameters

The Dupuis algorithm and other similar treatments are basically founded on mathematical considerations, and do not exploit the physical implications embodied in the hierarchy of Eqs. (9). In this section we give a new and simple way for extracting the parameters of the Mori chain from the moments.

We start from the first equation of the hierarchy

$$\frac{d}{dt}\Phi_0(t)=\lambda_0\Phi_0(t) - \Delta_1^2\int_0^t \Phi_1(t-\tau)\Phi_0(\tau)d\tau \ . \tag{16}$$

Then we expand in the Taylor series both the correlation function $\Phi_0(t)$ and its memory function $\Phi_1(t)$:

$$\Phi_0(t)=\sum_{n=0}^{\infty}\frac{s_n}{n!}t^n \ , \tag{17a}$$

$$\Phi_1(t)=\sum_{n=0}^{\infty}\frac{\sigma_n}{n!}t^n \ . \tag{17b}$$

The convolution integral appearing in Eq. (16) can be written as follows:

$$\int_0^t\Phi_1(t-\tau)\Phi_0(\tau)d\tau=\int_0^t d\tau\sum_{n=0}^{\infty}\frac{1}{n!}\sigma_n\sum_{k=0}^{n}\frac{n!}{k!(n-k)!}t^{n-k}(-\tau)^k\sum_{m=0}^{\infty}\frac{1}{m!}s_m\tau^m$$

$$=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{1}{m!}\sigma_n s_m\sum_{k=0}^{n}\frac{(-1)^k}{k!(n-k)!}\frac{t^{n+m+1}}{m+k+1} \ .$$

Using the identity

$$\sum_{k=0}^{n}\frac{(-1)^k}{k!(n-k)!(m+k+1)}\equiv\frac{m!}{(m+n+1)!} \ ,$$

we obtain

$$\int_0^t\Phi_1(t-\tau)\Phi_0(\tau)d\tau=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\sigma_n s_m\frac{1}{(n+m+1)!}t^{n+m+1} \ . \tag{18}$$

Replacing Eqs. (17) and (18) into Eq. (16), and comparing term by term the coefficients of the same power in t (remember the implicit assumption $s_0\equiv\sigma_0\equiv 1$), we obtain the following results:

$$\lambda_0=s_1 \ , \tag{19a}$$

$$\Delta_1^2=s_1^2-s_2 \ , \tag{19b}$$

$$\sigma_n=\frac{s_1s_{n+1}-s_{n+2}}{s_1^2-s_2}-\sum_{k=0}^{n-1}\sigma_k s_{n-k} \quad \text{if } \Delta_1^2\neq 0 \ , \tag{19c}$$

$$s_n=s_1^n \quad \text{if } \Delta_1^2=0 \ . \tag{19d}$$

Equations (19) constitute the basically new (and elegant) result of this paper, which allows an efficient and stable procedure for calculating the parameters of the Mori chain. Suppose that the first $\bar{n}$ moments of a correlation function are known. Then we can say the following:

(i) The first parameter λ_0 of the Mori chain equals s_1.

(ii) The first parameter Δ_1^2 of the Mori chain equals $s_1^2-s_2$.

(iii) The first $\bar{n}-2$ moments of the memory function are trivially given by Eq. (19c) (except in the very particular case of exact truncation $\Delta_1^2\equiv 0$).

At this stage the procedure can be repeated for the memory function itself, and the next step parameters of the Mori chain can be easily worked out.

Our procedure comes to an end when the knowledge of $\bar{n}$ moments is fully exploited or if a Δ_i^2 parameter vanishes. The latter case implies a severe constraint on all residual moments, which are automatically fixed by such an event.

III. A FEW ILLUSTRATIVE EXAMPLES

In this section we give two illustrative examples of the new procedure in order to make transparent its simplicity. We consider the case of the Gaussian spectrum and of the Hubbard model.

In the case of a Gaussian spectrum the moments s_n are given by

$$s_n=(-1)^{n/2}[(n-1)!!]B^n \tag{20}$$

for even n, and are zero for odd n; B is the root-mean-square amplitude of the Gaussian distribution $(1/\sqrt{2\pi}B)\exp[-E^2/2B^2]$. The first few moments, if we measure the energies in units of B, are

$$s_0=1,\ s_2=-1,\ s_4=3,\ s_6=-15\ , \tag{21}$$
$$s_8=105,\ s_{10}=-945\ ,$$

etc.

If we calculate the Hankel determinants (12) using the moments (20) or (21), we verify by inspection the ill-conditioned nature of the Dupuis procedure; we have in fact, for instance $D_5=-0.3456\times10^5$, $D_{10}=-0.6658\times10^{28}$, and $D_{14}=-0.6911\times10^{65}$. If instead we apply our procedure summarized by Eqs. (19), we have $\lambda_0=0$, $\Delta_1^2=1$; $\sigma_2=-2$, $\sigma_4=10$, $\sigma_6=-74$, $\sigma_8=706$, etc. It is straightforward to apply our procedure more and more, and verify directly for a number of steps that $\Delta_n^2=n$. We thus arrive at the well-known continued-fraction expansion of a Gaussian function

$$\hat{\Phi}_0(z)=\cfrac{1}{z+\cfrac{B^2}{z+\cfrac{2B^2}{z+\cdots}}}\ .$$

As a second example we consider the Hubbard model.[23] In this case the moments s_n are given by

$$s_n=(-1)^{n/2}2\frac{(n-1)!!}{(n+2)!!}B^n \tag{22}$$

for even n, and are zero for odd n; the moments can be easily obtained starting from the parabolic spectral density (normalized to 1) $(2/\pi B^2)(B^2-E^2)^{1/2}$ for $|E|<B$. The first few moments are $s_0=1$; $s_2=-\frac{1}{4}B^2$, $s_4=\frac{1}{8}B^4$, $s_6=-\frac{5}{64}B^6$, $s_8=\frac{7}{128}B^8$, etc.

If we apply our procedure summarized by Eqs. (19), we have $\lambda_0=0$, $\Delta_1^2=\frac{1}{4}B^2$; $\sigma_2=-\frac{1}{4}B^2$, $\sigma_4=\frac{1}{8}B^4$, $\sigma_6=-\frac{5}{64}B^6$, etc. In this case we see that the memory kernel coincides with the correlation function; this interesting result is a by-product of our unorthodox manner to face the model. We arrive at the continued-fraction expansion

$$\hat{\Phi}_0(z)=\cfrac{1}{z+\cfrac{B^2/4}{z+\cfrac{B^2/4}{z+\cdots}}}$$

which can be exactly summed up with the methods discussed, for instance, by Turchi *et al.*[22] These examples show operatively how flexible the computation of the Mori parameters is from Eqs. (19) once a number of moments are known.

IV. CONCLUSIONS

In this paper we have provided a new method for extracting the parameters of the Mori chain from the knowledge of the moments. The novelty of our procedure is that it fully exploits the physical implications of the Mori formalism. The simplicity and the elegance of the results of this paper further strengthen the leading role that the Mori-type formalism is having in the theory of relaxation.

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