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A Simple Algebraic Technique in the Generalized Continued-Fraction Representation

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We obtained a generalized continued fraction representation containing two memory functions by proceeding directly from the Laplace transform of time correlation function and taking algebraic expansion of the inverse operator. The result is identical with the representation of Nagano et al. based on Mori's memory function formalism.

Recently there has been growing interest in the foundation of the methods for calculating correlation functions. So far various ways have been found to approach the actual physical problems in this area.[1)~4)] Among these, the countinued fraction representation approach[5)~11)] originally presented by Mori[5)] seems to play a central role. Actually it has been applied to a variety of interesting physical problems including investigation of line-shapes and critical slowing-downs in the electronic systems and lattice spin systems.[11)~16)]

Later, Karasudani, Nagano, Okamoto and Mori[6)] generalized Mori's continued fraction representation which takes into account two effects expressed by macroscopic and microscopic memory functions. Furthermore, they[7)] obtained reduced equations of motion for generalized flux variables. It contains two kinds of fluctuating forces.

On the other hand, some different kinds of approach have been studied for the representation. Lado, Memory and Parker[11)] obtained the representation by expanding the dynamical variable in terms of an orthogonal set. Lee[8)]got the representation by utilizing the recurrence relation method.

It is well known that the formal solutions for time evolution can be obtained by solving the generalized Langevin equation which was first derived and formally solved by Mori using a projection operator technique. However, this generalized Langevin equation can also be derived by proceeding directly from the Laplace transform of time correlation function.[17]

In this paper, by applying the similar way we would like to obtain the generalized continued fraction representation containing two kinds of memory function which correspond to higher order and low order fluxes, respectively.

If, for the column matrix of state variables $\mathbf{A}(t)$ in a many body system with the Hamiltonian H, $[H,A]\equiv H-AH\neq 0$, then the time evolution in the Heisenberg picture is formally given by $\mathbf{A}(t)=\exp(i\mathbf{H}t)\mathbf{A}\exp(-i\mathbf{H}t)$, where $\mathbf{A}=\mathbf{A}(0)$ and h=1. The information about $\mathbf{A}(t)$ helps us to obtain the time correlation function.

The equation of motion is given by

$$\frac{d\mathbf{A}(t)}{dt}=iLA(t) \tag{1}$$

where L is the Liouville operator corresponding to H. The standard Mori theory is based on the assumption that L is the Hermitian, i.e.,

$$(LF,G^*)=(F,[LG]^*) \tag{2}$$

for arbitrary linear operators F and G, where G^* is the Hermitian conjugate of G, and (A,B) is any binary operation of two variables A and B. The operation can be the usual inner product, the Kubo product, or the trace operation.

For our purpose we construct a biorthogonal set of vectors and the corresponding projection operators. The quantity A defines a vector in a Hilbert space. The projection operator P_0 onto the A-axis is defined by

$$P_0X\equiv(X,A^*)\cdot(A,A^*)^{-1}\cdot A \tag{3}$$

With the aid of P_0, we split $\dot{A}=iLA$ into two parts:

$$iLA=P_0iLA+a_1, \tag{4}$$

where

$$a_1\equiv(1-P_0)iLA \tag{5}$$

The new quantity a_1 stands for the first order flux. Proceeding similarly, we define the j-th order flux $a_j\equiv a_j(0)$ through the recurrence equation

$$a_j \equiv \tilde{Q}_{j-1}iLa_{j-1} \quad (j=1,2,\cdots) \tag{6}$$

with $a_0 \equiv A$, where

$$\hat{Q}_{j-1} \equiv Q_{j-1}Q_{j-2}\cdots Q_1Q_0 = 1-\hat{P}_{j-1}, \quad (7)$$

$$Q_i \equiv 1-P_i,$$

$$P_iX \equiv (X,a_i^*)\cdot(a_i,a_i^*)^{-1}\cdot a_i, \quad (9)$$

$$\hat{P}_{j-1}=\sum_{m=0}^{j-1} P_m=P_{j-1}+\hat{P}_{j-2}. \quad (10)$$

Here P_i is the projection operator onto the a_i-axis and $\hat{P}_j$ represents the projection operator onto the $(j+1)$ dimensional subspace spanned by $a_0, a_1, \cdots, a_j$ which satisfy the orthogonality condition $(a_i,a_j^*)=0,(i\neq j)$

Now let us consider the rime evolution of the generalized flux variables $a_j(t)$ as

$$(d/dt)a_j(t)=iLa_j(t) \quad (11)$$

or

$$a_j(t)=\exp(itL)a_j \quad (12)$$

and define *j-j* element of the time-correlation function $\Xi(t)$ as

$$\Xi_{jj}(t)\equiv(a_j(t),a_j^*)/(a_j,a_j^*) \quad (13)$$

By Laplace transforming Eq. (13), we obtain the relaxation function

$$\tilde{\Xi}_{jj}[z]=\int_0^{\infty}\exp(-zt)\Xi_{jj}(t)dt$$

$$=((z-iL)^{-1}a_j,a_j^*)/(a_j,a_j^*), \quad (14)$$

which can be rewritten into the following form:

$$\Xi_{jj}=(\{(z-iL(\hat{P}_{j-1}+\hat{Q}_j))^{-1}+(z-iL(\hat{P}_{j-1}+\hat{Q}_j))^{-1}iLP_j(z-iL(\hat{P}_{j-1}+\hat{Q}_j+P_j))^{-1}\}a_j,a_j^*)/(a_j,a_j^*), \quad (15)$$

where $\hat{P}_{j-1}+\hat{Q}_j+P_j=1$ and the operator identity $(A+B)^{-1}=A^{-1}-A^{-1}\cdot B\cdot(A+B)^{-1}$ have been used.

Since $\hat{P}_{j-1}a_j=\hat{Q}_ja_j=0$,the first term of Eq.(15) becomes

$$((z-iL(\hat{P}_{j-1}+\hat{Q}_j))^{-1}a_j,a_j^*)=(a_j,a_j^*)/z. \quad (16)$$

Using the property

$$(\hat{P}_{j-1}+\hat{Q}_j)\{z-iL(\hat{P}_{j-1}+\hat{Q}_j)\}^{-1}=\{z-(\hat{P}_{j-1}+\hat{Q}_j)iL\}^{-1}(\hat{P}_{j-1}+\hat{Q}_j), \quad (17)$$

we obtain

$$\tilde{\Xi}_{jj}[z]=[z-(iLa_j,a_j^*)\cdot(a_j,a_j^*)^{-1}-(iL\{z-(\hat{P}_{j-1}+\hat{Q}_j)iL\}^{-1}(\hat{P}_{j-1}+\hat{Q}_j)iLa_j,a_j^*)\cdot(a_j,a_j^*)^{-1}]^{-1}. \quad (18)$$

In order to calculate Eq. (18) further, we take into account the following relations.[6)]

$$(iLa_j,a_m^*)=\begin{cases} 0 & \text{if } m\geq j+2. \\ (a_{j+1},a^*_{j+1}) & \text{if } m=j+1. \\ (iLa_j,a_j^*) & \text{if } m=j. \\ -(a_j,a_j^*) & \text{if } m=j-1 \\ 0 & \text{if } m\leq j-2. \end{cases} \quad (19)$$

The last term in the denominator of Eq. (18) can be written as

$$(iL\{z-(P_{j-1}+Q)iL\}^{-1}(P_{j-1}+Q_j)iLa_j,a_j^*)$$

$$= -\left\{\{z-\hat{P}_{j-1}iL\}^{-1}\sum_{n=0}^{\infty}\left[\hat{Q}_j iL\left\{\frac{1}{z}\sum_{m=0}^{\infty}\left(\frac{\hat{P}_{j-1}iL}{z}\right)^m\right\}\right]^n \hat{P}_{j-1}iLa,(iLa_j)^*\right\}$$

$$-\left\{\{z-\hat{Q}iL\}^{-1}\sum_{n=0}^{\infty}\left[\hat{P}_{j-1}iL\left\{\frac{1}{z}\sum_{m=0}^{\infty}\left(\frac{\hat{Q}_{j-1}iL}{z}\right)^m\right\}\right]^n \hat{Q}_j iLa_j,(iLa_j)^*\right\} \quad (20)$$

In Eq. (20) all the terms become zero except the first term for n=0, since $[\hat{Q}_j iL(\hat{P}_{j-1}iL)^m]\hat{P}_{j-1}iLa_j$ and $[\hat{P}_{j-1}iL(\hat{Q}_j iL)^m]\hat{Q}_j iLa_j$ contained in the first and second parts, respectively, become zero. The proof for a few terms is demonstrated as follows: We start with the first part. For m=0, $\hat{Q}_j iL\hat{P}_{j-1}iLa_j=0$ is easily checked by using the properties of Eq. (19), $\hat{P}_{j-1}iLa_j=-(a_j,a_j^*)\cdot(a_{j-1},a^*_{j-1})^{-1}\cdot a_{j-1}$ and $\hat{Q}_j iLa_{j-1} =\hat{Q}_j\hat{Q}_{j-1}iLa_{j-1}=\hat{Q}_j a_j=0$. For m=1, $\hat{Q}_j iL\hat{P}_{j-1}iL\hat{P}_{j-1}iLa_j$ becomes zero since $\hat{P}_{j-1}iLa_{j-1}=-(a_{j-1},(iLa_{j-1})^*)\cdot(a_{j-1},a^*_{j-1})^{-1}\cdot a_{j-1}-(a_{j-1},(iLa_{j-2})^*)\cdot(a_{j-2},a^*_{j-2})^{-1}\cdot a_{j-2}$ and $\hat{Q}_j iL(a_{j-1}+a_{j-2})=\hat{Q}_j\hat{Q}_{j-1}iLa_{j-1}+\hat{Q}_j\hat{Q}_{j-1}\hat{Q}_{j-2}iLa_{j-2} =\hat{Q}_j a_j+\hat{Q}_j\hat{Q}_{j-1}a_{j-1}=0$. The proof for the second part can be performed similarly. For m=0 and m=1 we can obtain $\hat{P}_{j-1}iL\hat{Q}_j iLa_j=\hat{P}_{j-1}iLa_{j+1}=0$ and $\hat{P}_{j-1}iL\hat{Q}_j iL\hat{Q}_j iLa_j=\hat{P}_{j-1}iL(\hat{Q}_{j+1}+P_{j+1})iLa_{j+1}=\hat{P}_{j-1}iL(a_{j+2}+P_{j+1}iLa_{j+1})=0$, respectively, using Eqs(6) and (19). The proof for m=2 can be shown by considering $\hat{Q}_j=\hat{Q}_{j+1}+P_{j+1}$ and $\hat{Q}_j=\hat{Q}_{j+2}+P_{j+1}+P_{j+2}$. We can show in similar ways that the higher order terms in the two parts in Eq.(20) disappear.

Thus the relaxation function given by Eq.(18) becomes

$$\tilde{\Xi}_{jj}[z]=[z-i\omega_j+\tilde{\Psi}_j[z]+\tilde{\phi}_j[z]]^{-1}, \quad (21)$$

where the frequency matrix element and the two memory functions are defined by

$$i\omega_j\equiv(iLa_j,a_j^*)/(a_j,a_j^*), \quad (22)$$

$$\tilde{\Psi}_j[z]\equiv(\{z-\hat{P}_{j-1}iL\}^{-1}\hat{P}_{j-1}iLa_j,(\hat{P}_{j-1}iLa_j)^*)/(a_j,a_j^*), \quad (23)$$

$$\tilde{\phi}_j[z]\equiv(\{z-\hat{Q}_j iL\}^{-1}\hat{Q}_j iLa_j,(\hat{Q}_j iLa_j)^*)/(a_j,a_j^*), \quad (24)$$

respectively.

By considering $\hat{Q}_j=\hat{Q}_{j+1}+P_{j+1}$ in Eq.(24), $\hat{P}_{j-1}=P_{j-1}+\hat{P}_{j-2}$ in Eq.(23) and taking the similar procedure successively, $\tilde{\Psi}_j[z]$ and $\tilde{\phi}_j[z]$ can be put into the following continued fraction representation:

$$\tilde{\Psi}_j[z]= \cfrac{\Delta_j^2}{z-i\omega_{j-1}+\cfrac{\Delta^2_{j-1}}{z-i\omega_{j-2}+\ddots+\cfrac{\Delta_1^2}{z-i\omega_0}}}\ ,(j\geq 1) \qquad (25)$$

$$\tilde{\phi}_j[z]= \cfrac{\Delta^2_{j+1}}{z-i\omega_{j+1}+\cfrac{\Delta^2_{j+2}}{z-i\omega_{j+2}+\ddots+\cfrac{\Delta_n^2}{z-i\omega_n+\tilde{\phi}_n[z]}}}\ ,(n-1\geq j>0) \qquad (26)$$

$$\Delta_j^2=(a_j,a_j^*)/(a_{j-1},a^*_{j-1}), \qquad (27)$$

which is identical with the result of Nagano et al.[7] This shows $\tilde{\Xi}_{jj}[z]$ can be directly expressed as the continued fraction representation without using the momory function formalism.

We may conclude as follows. In the standard Mori approach, the relaxation function is iterated by applying the memory function formalism for $\Xi_{jj}[t]$ successively. On the other hand, the present work has dealt with the algebraic expansion of the inverse operator. By doing so, the relaxation function has been given in the generalized continued fraction representation containing two memory functions. One is the usual continued fraction representation previously found by Mori and the other the inverted continued fraction of finite order.

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