Derivation of Correlation Spectra by the Operator Algebra Technique

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Abstract

Cross and autocorrelation spectra are dealt with in a unified category by a straightforward method, which is called the operator algebra technique. In this technique the Laplace transform of the correlation functions is performed prior to calculating the Liouville operators. It is shown that this derivation procedure is very simple and the results are identical with those of some other authors.

1. Introduction

Dynamical properties of macroscopic systems can be expressed in terms of the time correlation functions of appropriate physical variables. For instance, the thermal conductivity is given by the time correlation function of the heat flux fluctuation, the polarizability by that of the dipole moment, the magnetic susceptibility by that of the magnetic moment, and the electric conductivity tensor by that of the current density. Studies of correlation spectra are classified into two categories: autocorrelation spectra and cross-correlation spectra. Most of the studies performed so far are related with the former one.

Zwanzig developed a projection technique to select out only the relevant information contained in the dynamical variable. Mori presented a projection operator technique and obtained an expression for the Laplace transform of an autocorrelation function as a continued fraction representation. On the other hand, several different types of approach have also been reported. Lado et al. obtained the representation by expanding the dynamical variable in terms of the orthogonal set of basis vectors in the Hilbert space. Lee got the representation by utilizing the recurrence relation method. Yi et al. used the so-called operator algebra method in getting the representation. In this method the Laplace transform of the time correlation function is performed prior to calculating the Liouville operators, while it is carried out reversely in Mori’s work. The operator algebra technique, when applied to this representation, turned out to be simple and straightforward.

The studies introduced above contain only one kind of fluctuation force. It should be mentioned that introduction of two kinds of fluctuating forces yields both cross- and autocorrelations. The study containing two kinds of
fluctuating forces was initiated by Karasudani et al. They took into account two effects expressed by macroscopic and microscopic memory functions in Mori's representation, but they got an expression for only autocorrelation spectra. Yi et al. reviewed the work by using the operator algebra technique.

Among the studies on cross-correlation spectra, the work of Nagano et al. draws attention of the present authors. Since it is based on Mori's memory function formalism, the derivation is somewhat complicated. In this paper, we shall show that the cross- and autocorrelation spectra can be obtained in a unified category by the operator algebra technique and that this method is simple and straightforward.

2. Operator algebra

For a state variable $a_0$ in a many-body system with Hamiltonian $H$, the time evolution in the Heisenberg representation is given by

$$a_0(t) = \exp(iHt) a_0(0) \exp(-iHt),$$

which is identical with

$$\frac{da_0(t)}{dt} = iLa_0(t),$$

where $L$ is the Liouville operator corresponding to $H$ and is assumed to be Hermitian, i.e.,

$$\langle LF \mid G \rangle = \langle F \mid LG \rangle$$

for arbitrary linear operators $F$ and $G$. Here $\langle A \mid B \rangle$ is the usual inner product and we use the units in which $\hbar = 1$.

We now define the $j$th order flux $a_j$ in terms of the zeroth flux $a_0$ as

$$a_j = \tilde{Q}_j^{-1} iLa_j^{-1} \quad (j = 1, 2, 3, \cdots),$$

where

$$\tilde{Q}_j = 1 - \tilde{P}_j,$$

for an arbitrary operator $X$ and for $k = 0, 1, 2, \cdots$. It is to be noted that Eq.(6) implies projection of $X$ onto the $a_k$ axis and $\tilde{Q}_jX$ means projection of $X$ onto the $(j+1)$ dimensional subspace spanned by the basis functions $a_0, a_1, \cdots, a_j$, which satisfy the orthogonality condition

$$\langle a_k \mid a_i \rangle = \delta_{ki},$$

were $k, l = 0, 1, 2, \cdots, j$.

We now consider the time evolution of the generalized flux variables $a_j(t)$ defined by

$$a_j(t) = \exp(iLt)a_j$$

or

$$\frac{da_j(t)}{dt} = iLa_j(t).$$

As will be clarified later, the information about the dynamical behavior of the system comes from the Laplace transform of Eq.(7), i.e.,

$$a_j(z) = \int_0^\infty \exp(-zt) \exp(iLt)a_j dt = (z - iL)^{-1} a_j.$$

Now it suffices to expand $(z - iL)^{-1}$ properly. The way of expansion depends on choosing the projection operators.

Among many operator identities, we choose $\tilde{P}_j + \tilde{Q}_j = 1$. Then we have (Appendix A)

$$(z - iL)^{-1} = \tilde{P}_j(z - iL)^{-1} + (z - \tilde{Q}_j iL)^{-1} \tilde{Q}_j$$

$$+ (z - \tilde{Q}_j iL)^{-1} \tilde{Q}_j iL \tilde{P}_j (z - iL)^{-1},$$

$$= \tilde{Q}_j (z - iL)^{-1} + (z - \tilde{P}_j iL)^{-1} \tilde{P}_j$$

$$+ (z - \tilde{P}_j iL)^{-1} \tilde{P}_j iL \tilde{Q}_j (z - iL)^{-1},$$

In order to proceed further we take into account the following properties:

$$\tilde{P}_j \tilde{P}_j = \tilde{P}_j = \tilde{P}_j \delta_{ij},$$

$$\tilde{P}_j \tilde{P}_m = \tilde{P}_j \quad (j \leq m),$$

$$\tilde{Q}_j \tilde{P}_j = 0,$$

$$\tilde{Q}_m \tilde{Q}_j = \tilde{Q}_j \quad (m < j),$$
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\[ P_{j-1}a_j = \bar{Q}_j a_j = 0, \quad (16) \]
\[ \bar{P}_j(z - \bar{P}_j L)^{-1} = (z - \bar{P}_j L)^{-1}. \quad (17) \]

In the following two sections we shall derive the expressions for cross- and autocorrelation spectra. The two spectra are defined in the following way. We consider projections of \( a_j(z) \) onto \( a_j \) and \( a_k(k \neq j) \), respectively, specified by

\[ P_j a_j(z) = \mathcal{E}_j(z) a_j, \quad (18) \]
\[ \mathcal{E}_j(z) = <a_j | a_j > <a_j | a_j>^{-1}, \quad (19) \]

and

\[ P_k a_j(z) = \mathcal{E}_k(z) a_k, \quad (20) \]
\[ \mathcal{E}_k(z) = <a_k | a_k > <a_k | a_k>^{-1}. \quad (21) \]

Here \( \mathcal{E}_j(z) \) and \( \mathcal{E}_k(z) \) are named the autocorrelation and the cross-correlation spectra, respectively.

3. Cross-Correlation

Now we shall derive the expression for the cross-correlation spectra using the operator properties introduced so far. We start with

\[ a_j(z) = (P_j + \bar{P}_{j-1} + \bar{Q}_j) a_j(z). \quad (22) \]

The first term of Eq. (22) becomes \( P_j a_j(z) = \mathcal{E}_j(z) a_j \) from Eq. (18). The second term of Eq. (22) becomes (Appendix B)

\[ \bar{P}_{j-1} a_j(z) = g_j(z) \mathcal{E}_j(z), \]

where

\[ g_j(z) = (z - \bar{P}_{j-1} i L)^{-1} g_j, \quad (23) \]
\[ g_j = \Delta j^{-1} a_j, \quad (24) \]
\[ \Delta j <a_j | a_j> <a_j | a_j>^{-1}. \quad (25) \]

By considering Eqs. (3), (5), (6), (11) – (17), the orthogonality condition and Eq. (24), \( g_j(z) \) can be changed as (Appendix C)

\[ g_j(z) = \psi_j(z) [a_{j-1} + g_{j-1}(z)], \quad (26) \]

where

\[ \psi_j(z) = <g_j(z) | g_j > <a_j | a_j>^{-1} \quad (27) \]

or

\[ g_j(z) = \psi_j(z) [a_{j-1} + (\psi_{j-2} a_{j-2} + g_{j-2}(z))] \]
\[ = \sum_{m=0}^{\infty} (-1)^m \psi_j(z) \psi_{j-1}(z) \]
\[ \cdot \cdot \cdot \psi_{m+1}(z) a_m \]
\[ = \sum_{m=0}^{\infty} \Lambda_{jm}(z) a_m, \quad (28) \]

where

\[ \Lambda_{jm}(z) = (-1)^m \psi_j(z) \psi_{m+1}(z) \quad (m = 0, 1, 2, \cdot \cdot \cdot, j - 1). \quad (29) \]

Similarly, the third term of Eq. (22) becomes

\[ \bar{Q}_j a_j(z) = (z - \bar{Q}_j i L)^{-1} \bar{Q}_j i L \bar{P}_j a_j(z) = f_j(z) \mathcal{E}_j(z), \quad (30) \]

where

\[ f_j(z) = (z - \bar{Q}_j i L)^{-1} f_j, \quad (31) \]
\[ f_j = \bar{Q}_j i L a_j. \quad (32) \]

By using Eqs. (3), (6), (10) – (17), and the orthogonality condition, \( f_j(z) \) can be changed as (Appendix D)

\[ f_j(z) = \Phi_j(z) [f_{j+1} + f_{j+1}(z)], \quad (33) \]

where

\[ \Phi_j(z) = <f_j | f_j > <a_{j+1} | a_{j+1}>^{-1} \quad (34) \]

or

\[ f_j(z) = \Phi_j(z) [f_i + \Phi_{j+1}(z) (f_{j+1} + f_{j+1}(z))]
\[ = \sum_{m=j+1}^{\infty} \Phi_j(z) \Phi_{j+1}(z) \cdots \Phi_{j+m-1}(z) f_{m-1} \]
\[ + \Phi_j(z) \Phi_{j+2}(z) \cdots \Phi_{j+m-1}(z) f_{m-1}
\[ = \sum_{m=j+1}^{\infty} \Phi_{j,m}(z) a_m + H_{jm}(z) a_m, \quad (35) \]

where

\[ H_{jm}(z) = \Phi_j(z) \Phi_{j+m}(z) \cdots \Phi_{j+m-1}(z) \quad (m \geq j + 1). \quad (36) \]

Adding up the first, second, and third terms of Eq. (22), we obtain
\[ a_j(z) = \mathcal{S}_{j}(z) \left[ a_j + \sum_{m=0}^{j} A_{jm}(z)a_m \right] \]
\[ = \mathcal{S}_{j}(z) \left[ a_j + \sum_{m=j+1}^{\infty} H_{jm}(z)a_m + H_{jj}(z)a_j \right]. \]

If we insert Eq. (37) into Eq. (21), we have
\[ \mathcal{E}_{j}(z) = \begin{cases} \mathcal{S}_{j}(z)A_{jk}(z) & (j > k), \\ \mathcal{S}_{j}(z)H_{jk}(z) & (j < k), \end{cases} \quad (39) \]

where \( A_{jk}(z) \) and \( H_{jk}(z) \) have been defined in Eqs. (29) and (36), respectively. We now see that Eq. (39) is identical with the result of Nagano et al.\textsuperscript{13} The explicit form for \( \mathcal{E}_{j}(z) \) will be dealt with in the next section.

### 4. Autocorrelation

The autocorrelation spectra \( \mathcal{E}_{j}(z) \) can be obtained from Eq. (8). The Laplace transform of Eq. (8) becomes
\[ -a_j(0) + z a_j(z) = (z - iL)^{-1} iL a_j. \quad (40) \]

The right-hand side of this expression can be rewritten as
\[ (z - iL)^{-1} iL a_j = (z - iL)^{-1} (P_j + \bar{P}_{j-1} + \bar{Q}_j)iL a_j, \quad (41) \]

each part of which is calculated as (Appendix E)
\[ (z - iL)^{-1} P_j L a_j = i \omega_j a_j(z), \quad (42) \]
\[ (z - iL)^{-1} P_{j-1} L a_j = g_j(z) - \psi_j(z)a_j(z), \quad (43) \]
\[ (z - iL)^{-1} \bar{Q}_j L a_j = f_j(z) - \phi_j(z)a_j(z), \quad (44) \]

where
\[ \omega_j = \langle L a_j | a_j \rangle \langle a_j | a_j \rangle^{-1}, \quad (45) \]
\[ \psi_j(z) = \langle f_j(z) | f_j \rangle \langle a_j | a_j \rangle^{-1} \quad (46) \]
\[ \phi_j(z) = \Phi_j(z) \Delta_j^{\ast} + 1, \quad (47) \]
and \( g_j(z) \), \( \psi_j(z) \), \( f_j(z) \), and \( \Phi_j(z) \) have been defined in Eqs. (23), (27), (31), and (34), respectively. Inserting Eqs. (42), (43), and (44) into Eq. (41) we have, from Eq. (40),
\[ a_j(z) = [z - i \omega_j + \psi_j(z) + \phi_j(z)]^{-1} \times (a_j + g_j(z) + f_j(z)). \quad (48) \]

Comparing Eq. (37) with Eq. (48), we have
\[ \mathcal{E}_{j}(z) = [z - i \omega_j + \psi_j(z) + \phi_j(z)]^{-1}, \quad (49) \]

which is identical with the result of Karasudani et al.\textsuperscript{11}

### 5. Conclusion

So far we have shown that the cross- and autocorrelation spectra can be easily dealt with in a unified category by using the operator algebra technique. We may claim that this method is simple since the procedure is straightforward. The autocorrelation with one or two fluctuating forces is involved in calculating lineshapes and critical slowing downs in electronic and electron phonon systems\textsuperscript{11-10}. The methods of Mori\textsuperscript{9} and of Nagano et al.\textsuperscript{13} have been successfully utilized in those problems. Thus we may expect that theoretical investigation of the cross-correlation spectra can also be easily carried out if we use this method effectively.

### Appendix A: Proof of Eqs.(10) and (11)

Here \((z - iL)^{-1}\) can be expanded as
\[ (z - iL)^{-1} = z^{-1} \left( 1 - i \frac{\bar{P}_j + \bar{Q}_j}{z} \right)^{-1} \]
\[ = z^{-1} \sum_{n=0}^{\infty} \left( i \frac{\bar{P}_j + \bar{Q}_j}{z} \right)^n \]
\[ = z^{-1} (\bar{P}_j + \bar{Q}_j) + z^{-2} (\bar{P}_j + \bar{Q}_j)^2 + \cdots \]
\[ = (P_j L P_j L + \bar{P}_j L \bar{Q}_j L + \bar{Q}_j L P_j L + \bar{Q}_j L \bar{Q}_j L) \cdots. \quad (A1) \]

By using \( \bar{Q}_j L = \bar{Q}_j L (\bar{P}_j + \bar{Q}_j) \) and \( \bar{P}_j L = (1 - \bar{Q}_j) \)
\( iL \), we have
\[ (z - iL)^{-1} = z^{-1} \bar{P}_j [1 + z^{-1} (iL) + z^{-2} (iL)^{-2} + \cdots] \]
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\[ +z^{-1}\left[1+z^{-1}(\tilde{Q}_iL)^{q_1}+z^{-1}(\tilde{Q}_iL)^{q_2}+\cdots+\tilde{Q}_i\right] \]

\[ +z^{-1}\left[\sum_{i=0}^{\infty}\sum_{m=0}^{\infty}(z^{-m})^{-1}(\tilde{Q}_iL)^{q_1}iLP_s(z^{-m})\tilde{Q}_i\right] \]

\[ =\tilde{P}_j\left[z^{-1}\sum_{m=0}^{\infty}\left(\frac{IL}{z}\right)^m\right] +\left[z^{-1}\sum_{i=0}^{\infty}\left(\frac{\tilde{Q}_iL}{z}\right)^m\right] \]

\[ +\left[z^{-1}\sum_{i=0}^{\infty}\left(\frac{\tilde{Q}_iL}{z}\right)^m\right] \tilde{Q}_iLP_s\left[z^{-1}\sum_{m=0}^{\infty}\left(\frac{IL}{z}\right)^m\right] \]

\[ =\tilde{P}_j(z-iL)^{-1} +\left(z - \tilde{Q}_iL\right)^{-1}\tilde{Q}_i \]

\[ +\left(z - \tilde{Q}_iL\right)^{-1}\tilde{Q}_iLP_s(z-iL)^{-1}. \]

Similarly,

\[ (z-iL)^{-1} = \tilde{Q}_i(z-iL)^{-1} + (z - \tilde{Q}_iL)^{-1} \tilde{P}_j \]

\[ + (z - \tilde{P}_jL)^{-1} \tilde{P}_jL\tilde{Q}_i(z-iL)^{-1} \]

\[ = (z-iL)^{-1}\tilde{Q}_i + (z - \tilde{Q}_iL)^{-1} \tilde{P}_j \]

\[ + (z - iL)^{-1} \tilde{Q}_iLP_s(z-iL)^{-1} \]

\[ = (z-iL)^{-1}\tilde{P}_j + (z - \tilde{Q}_iL)^{-1} \tilde{Q}_i \]

\[ + (z - iL)^{-1} \tilde{P}_jL\tilde{Q}_i(z-iL)^{-1}. \]

**Appendix B : Derivation of the second term in Eq.(22)**

Here \( \tilde{P}_j = (z-iL)\tilde{Q}_i(z-iL)^{-1} + (z - \tilde{Q}_iL)^{-1} \tilde{P}_j \)

\[ + (z - \tilde{P}_jL)^{-1} \tilde{P}_jL\tilde{Q}_i(z-iL)^{-1} \]

by using Eq. (11). By taking into account Eqs. (12) – (16), we have

\[ \tilde{P}_j - 1\tilde{Q}_i(z-iL)^{-1} + (z - \tilde{Q}_iL)^{-1} \tilde{P}_j \]

\[ + (z - \tilde{P}_jL)^{-1} \tilde{P}_jL\tilde{Q}_i(z-iL)^{-1} \]

\[ = (z-iL)^{-1}\tilde{Q}_i + (z - \tilde{Q}_iL)^{-1} \tilde{P}_j \]

\[ + (z - iL)^{-1} \tilde{Q}_iLP_s(z-iL)^{-1} \]

\[ <a_m|a_m>\] and Eq. (3), we obtain

\[ \tilde{P}_j - 1\tilde{Q}_i(z-iL)^{-1} \tilde{Q}_i(z-iL)^{-1} <a_j|a_j> \]

\[ <a_{j-1}|a_{j-1}> <a_j|a_j> \]

**Appendix C : Derivation of Eq. (26)**

Here \( g(z) \) can be changed as

\[ g(z) = (z - \tilde{P}_jL)^{-1} g_j = \tilde{P}_j - 1(z - \tilde{P}_jL)^{-1} g_j \]

\[ = (\tilde{P}_j - 1 + \tilde{P}_j - 2) g_j(z), \]

by using Eq. (17).

The first term of Eq. (C1) becomes

\[ \tilde{P}_j - 1 g_j(z) = <g(z)|a_{j-1}> <a_{j-1}|a_{j-1}> <a_{j-1}|z-iL|a_{j-1}> \]

\[ = <g(z)|(-\frac{\Delta_j}{a_{j-1}}) <a_{j-1}|a_{j-1}> <a_{j-1}|z-iL|a_{j-1}> \]

\[ = \psi_j(z) g_j. \]

The second term of Eq. (C1) becomes

\[ \tilde{P}_j - 2 g_j(z) = \tilde{P}_j - 1(z - \tilde{P}_jL)^{-1} g_j \]

\[ = \tilde{P}_j - 1(z - \tilde{P}_jL)^{-1} g_j \]

by using Eqs. (11) – (14), (16), and (17), or

\[ \tilde{P}_j - 1 g_j(z) = \tilde{P}_j - 1(z - \tilde{P}_jL)^{-1} \tilde{Q}_i(z-iL)^{-1} g_j(z) \]

\[ = (z - \tilde{P}_jL)^{-1} \sum_{m=0}^{\infty} <iL\tilde{Q}_i(z-iL)^{-1} a_m|a_m> \]

\[ <a_m|a_m> \]

or

\[ \tilde{P}_j - 1 g_j(z) = (z - \tilde{P}_jL)^{-1} <g(z)|a_{j-1}> \]

\[ <a_{j-2}|a_{j-2}> <a_{j-2}|z-iL|a_{j-2}> \]

\[ = (-\frac{\Delta_j}{a_{j-2}}) <a_{j-2}|z-iL|a_{j-2}> \]

\[ = (-\frac{\Delta_j}{a_{j-2}}) <a_{j-2}|z-iL|a_{j-2}> \]

\[ = (-\frac{\Delta_j}{a_{j-2}}) <a_{j-2}|z-iL|a_{j-2}> \]

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\[ = (-\frac{\Delta_j}{a_{j-2}}) <a_{j-2}|z-iL|a_{j-2}> \]

\[ = (-\frac{\Delta_j}{a_{j-2}}) <a_{j-2}|z-iL|a_{j-2}> \]

\[ = (-\frac{\Delta_j}{a_{j-2}}) <a_{j-2}|z-iL|a_{j-2}> \]
By using Eq. (24) and E. (27) we have
\[ \tilde{P}_j \cdot \tilde{g}(z) = \tilde{\psi}(z)(z - \tilde{P}_j - \tilde{q}L) \cdot \tilde{g}_{j-1} = \tilde{\psi}(z) \tilde{g}(z). \]

From Eqs. (C2) and (C3) we obtain
\[ \tilde{g}(z) = \tilde{\psi}(z)(\tilde{a}_j-2 + \tilde{g}_{j-1}(z)). \]

**Appendix D: Derivation of Eq. (33)**

Here \( f_j(z) \) can be changed as
\[ f_j(z) = (z - \tilde{Q}iL)^{-1} f_j = (P_j + i\tilde{P}) f_j, \]
\[ = f_j(z)(\tilde{a}_j+1) <a_{j+1}|a_j>, \]
\[ = f_j(z) f_j, \]
\[ = f_j(z)(\tilde{a}_j+1) <a_{j+1}|a_j>, \]
\[ = f_j(z) f_j, \]
\[ = \Phi(z)(z - \tilde{Q}_j + iL) - \tilde{Q}_j + iL \Phi f_j = \Phi(z) f_j, \]
\[ \text{by using Eqs. (15) and (32). From Eqs. (D2) and (D3) we have} \]
\[ f_j(z) = \Phi(z)(f_j + f_{j+1}(z)). \]

**Appendix E: Derivation of Eqs. (42) – (44)**

we start with the identity
\[ (z - iL)^{-1} \tilde{L} a_j = (z - iL)^{-1} (P_j + \tilde{P}_j - iL) \tilde{L} a_j. \]

The first term of Eq. (E1) becomes
\[ (z - iL)^{-1} \tilde{L} a_j = (z - iL)^{-1} \tilde{L} a_j = (z - iL)^{-1} \tilde{L} a_j. \]

The second term of Eq. (E1) becomes
\[ (z - iL)^{-1} \tilde{P}_j - iL a_j = (z - iL)^{-1} \tilde{P}_j - iL a_j. \]

by using Eqs. (A2). Taking into account \( \tilde{P}_j - iL a_j = -\Delta \tilde{a}_j - 1 \) and using Eqs. (11), (23), and (27), we have
\[ \tilde{P}_j - iL a_j = z - iL)^{-1} \tilde{Q}_j - iL \tilde{P}_j - iL a_j = \sum_{m=0}^{\infty} g(z) |a_m><a_m| \]
\[ = g(z) - (z - iL)^{-1} \tilde{Q}_j - iL g(z). \]

The third term of Eq. (E1) becomes
\[ (z - iL)^{-1} \tilde{Q}_j - iL a_j = (z - iL)^{-1} \tilde{Q}_j - iL a_j. \]

by using Eqs. (A3), (3) and (32).

**References**

6. S. W. Lovesey, Condensed Matter Physics;
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Dynamic Correlations (Benjamin, New York, 1980).

7) D. Forster, Hydrodynamic Fluctuations, Broken Symmetry and Correlation Functions (Benjamin, New York, 1975).


