

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 variables¹⁻⁷. 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^{6,7}. 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 variable². Mori presented a projection operator technique and obtained an expression for the Laplace trans-

form of an autocorrelation function as a continued fraction representation³. 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 space⁴. Lee got the representation by utilizing the recurrence relation method⁵. Yi *et al.* used the so – called operator algebra method in getting the representation⁹. 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 work³. 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 fluctuating 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*⁹⁾. 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 technique¹⁰⁾.

Among the studies on cross - correlation spectra, the work of Nagano *et al.* draws attention of the present authors¹¹⁾. 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 Heisenberg representation is given by

$$a_0(t) = \exp(iHt) a_0(0) \exp(-iHt), \quad (1)$$

which is identical with

$$\frac{da_0(t)}{dt} = iLa_0(t), \quad (2)$$

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

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

for arbitrary linear operators F and G . Here $\langle A | B \rangle$ 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

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

where

$$\tilde{Q}_j = 1 - \tilde{P}_j, \quad (4)$$

$$\tilde{P}_j \equiv \sum_{m=0}^j P_m = P_j + \tilde{P}_j - 1, \quad (5)$$

$$P_k X \equiv \langle X | a_k \rangle \langle a_k | a_k \rangle^{-1} a_k \quad (6)$$

for an arbitrary operator X and for $k = 0, 1, 2, \dots$. It is to be noted that Eq.(6) implies projection of X onto the a_k axis and $\tilde{P}_j X$ means projection of X onto the $(j+1)$ dimensional subspace spanned by the basis functions a_0, a_1, \dots, a_j , which satisfy the orthogonality condition $\langle a_k | a_l \rangle = \delta_{kl}$, where $k, l = 0, 1, 2, \dots, j$.

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

$$a_j(t) = \exp(iLt) a_j \quad (7)$$

or

$$\frac{da_j(t)}{dt} = iLa_j(t). \quad (8)$$

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

$$a_j(z) \equiv \int_0^\infty \exp(-zt) \exp(iLt) a_j dt = (z - iL)^{-1} a_j. \quad (9)$$

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)

$$(z - iL)^{-1} = \tilde{P}_j (z - iL)^{-1} + (z - \tilde{Q}_j iL)^{-1} \tilde{Q}_j + (z - \tilde{Q}_j iL)^{-1} \tilde{Q}_j iL \tilde{P}_j (z - iL)^{-1}, \quad (10)$$

$$= \tilde{Q}_j (z - iL)^{-1} + (z - \tilde{P}_j iL)^{-1} \tilde{P}_j + (z - \tilde{P}_j iL)^{-1} \tilde{P}_j iL \tilde{Q}_j (z - iL)^{-1} \quad (11)$$

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

$$P_i P_j = P_j P_i = P_i \delta_{ij}, \quad (12)$$

$$\tilde{P}_j \tilde{P}_m = \tilde{P}_j \quad (j \leq m), \quad (13)$$

$$\tilde{Q}_j \tilde{P}_j = 0, \quad (14)$$

$$\tilde{Q}_j \tilde{Q}_m = \tilde{Q}_j \quad (m < j), \quad (15)$$

$$\bar{P}_{j-1}a_j = \bar{Q}_j a_j = 0, \quad (16) \quad \psi_j(z) \equiv \langle g_i(z) | g_j \rangle \langle a_j | a_j \rangle^{-1} \quad (27)$$

$$\bar{P}_j(z - \bar{P}_j iL)^{-1} = (z - \bar{P}_j iL)^{-1}. \quad (17)$$

or

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

$$\begin{aligned} g_i(z) &= \psi_j(z)[a_{j-1} + (-\psi_{j-2}(a_{j-2} + g_{j-2}(z)))] \\ &= \sum_{m=0}^{j-1} (-1)^m \psi_j(z) \psi_{j-1}(z) \\ &\quad \cdots \psi_{m+2}(z) \psi_{m+1}(z) a_m \\ &= \sum_{m=0}^{j-1} A_{jm}(z) a_m, \end{aligned} \quad (28)$$

$$P_j a_j(z) = \mathcal{E}_{ij}(z) a_j, \quad (18)$$

$$\mathcal{E}_{ij}(z) = \langle a_j(z) | a_j \rangle \langle a_j | a_j \rangle^{-1}, \quad (19)$$

where

$$\begin{aligned} A_{jm}(z) &\equiv (-1)^m \psi_j(z) \psi_{j-1}(z) \cdots \psi_{m+1}(z) \\ (m=0, 1, 2, \dots, j-1). \end{aligned} \quad (29)$$

and

$$P_k a_j(z) = \mathcal{E}_{jk}(z) a_k \quad (20)$$

$$\mathcal{E}_{jk}(z) \equiv \langle a_j(z) | a_k \rangle \langle a_k | a_k \rangle^{-1}. \quad (21)$$

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

$$\bar{Q}_j a_j(z) = (z - \bar{Q}_j iL)^{-1} \bar{Q}_j iL \bar{P}_j a_j(z) = f_j(z) \mathcal{E}_{ij}(z), \quad (30)$$

Here $\mathcal{E}_{ij}(z)$ and $\mathcal{E}_{ik}(z)$ are named the autocorrelation and the cross-correlation spectra, respectively.

where

$$f_j(z) \equiv (z - \bar{Q}_j iL)^{-1} f_j, \quad (31)$$

$$f_j \equiv \bar{Q}_j iL a_j. \quad (32)$$

3. Cross - Correlation

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

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

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

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

where

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

$$\Phi_j(z) \equiv \langle f_j | f_j \rangle \langle a_{j+1} | a_{j+1} \rangle^{-1} \quad (34)$$

or

$$\bar{P}_{j-1} a_j(z) = g_j(z) \mathcal{E}_{ij}(z),$$

where

$$g_j(z) \equiv (z - \bar{P}_{j-1} iL)^{-1} g_j, \quad (23)$$

$$g_j \equiv -\Delta_j^2 a_{j-1}, \quad (24)$$

$$\Delta_j^2 \equiv \langle a_j | a_j \rangle \langle a_{j-1} | a_{j-1} \rangle^{-1}. \quad (25)$$

$$\begin{aligned} f_i(z) &= \Phi_j(z) [f_i + \Phi_{j+1}(z) (f_{j+1} + f_{j+2}(z))] \\ &= \sum_{m=j+1}^{n-1} \Phi_j(z) \Phi_{j+2}(z) \cdots \Phi_{m-1}(z) f_{m-1} \\ &\quad + \Phi_j(z) \Phi_{j+2}(z) \cdots \Phi_{n-1}(z) f_{n-1} \\ &= \sum_{m=j+1}^{n-1} H_{jm}(z) a_m + H_{jn}(z) a_n, \end{aligned} \quad (35)$$

where

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

$$H_{jm}(z) \equiv \Phi_j(z) \Phi_{j+2}(z) \cdots \Phi_{m-1}(z) \quad (m \geq j+1). \quad (36)$$

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

where

Adding up the first, second, and third terms of Eq. (22), we obtain

$$a_j(z) = \mathcal{E}_{ij}(z) [a_j + g_j(z) + f_j(z)] \quad (37)$$

$$= \mathcal{E}_{ij}(z) \left[a_j + \sum_{m=0}^{j-1} A_{jm}(z) a_m + \sum_{m=j+1}^{j-1} H_{jm}(z) a_m + H_{jn}(z) a_n \right]. \quad (38)$$

If we insert Eq. (37) into Eq. (21), we have

$$\mathcal{E}_{jk}(z) = \begin{cases} \mathcal{E}_{ij}(z) A_{jk}(z) & (j > k), \\ \mathcal{E}_{ij}(z) H_{jk}(z) & (j < k), \end{cases} \quad (39)$$

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.*¹¹ The explicit form for $\mathcal{E}_{ij}(z)$ will be dealt with in the next section.

4. Autocorrelation

The autocorrelation spectra $\mathcal{E}_{ij}(z)$ can be obtained from Eq. (8). The Laplace transform of Eq. (8) becomes

$$-a_j(0) + za_j(z) = (z - iL)^{-1} iLa_j. \quad (40)$$

The right-hand side of this expression can be rewritten as

$$(z - iL)^{-1} iLa_j = (z - iL)^{-1} (P_j + \tilde{P}_{j-1} + \tilde{Q}_j) iLa_j, \quad (41)$$

each part of which is calculated as (Appendix E)

$$(z - iL)^{-1} P_j iLa_j = i\omega_j a_j(z), \quad (42)$$

$$(z - iL)^{-1} \tilde{P}_{j-1} iLa_j = g_j(z) - \psi_j(z) a_j(z), \quad (43)$$

$$(z - iL)^{-1} \tilde{Q}_j iLa_j = f_j(z) - \phi_j(z) a_j(z), \quad (44)$$

where

$$\omega_j \equiv \langle La_j | a_j \rangle \langle a_j | a_j \rangle^{-1}, \quad (45)$$

$$\phi_j(z) \equiv \langle f_i(z) | f_i \rangle \langle a_j | a_j \rangle^{-1} \quad (46)$$

$$= \Phi_j(z) \Delta_j^2, \quad (47)$$

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

$$\mathcal{E}_{ij}(z) = [z - i\omega_j + \psi_j(z) + \phi_j(z)]^{-1}, \quad (49)$$

which is identical with the result of Karasudani *et al.*⁹⁾

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 systems¹¹⁻¹⁸⁾. The methods of Mori⁹⁾ and of Nagano *et al.*¹¹⁾ 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

$$\begin{aligned} (z - iL)^{-1} &= z^{-1} \left(1 - i(\tilde{P}_j + \tilde{Q}_j) \frac{L}{z} \right)^{-1} \\ &= z^{-1} \sum_{n=0}^{\infty} \left(\frac{i(\tilde{P}_j L + \tilde{Q}_j L)}{z} \right)^n \\ &= z^{-1} (\tilde{P}_j + \tilde{Q}_j) + z^{-2} i(\tilde{P}_j L + \tilde{Q}_j L) + z^{-3} i^2 \\ &\quad (\tilde{P}_j L \tilde{P}_j L + \tilde{P}_j L \tilde{Q}_j L + \tilde{Q}_j L \tilde{P}_j L \\ &\quad + \tilde{Q}_j L \tilde{Q}_j L) \cdots. \end{aligned} \quad (A1)$$

By using $\tilde{Q}_j iL = \tilde{Q}_j iL(\tilde{P}_j + \tilde{Q}_j)$ and $\tilde{P}_j iL = (1 - \tilde{Q}_j) iL$, we have

$$(z - iL)^{-1} = z^{-1} \tilde{P}_j [1 + z^{-1} iL + z^{-2} (iL)^2 + \cdots]$$

$$\begin{aligned}
 & +z^{-1}[1+z^{-1}(\tilde{Q}_j iL)^1+z^{-2}(\tilde{Q}_j iL)^2+\dots]\tilde{Q}_j \\
 & +z^{-1}\left[\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}(z^{+m})^{-1}(\tilde{Q}_j iL)^l\tilde{Q}_j iLP_j(iL)^m\right] \\
 & =\tilde{P}_j\left[z^{-1}\sum_{m=0}^{\infty}\left(\frac{iL}{z}\right)^m\right]+\left[z^{-1}\sum_{l=0}^{\infty}\left(\frac{\tilde{Q}_j iL}{z}\right)^l\right]\tilde{Q}_j \\
 & +\left[z^{-1}\sum_{l=0}^{\infty}\left(\frac{\tilde{Q}_j iL}{z}\right)^l\right]\tilde{Q}_j iLP_j\left[z^{-1}\sum_{m=0}^{\infty}\left(\frac{iL}{z}\right)^m\right] \\
 & =\tilde{P}_j(z-iL)^{-1}+(z-\tilde{Q}_j iL)^{-1}\tilde{Q}_j \\
 & +(z-\tilde{Q}_j iL)^{-1}\tilde{Q}_j iLP_j(z-iL)^{-1}.
 \end{aligned}$$

Similarly,

$$\begin{aligned}
 (z-iL)^{-1} & =\tilde{Q}_j(z-iL)^{-1}+(z-\tilde{P}_j iL)^{-1}\tilde{P}_j \\
 & +(z-\tilde{P}_j iL)^{-1}\tilde{P}_j iL\tilde{Q}_j(z-iL)^{-1} \quad (11)
 \end{aligned}$$

$$\begin{aligned}
 & =(z-iL)^{-1}\tilde{Q}_j+(z-\tilde{P}_j iL)^{-1}\tilde{P}_j \\
 & +(z-iL)^{-1}\tilde{Q}_j iL\tilde{P}_j(z-\tilde{P}_j iL)^{-1} \quad (A2)
 \end{aligned}$$

$$\begin{aligned}
 & =(z-iL)^{-1}\tilde{P}_j+(z-\tilde{Q}_j iL)^{-1}\tilde{Q}_j \\
 & +(z-iL)^{-1}\tilde{P}_j iL\tilde{Q}_j(z-\tilde{Q}_j iL)^{-1} \quad (A3)
 \end{aligned}$$

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

Here $\tilde{P}_{j-1}(z)a_j(z)$ can be changed as

$$\begin{aligned}
 \tilde{P}_{j-1}^{-1}a_j(z) & =\tilde{P}_{j-1}^{-1}[\tilde{Q}_{j-1}(z-iL)^{-1}+(z-\tilde{P}_{j-1}iL)^{-1}\tilde{P}_{j-1}] \\
 & +(z-\tilde{P}_{j-1}iL)^{-1}\tilde{P}_{j-1}iL\tilde{Q}_{j-1}(z-iL)^{-1}a_j, \quad (B1)
 \end{aligned}$$

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

$$\begin{aligned}
 \tilde{P}_{j-1}^{-1}a_j(z) & =(z-\tilde{P}_{j-1}iL)^{-1}\tilde{P}_{j-1}iL\tilde{Q}_{j-1}(z-iL)^{-1}a_j \\
 & =(z-\tilde{P}_{j-1}iL)^{-1}\sum_{m=0}^{j-1}P_m iL\tilde{Q}_{j-1}a_j(z) \\
 & =(z-\tilde{P}_{j-1}iL)^{-1}\sum_{m=0}^{j-1}\langle iL\tilde{Q}_{j-1}a_j(z)|a_m\rangle \\
 & \quad \langle a_m|a_m\rangle^{-1}a_m \\
 & =-(z-\tilde{P}_{j-1}iL)^{-1}\sum_{m=0}^{j-1}\langle a_j(z)|\tilde{Q}_{j-1}iLa_m\rangle \\
 & \quad \langle a_m|a_m\rangle^{-1}a_m
 \end{aligned}$$

By considering $\langle a_k|a_l\rangle = \sigma_{kl}$ and Eq. (3), we obtain

$$\begin{aligned}
 \tilde{P}_{j-1}^{-1}a_j(z) & =-(z-\tilde{P}_{j-1}iL)^{-1}\mathcal{E}_{jj}(z)\langle a_j|a_j\rangle \\
 & \quad \langle a_{j-1}|a_{j-1}\rangle^{-1}a_{j-1}.
 \end{aligned}$$

Appendix C : Derivation of Eq. (26)

Here $g_j(z)$ can be changed as

$$\begin{aligned}
 g_i(z) & =(z-\tilde{P}_{j-1}iL)^{-1}g_i=\tilde{P}_{j-1}(z-\tilde{P}_{j-1}iL)^{-1}g_j \\
 & =(P_{j-1}+\tilde{P}_{j-2})g_i(z), \quad (C1)
 \end{aligned}$$

by using Eq. (17)

The first term of Eq. (C1) becomes

$$\begin{aligned}
 P_{j-1}g_j(z) & =\langle g_j(z)|a_{j-1}\rangle\langle a_{j-1}|a_{j-1}\rangle^{-1}a_{j-1} \\
 & =\langle g_j(z)|(-\Delta_j^3)a_{j-1}\rangle\langle a_{j-1}|a_{j-1}\rangle^{-1} \\
 & \quad (-\Delta_j^2)^{-1}a_{j-1} \\
 & =\langle g_j(z)|g_i\rangle\langle a_j|a_j\rangle^{-1}\langle a_j|a_j\rangle \\
 & \quad \langle a_{j-1}|a_{j-1}\rangle^{-1}(-\Delta_j^3)^{-1}a_{j-1} \\
 & =\Psi_j(z)g_j. \quad (C2)
 \end{aligned}$$

The second term of Eq. (C1) becomes

$$\begin{aligned}
 \tilde{P}_{j-2}g_i(z) & =\tilde{P}_{j-2}(z-\tilde{P}_{j-1}iL)^{-1}g_j \\
 & =\tilde{P}_{j-2}[\tilde{Q}_{j-2}(z-\tilde{P}_{j-1}iL)^{-1} \\
 & \quad +(z-\tilde{P}_{j-2}\tilde{P}_{j-1}iL)^{-1}\tilde{P}_{j-2} \\
 & \quad +(z-\tilde{P}_{j-2}\tilde{P}_{j-1}iL)^{-1}\tilde{P}_{j-2}\tilde{P}_{j-1}iL\tilde{Q}_{j-2} \\
 & \quad (z-\tilde{P}_{j-1}iL)^{-1}]g_j \\
 & =\tilde{P}_{j-2}(z-\tilde{P}_{j-2}iL)^{-1}\tilde{P}_{j-2}iL\tilde{Q}_{j-2} \\
 & \quad (z-\tilde{P}_{j-1}iL)^{-1}g_j,
 \end{aligned}$$

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

$$\begin{aligned}
 \tilde{P}_{j-2}g_j(z) & =(z-\tilde{P}_{j-2}iL)^{-1}\tilde{P}_{j-2}iL\tilde{Q}_{j-2}g_j(z) \\
 & =(z-\tilde{P}_{j-2}iL)^{-1}\sum_{m=0}^{j-2}\langle iL\tilde{Q}_{j-2}g_j(z)|a_m\rangle \\
 & \quad \langle a_m|a_m\rangle^{-1}a_m \\
 & =-(z-\tilde{P}_{j-2}iL)^{-1}\sum_{m=0}^{j-2} \\
 & \quad \langle g_j(z)|\tilde{Q}_{j-2}iLa_m\rangle\langle a_m|a_m\rangle^{-1}a_m
 \end{aligned}$$

or

$$\begin{aligned}
 \tilde{P}_{j-2}g_j(z) & =-(z-\tilde{P}_{j-2}iL)^{-1}\langle g_j(z)|a_{j-1}\rangle \\
 & \quad \langle a_{j-2}|a_{j-2}\rangle^{-1}a_{j-2} \\
 & =-(z-\tilde{P}_{j-2}iL)^{-1}\langle g_i(z)|(-\Delta_j^3)a_{j-1}\rangle \\
 & \quad \langle a_j|a_j\rangle^{-1}\langle a_j|a_j\rangle\langle a_{j-1}|a_{j-1}\rangle^{-1} \\
 & \quad \times\langle a_{j-1}|a_{j-1}\rangle\langle a_{j-2}|a_{j-2}\rangle^{-1} \\
 & \quad (-\Delta_j^2)^{-1}a_{j-2} \\
 & =-(z-\tilde{P}_{j-2}iL)^{-1}\langle g_i(z)|g_j\rangle\langle a_j|a_j\rangle^{-1} \\
 & \quad \Delta_j^2(\Delta_{j-1}^2)(-\Delta_j^3)^{-1}a_{j-2} \\
 & =-(z-\tilde{P}_{j-2}iL)^{-1}\langle g_i(z)|g_j\rangle\langle a_j|a_j\rangle^{-1}
 \end{aligned}$$

$$(-\Delta_j^2)a_{j-2}. \quad (C3)$$

By using Eq. (24) and E. (27) we have

$$\tilde{P}_{j-2}g_j(z) = \psi_j(z)(z - P_{j-2}iL)^{-1}g_{j-1} = \psi_j(z)g_i(z).$$

From Eqs. (C2) and (C3) we obtain

$$g_i(z) = \psi_j(z)[a_{j-2} + g_{j-1}(z)].$$

Appendix D : Derivation of Eq. (33)

Here $f_j(z)$ can be changed as

$$\begin{aligned} f_j(z) &\equiv (z - \tilde{Q}_j iL)^{-1} f_j \\ &= [\tilde{P}_{j+1}(z - \tilde{Q}_j iL)^{-1} + (z - \tilde{Q}_{j+1} \tilde{Q}_j iL)^{-1} \tilde{Q}_{j+1} \\ &\quad + (z - \tilde{Q}_{j+1} \tilde{Q}_j iL)^{-1} \tilde{Q}_{j+1} \tilde{Q}_j iL \tilde{P}_{j+1} (z - \tilde{Q}_j iL)^{-1}] f_j \\ &= [\tilde{P}_{j+1}(z - \tilde{Q}_j iL)^{-1} + (z - \tilde{Q}_{j+1} iL)^{-1} \tilde{Q}_{j+1} iL \tilde{P}_{j+1} \\ &\quad (z - \tilde{Q}_j iL)^{-1}] f_j \end{aligned} \quad (D1)$$

by using Eq. (15) and the property $\tilde{Q}_{j+1} f_j = 0$.

The first term of Eq. (D1) becomes

$$\begin{aligned} \tilde{P}_{j+1}(z - \tilde{Q}_j iL)^{-1} f_j &= (P_{j+1} \tilde{P}_j) f_j(z) = P_{j+1} f_j(z) \\ &= \langle f_j(z) | a_{j+1} \rangle \langle a_{j+1} | a_{j+1} \rangle^{-1} a_{j+1} \\ &= \langle f_j(z) | f_j \rangle \langle f_j | f_j \rangle^{-1} f_j = \Phi_j(z) f_j. \end{aligned} \quad (D2)$$

The second term of Eq. (D1) becomes

$$\begin{aligned} (z - \tilde{Q}_{j+1} iL)^{-1} \tilde{Q}_{j+1} iL \tilde{P}_{j+1} (z - \tilde{Q}_j iL)^{-1} f_j \\ = (z - \tilde{Q}_{j+1} iL)^{-1} \tilde{Q}_{j+1} iL \Phi_j(z) f_j \\ = \Phi_j(z) (z - \tilde{Q}_{j+1} iL)^{-1} \tilde{Q}_{j+1} iL f_j = \Phi_j(z) f_{j+1}(z) \end{aligned} \quad (D3)$$

by using Eqs. (15) and (32). From Eqs. (D2) and (D3) we have

$$f_j(z) = \Phi_j(z) [f_j + f_{j+1}(z)].$$

Appendix E : Derivation of Eqs. (42) - (44)

we start with the identity

$$(z - iL)^{-1} iL a_j = (z - iL)^{-1} (P_j + \tilde{P}_{j-1} + \tilde{Q}_j) iL a_j. \quad (E1)$$

The first term of Eq. (E1) becomes

$$\begin{aligned} (z - iL)^{-1} P_j iL a_j &= (z - iL)^{-1} \langle iL a_j | a_j \rangle \langle a_j | a_j \rangle^{-1} a_j \\ &= (z - iL)^{-1} i\omega_j a_j = i\omega_j a_j(z) \end{aligned}$$

by using Eqs. (15) and (44). The second term of Eq. (E1) becomes

$$\begin{aligned} (z - iL)^{-1} \tilde{P}_{j-1} iL a_j \\ = [(z - iL)^{-1} \tilde{Q}_{j-1} + (z - \tilde{P}_{j-1} iL)^{-1} \tilde{P}_{j-1} \\ + (z - iL)^{-1} \tilde{Q}_{j-1} iL \tilde{P}_{j-1} (z - \tilde{P}_{j-1} iL)^{-1}] \tilde{P}_{j-1} iL a_j \end{aligned}$$

by using Eq. (A2). Taking into account $\tilde{P}_{j-1} iL a_j = -\Delta_j^2 a_{j-1}$ and using Eqs. (11), (23), and (27), we have

$$\begin{aligned} \tilde{P}_{j-1} iL a_j(z) &= g_j(z) + (z - iL)^{-1} \tilde{Q}_{j-1} iL \tilde{P}_{j-1} g_j(z) \\ &= g_j(z) + (z - iL)^{-1} \tilde{Q}_{j-1} iL \sum_{m=0}^{j-1} \langle g_j(z) | a_m \rangle \\ &\quad \langle a_m | a_m \rangle^{-1} a_m \\ &= g_j(z) - (z - iL)^{-1} \tilde{Q}_{j-1} iL \langle g_j(z) | (-\Delta_j^2) a_{j-1} \rangle \\ &\quad \langle a_j | a_j \rangle^{-1} a_{j-1} = g_j(z) - \psi_j(z) a_j(z). \end{aligned}$$

The third term of Eq. (E1) becomes

$$\begin{aligned} (z - iL)^{-1} \tilde{Q}_j iL a_j &= [(z - iL)^{-1} \tilde{P}_j + (z - \tilde{Q}_j iL)^{-1} \tilde{Q}_j \\ &\quad + (z - iL) \tilde{P}_j iL \tilde{Q}_j (z - \tilde{Q}_j iL)^{-1}] \tilde{Q}_j iL a_j \\ &= f_j(z) + (z - iL)^{-1} \tilde{P}_j iL f_j(z) \\ &= f_j(z) + (z - iL)^{-1} \sum_{m=0}^j \langle iL f_j(z) | a_m \rangle \langle a_m | a_m \rangle^{-1} a_m \\ &= f_j(z) - (z - iL)^{-1} \langle f_j(z) | a_{j+1} \rangle \\ &\quad \langle a_j | a_j \rangle^{-1} a_j = f_j(z) - \Phi_j(z) a_j(z), \end{aligned}$$

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

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