On the Expansion of Linear Response Functions—
Application to Electrical Conductivity
of Disordered Metals

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Two expansions for linear response functions which are based on different time-ordering prescriptions are presented. The expansions are associated with the derivation of reduced equations of motion (REM) which are nonlocal and local in time, respectively. Both expansions are formally exact and are written in a closed form but they may yield very different results once approximations are made. Therefore they are expected to be useful for different statistical properties of the system. The time-local expansion has certain formal advantages over the nonlocal one, which makes it applicable to a wide class of problems. In the weak-coupling Markovian limit the two expansions are identical. Application is made to disordered metals where explicit expressions are derived for the electrical conductivity using both reduction schemes.

1. INTRODUCTION

The theory of linear response enables us to calculate the effect of a weak external driving field on a macroscopic system and is one of the basic tools of nonequilibrium statistical mechanics.[1-5] It is widely used for the microscopic calculation of transport coefficients. A few examples are the hydrodynamic transport coefficients, electrical conductivity, light scattering cross sections, absorption line shapes, etc. The linear response formalism requires the microscopic evaluation of correlation functions corresponding

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to the external perturbation and to the detection process associated with the desired transport coefficient. The exact evaluation of the latter is equivalent to finding the true eigenstates of the unperturbed system. This is a formidable task and is feasible only for few, extremely simple, microscopic models (e.g., ideal gases, harmonic lattices etc.). For this reason there were developed various methods for the approximate calculation of equilibrium correlation functions and linear-response functions. These include, e.g., Monte Carlo methods, Langevin equations, Master equations, and projection operator techniques. A common method involves the derivation of reduced equations of motion (REM) for the necessary correlation functions. It is our purpose in this paper to present and compare two methods for the calculation of correlation functions, which are based on the derivation of REM making use of different time-ordering prescriptions. The first, denoted COP (chronological ordering prescription), is the more common and results in REM which are nonlocal in time (integral equations).[6] The second, denoted POP (partial ordering prescription), was developed recently[7-12] and the resulting REM are local in time. Recent applications of the POP equations to molecular radiative processes and line shape problems have proven very useful.[8-10] In Section 2 we present the COP and POP REM for the evaluation of correlation functions. In Section 3 we summarize the linear response formalism and develop the COP and the POP expansions for the response functions. In Section 4 we specialize the formalism to a single conserved variable, and finally in Section 5 we consider a simple model of a disordered metal and calculate the electrical conductivity using both methods.

2. EVALUATION OF CORRELATION FUNCTIONS USING THE COP AND THE POP REDUCED EQUATIONS OF MOTION

Within the framework of nonequilibrium statistical mechanics, the microscopic information relevant for macroscopic observables such as transport coefficients is usually put in the form of appropriate correlation functions. Given two dynamical operators A_ν and A_μ we define their correlation function as

$$C_{\nu\mu}(\tau) \equiv \text{Tr}\Big[\exp(iH\tau)A_\nu^\dagger \exp(-iH\tau)A_\mu f \Big] \equiv \text{Tr}\Big[A_\nu^\dagger(\tau)A_\mu f \Big] \qquad (1)$$

Here H is the total Hamiltonian of the system and $f = f(H)$ is the equilibrium distribution function which is a function of H and therefore commutes with it, $[H, f] = 0$.

The rigorous evaluation of the correlation functions (1) requires the knowledge of the exact eigenstates $|\alpha\rangle$ of H and their eigenvalues E_α, in

terms of which we have

$$C_{\nu\mu}(\tau) = \sum_{\alpha\beta} f(\alpha)\left(A_\nu^\dagger\right)_{\alpha\beta}(A_\mu)_{\beta\alpha} \exp\left(i\omega_{\alpha\beta}\tau\right) \tag{2}$$

where

$$f = \sum_\alpha |\alpha\rangle f(\alpha)\langle\alpha| \tag{3}$$

and

$$\omega_{\alpha\beta} = E_\alpha - E_\beta \tag{4}$$

Equation (2) does not usually provide a practical way for the evaluation of correlation functions. The reason is that we seldom know the true eigenstates of a complicated many-body system. Moreover, the information content of the true eigenstates is often much larger than required for the knowledge of the correlation functions in the desired accuracy dictated by experiment. We should thus adopt appropriate approximation schemes for the evaluation of the correlation functions (1). To that end let us introduce a Liouville space (tetradic) notation which simplifies our subsequent formal manipulations. In Liouville space, an ordinary operator A_ν is a vector and we define a ket vector $|A_\nu\rangle\rangle$ corresponding to A_ν. Similarly to $A_\nu^\dagger$ we assign a bra $\langle\langle A_\nu|$. The scalar product of two vectors is defined as

$$S_{\nu\mu} \equiv \langle\langle A_\nu \,|\, A_\mu\rangle\rangle \equiv \mathrm{Tr}\left(A_\nu^\dagger A_\mu f\right) \tag{5}$$

A tetradic (Liouville space) operator is defined by its action on a set of ordinary operators,

$$\mathfrak{I}A_\nu = A_\mu \tag{6}$$

and we define a tetradic "matrix element"

$$\langle\mathfrak{I}\rangle_{\nu\mu} \equiv \langle\langle A_\nu|\mathfrak{I}|A_\mu\rangle\rangle \equiv \mathrm{Tr}\left(A_\nu^\dagger \mathfrak{I}A_\mu f\right) \tag{7}$$

If $\{A_\nu\}$ is a complete set of operators, then the unit operator in Liouville space has the form

$$I = \sum_\nu |A_\nu\rangle\rangle S_{\nu\mu}^{-1}\langle\langle A_\mu| \tag{8}$$

If the set of operators $\{A_\nu\}$ is orthonormal then

$$S_{\nu\mu} = \delta_{\nu,\mu} \tag{9a}$$

and we have

$$I = \sum_\nu |A_\nu\rangle\rangle\langle\langle A_\nu| \tag{9b}$$

Using the matrix notation introduced by Eqs. (6)–(8) we may write any tetradic operator $\mathfrak{I}$ in the following matrix form:

$$\mathfrak{I} \equiv \sum_{\substack{\nu\mu \\ \nu'\mu'}} |A_\nu\rangle\rangle S_{\nu\mu}^{-1} \langle\mathfrak{I}\rangle_{\mu\mu'} S_{\mu'\nu'}^{-1} \langle\langle A_{\nu'}| \tag{10}$$

When the sum in Eq. (8) is restricted to a finite set of operators A_ν, $\nu = 1, \ldots, N$ which do not span the entire phase space, we get a Mori projection onto the subspace defined by these operators, i.e.,

$$P \equiv \sum_{\nu,\mu=1}^{N} |A_\nu\rangle\rangle S_{\nu\mu}^{-1} \langle\langle A_\mu| \tag{11}$$

Equations (6)–(11) are direct analogs of ordinary (Hilbert space) formalism; the only difference is the definition of the scalar product [Eq. (5)]. The Liouville operator (Liouvillian) L is the tetradic operator corresponding to the Hamiltonian H, i.e.,

$$LA_\nu \equiv [H, A_\nu] \tag{12}$$

We may then write

$$A_\nu(\tau) = \exp(iH\tau)A_\nu \exp(-iH\tau) \equiv \exp(iL\tau)A_\nu \tag{13}$$

and using our vector notation:

$$|A_\nu(\tau)\rangle\rangle = \exp(iL\tau)|A\rangle\rangle \tag{14a}$$

$$\langle\langle A_\nu(\tau)| = \langle\langle A_\nu|\exp(-iL\tau) \tag{14b}$$

we have

$$C_{\nu\mu}(\tau) = \langle\langle A_\nu(\tau) | A_\mu(0)\rangle\rangle \equiv \langle\langle A_\nu|\exp(-iL\tau)|A_\mu\rangle\rangle \tag{15}$$

We shall now turn to discuss practical ways for the evaluation of the correlation functions $C_{\nu\mu}(\tau)$, using the tetradic notation introduced in Eqs. (5)–(14). A straightforward perturbative approach involves the partitioning of H in the form

$$H = H_0 + H' \tag{16}$$

and correspondingly in Liouville space we have

$$L = L_0 + L' \tag{17}$$

Using Eq. (17) we have the following iterative relations:

$$\exp(-iLt) = \exp(-iL_0t) - i\int_0^t d\tau \exp[-iL_0(t-\tau)]L'\exp(-iL\tau) \tag{18}$$

$$f = f_0 + \frac{1}{-L_0 + i\epsilon}L'f \tag{19}$$

where $f_0 = f_0(H_0)$ is the distribution function corresponding to H_0. Equations (18) and (19) may be used to generate a perturbative series for $C_{\nu\mu}(\tau)$ as a power series in L'. This is done by substituting these equations in Eq. (15). Perturbative series of this type are usually valid for short times but they fail completely at long times owing to the accumulation of errors. It is therefore desirable to find resummation techniques which will yield expressions for $C_{\nu\mu}(\tau)$ which are nonperturbative in L'. A commonly used resummation technique involves the derivation of reduced equations of motion (REM) for the correlation functions. The kernels appearing in the REM are then evaluated perturbatively but when solving the REM for $C_{\nu\mu}(\tau)$ the solution will be to infinite order. This corresponds to a partial resummation of the perturbative series for $C_{\nu\mu}(\tau)$. We shall focus here on two types of REM denoted COP (chronological time ordering prescription) and POP (partial time ordering prescription). The COP equations are derived in Appendix A and they read (in a matrix form)

$$\frac{d\mathbf{C}(t)}{dt} = -i\langle\Omega\rangle\mathbf{C}(t) - \int_0^t d\tau \,\langle\mathbf{K}(t-\tau)\rangle\mathbf{C}(\tau) \tag{20a}$$

or, more explicitly,

$$\frac{dC_{\nu\mu}(t)}{dt} = -\sum_\lambda i\langle\Omega\rangle_{\nu\lambda} C_{\lambda\mu}(t) - \sum_\lambda \int_0^t d\tau \,\langle K(t-\tau)\rangle_{\nu\lambda} C_{\lambda\mu}(\tau) \tag{20b}$$

The $\langle\Omega\rangle$ and $\langle\mathbf{K}\rangle$ matrices are defined as follows:

$$\langle\Omega\rangle = \langle\mathbf{L}\rangle\langle\mathbf{S}\rangle^{-1} \tag{21}$$

$$\langle\mathbf{K}(\tau)\rangle = \langle\mathbf{W}(\tau)\rangle\langle\mathbf{S}\rangle^{-1} \tag{22}$$

where

$$\langle\mathbf{L}\rangle_{\mu\nu} = \langle\langle A_\mu | L | A_\nu \rangle\rangle \tag{23a}$$

$$\langle\mathbf{S}\rangle_{\mu\nu} = \langle\langle A_\mu | A_\nu \rangle\rangle \tag{23b}$$

and

$$\langle\mathbf{W}(\tau)\rangle_{\mu\nu} = \langle\langle A_\mu | LQ \exp(-iQL\tau)\, QL | A_\nu \rangle\rangle \tag{24}$$

Here P is the projection operator Eq. (11) and

$$Q = 1 - P \tag{25}$$

The POP equations of motion are derived in Appendix B, and they read (using matrix notation)

$$\frac{d\mathbf{C}(t)}{dt} = -i\langle\Omega\rangle\mathbf{C}(t) - \int_0^t d\tau \,\langle\boldsymbol{\phi}(\tau)\rangle \cdot \mathbf{C}(t) \tag{26a}$$

or, more explicitly,

$$\frac{dC_{\nu\mu}(t)}{dt} = -\sum_{\lambda} i\langle\Omega\rangle_{\nu\lambda} C_{\lambda\mu}(t) - \sum_{\lambda} \int_{0}^{t} \langle\phi(\tau)\rangle_{\nu\lambda} d\tau\, C_{\lambda\mu}(t) \qquad (26b)$$

Here the $\langle\Omega\rangle$ matrix is given by Eq. (21) and

$$\langle\phi(\tau)\rangle = -\frac{d}{d\tau}\langle\dot{S}(\tau)\rangle\langle S(\tau)\rangle^{-1} \qquad (27)$$

or, alternatively,

$$\langle\phi(\tau)\rangle = -\langle\ddot{S}(\tau)\rangle\langle S(\tau)\rangle^{-1} + \langle\dot{S}(\tau)\rangle\langle S(\tau)\rangle^{-1}\langle\dot{S}(\tau)\rangle\langle S(\tau)\rangle^{-1} \qquad (28)$$

where a dot denotes derivative with respect to time and we have

$$\langle S(\tau)\rangle_{\nu\mu} = \langle\langle A_{\nu}|\exp(-iL\tau)|A_{\mu}\rangle\rangle \qquad (29)$$

$$\langle\dot{S}(\tau)\rangle_{\nu\mu} = -i\langle\langle A_{\nu}|L\exp(-iL\tau)|A_{\mu}\rangle\rangle \qquad (30)$$

and

$$\langle\ddot{S}(\tau)\rangle_{\nu\mu} = -\langle\langle A_{\nu}|L\exp(-iL\tau)L|A_{\mu}\rangle\rangle \qquad (31)$$

Equations (20) or (26) are convenient *starting points* for the approximate evaluation of the correlation functions $C_{\nu\mu}(\tau)$. The way to proceed is now to evaluate $\langle\Omega\rangle$ and $\langle K\rangle$ for the COP or $\langle\Omega\rangle$ and $\langle\phi\rangle$ for the POP perturbatively. A low-order perturbative expansion of these quantities in some parameter will result in an infinite-order approximation for $C_{\nu\mu}(\tau)$, which corresponds to a partial resummation. The nature of the perturbative expansion depends in general on A_{ν} and on the Hamiltonian H. If we use the partitioning [Eq. (17)] for L, where L_0 is a solvable zero-order Liouville operator and L' is a perturbation, then the POP kernel $\langle\phi(\tau)\rangle$ [Eq. (28)] may be expanded using Eqs. (18) and (19). The evaluation of the COP kernel $\langle K(\tau)\rangle$ [Eq. (22)] requires the expansion of $\exp(-iQL\tau)$. This is less straightforward than the expansion of $\exp(-iL\tau)$ [Eq. (18)]. In the common case where

$$L_0 A_{\nu} = 0 \qquad (32)$$

so that

$$L_0 P = 0 \qquad (33)$$

we may write

$$\exp(-iQL\tau) = \exp(-iL_0\tau - iQL'\tau)$$
$$= \exp(-iL_0\tau) - i\int_{0}^{\tau} d\tau_1 \exp\left[-iL_0(\tau - \tau_1)\right]$$
$$\times QL'\exp(-iQL\tau) \qquad (34)$$

Equations (19) and (34) are then used to evaluate the $\langle K(\tau)\rangle$ matrix, perturbatively in L'. The above discussion shows already one formal

advantage of the POP equations. Namely, the expansion of $\exp(-iL\tau)$ is easier and leaves us with more flexibility than the expansion of $\exp(-iQL\tau)$.[8-10]

3. THE EXPANSION OF LINEAR-RESPONSE FUNCTIONS

In this section we shall introduce the necessary notation for the definition of the linear-response functions and present their expansions using the COP and the POP reduction schemes.

We consider a complicated system with many degrees of freedom, characterized by a Hamiltonian H and subject to an external driving force $F(r, t)$. The total Hamiltonian for the driven system is

$$H_T = H + H_I \tag{35}$$

where

$$H_I = -\int dr\, B(r)F(r, t) \tag{36}$$

$B(r)$ is a dynamical variable which depends on the degrees of freedom of our system and which denotes its coupling with the external field. For a fluid consisting of many identical molecules we have

$$B(r) = \sum_m \tfrac{1}{2}\big[B_m, \delta(r - r_m) \big]_+ \tag{37}$$

where

$$[A, B]_+ \equiv AB + BA \tag{38}$$

and the summation is over the single molecule operators B_m.

If we measure the expectation value of an operator $A(r)$ which is again of the form

$$A(r) = \sum_m \tfrac{1}{2}\big[A_m, \delta(r - r_m) \big]_+ \tag{39}$$

Then, to lowest order in the field F we have

$$\langle A(r, t) \rangle = \int_{-\infty}^{t} d\tau \int dr'\, \phi_{AB}(r - r', t - \tau)F(r', \tau) \tag{40}$$

or

$$\langle A(r, t) \rangle = \sum_{k, \omega} \chi_{AB}(k, \omega)F_{k\omega}\exp\big[-i(kr - \omega t) \big] \tag{41}$$

where

$$F(r, t) = \sum_{k\omega} F_{k\omega}\exp\big[-i(kr - \omega t) \big] \tag{42}$$

$$\chi_{AB}(k, \omega) = \int_0^{\infty} d\tau \int dr\, \Phi_{AB}(r, \tau)\exp\big[i(kr - \omega\tau) \big] \tag{43}$$

Φ_{AB} or χ_{AB} are the *response functions* denoting the effect of driving with B on the expectation value of the operator A. The linear-response formalism gives a microscopic expression for these quantities.[1-5] Before writing it explicitly, we shall first introduce some notation. We define the advanced and retarded Green's functions G^+ and G^-, respectively:

$$G^{\pm}(\tau) \equiv \theta(\tau)\exp(\mp iL\tau) \tag{44}$$

where $\theta(\tau)$ is the Heaviside step function. In the frequency domain we define

$$G^{\pm}(\omega) = \frac{1}{\omega - L \pm i\epsilon} \tag{45}$$

we then have

$$G^+(\omega) = -i\int_0^\infty d\tau\, G^+(\tau)\exp(i\omega\tau) \tag{46a}$$

and

$$G^-(-\omega) = i\int_0^\infty d\tau\, G^-(\tau)\exp(i\omega\tau) \tag{46b}$$

Using Eqs. (15) and (44)–(46) we have

$$C_{\nu\mu}(\tau) = \langle\langle A_\nu(\tau)\,|\,A_\mu(0)\rangle\rangle = \langle\langle A_\nu|G^+(\tau)|A_\mu\rangle\rangle \tag{47a}$$

and

$$C_{\nu\mu}(-\tau) = \langle\langle A_\nu(-\tau)\,|\,A_\mu(0)\rangle\rangle = \langle\langle A_\nu(0)\,|\,A_\mu(\tau)\rangle\rangle \equiv \langle\langle A_\nu|G^-(\tau)|A_\mu\rangle\rangle \tag{47b}$$

We next introduce the Fourier transforms of $A(r)$ [Eq. (39)] and $B(r)$ [Eq. (37)], i.e.,

$$A_k = \sum_m \tfrac{1}{2}\big[A_m, \exp(ikr_m)\big]_+ \tag{48a}$$

$$B_k = \sum_m \tfrac{1}{2}\big[B_m, \exp(ikr_m)\big]_+ \tag{48b}$$

so that

$$A_k^\dagger(\tau) = A_{-k}(\tau) \tag{49}$$

Finally we define the matrix elements of the Green's functions

$$\langle G_{AB}^+(k,\tau)\rangle \equiv \langle\langle A_{-k}|G^+(\tau)|B_{-k}\rangle\rangle \equiv \mathrm{Tr}\big[A_k G^+(\tau)B_{-k}f\big] \tag{50a}$$

$$\langle G_{BA}^-(-k,\tau)\rangle \equiv \langle\langle B_k|G^-(\tau)|A_k\rangle\rangle \equiv \mathrm{Tr}\big[B_{-k}G^-(\tau)A_k f\big] \tag{50b}$$

Similarly, in the frequency domain we have

$$\langle G_{AB}^+(k,\omega)\rangle \equiv \langle\langle A_{-k}|G^+(\omega)|B_{-k}\rangle\rangle \equiv \mathrm{Tr}\big[A_k G^+(\omega)B_{-k}f\big] \tag{51a}$$

$$\langle G_{BA}^-(-k,-\omega)\rangle \equiv \langle\langle B_k|G^-(-\omega)|A_k\rangle\rangle \equiv \mathrm{Tr}\big[B_{-k}G^-(-\omega)A_k f\big] \tag{51b}$$

The linear response formalism results in the following microscopic expression for the response functions[1-5]:

$$\chi_{AB}(k,\omega) = i \int_0^\infty d\tau \, \chi_{AB}(k,\tau) \exp(i\omega\tau) \tag{52}$$

where

$$\chi_{AB}(k,\omega) = -\left\langle G_{AB}^+(k,\omega) \right\rangle - \left\langle G_{BA}^-(-k,-\omega) \right\rangle \tag{52a}$$

and where

$$\chi_{AB}(k,\tau) = \left\langle G_{AB}^+(k,\tau) \right\rangle - \left\langle G_{BA}^-(-k,\tau) \right\rangle \tag{52b}$$

The evaluation of the linear response functions thus reduces to the calculation of the equilibrium correlation functions [Eqs. (50)]. The correlation functions $\left\langle G_{AB}^+(k,\tau) \right\rangle$ may be directly obtained by solving the REM (20) or (26) where $C_{\nu\mu}(\tau)$ is replaced by $\left\langle G_{AB}^+(k,\tau) \right\rangle$. The retarded Green's functions $\left\langle G_{BA}^-(-k,\tau) \right\rangle$ may be obtained from similar REM where $-i\langle\Omega\rangle$, $\exp(-iQL\tau)$, and $\exp(-iL\tau)$ are replaced by $i\langle\Omega\rangle$, $\exp(iQL\tau)$ and $\exp(iL\tau)$, respectively. The appropriate (COP or POP) REM are defined by introducing the projection operators P and Q defined as follows:

$$P = \sum_\nu |A_{\nu k}\rangle\rangle S_{\nu\mu}^{-1} \langle\langle A_{\mu k}| \tag{53a}$$

$$Q = 1 - P \tag{53b}$$

The set of operators $\{A_{\nu k}\}$ has to include our relevant A and B operators. In addition it may include also other operators whose time evolution is correlated with that of our A and B. The solution of the COP equations [Eqs. (20)] is most easily carried out using a Laplace transform, resulting in

$$\left\langle G_{\nu\mu}^\pm(k,\omega) \right\rangle = \sum_\lambda \left[\omega - \left\langle R^\pm(k,\omega)\right\rangle\right]_{\nu\lambda}^{-1} \left\langle S(k)\right\rangle_{\lambda\mu} \tag{54}$$

where

$$\left\langle \mathsf{R}^\pm(k,\omega)\right\rangle \equiv \langle\Omega(k)\rangle + \left\langle \mathsf{K}^\pm(k,\omega)\right\rangle \tag{55a}$$

$$\langle\Omega(k)\rangle = \langle\mathsf{L}(k)\rangle\langle\mathsf{S}(k)\rangle^{-1} \tag{55b}$$

$$\left\langle \mathsf{K}^\pm(k,\omega)\right\rangle = \langle\mathsf{W}(k,\omega)\rangle\langle\mathsf{S}(k)\rangle^{-1} \tag{55c}$$

$$\left\langle \mathsf{L}(k)\right\rangle_{\nu\mu} = \langle\langle A_{\nu,-k}|L|A_{\mu,-k}\rangle\rangle \tag{55d}$$

$$\left\langle \mathsf{S}(k)\right\rangle_{\nu\mu} = \langle\langle A_{\nu,-k}|A_{\mu,-k}\rangle\rangle \tag{55e}$$

$$\left\langle \mathsf{W}^\pm(k,\omega)\right\rangle_{\nu\mu} = \langle\langle A_{\nu,-k}|LQ \frac{1}{\omega - QLQ \pm i\epsilon} QL|A_{\mu,-k}\rangle\rangle \tag{55f}$$

The formal solution of the POP equations (26) is also straightforward and reads

$$\left\langle G_{\nu\mu}^\pm(k,\pm\omega) \right\rangle = \mp i \int_0^\infty d\tau \exp(i\omega\tau) \left\langle G_{\nu\mu}^\pm(k,\tau) \right\rangle \tag{56a}$$

where

$$\left\langle G_{\nu\mu}^{\pm}(k,\tau)\right\rangle_{\nu\mu} = \sum_{\lambda} \exp_{+}\left[-i\int_{0}^{\tau} d\tau_1 \left\langle \Phi^{\pm}(k,\tau_1)\right\rangle\right]_{\nu\lambda} \left\langle S(k)\right\rangle_{\lambda\mu} \quad (56b)$$

Here

$$\left\langle \Phi^{\pm}(k,\tau)\right\rangle_{\nu\lambda} = \left\langle \Omega(k)\right\rangle_{\nu\lambda} - i\int_{0}^{\tau} d\tau_1 \left\langle \psi^{\pm}(k,\tau_1)\right\rangle_{\nu\lambda} \quad (57a)$$

$$\left\langle \psi^{\pm}(k,\tau)\right\rangle_{\nu\lambda} = -\frac{d}{d\tau}\sum_{\nu'}\left\langle \dot{S}^{\pm}(k,\tau)\right\rangle_{\nu\nu'}\left\langle S^{\pm}(k,\tau)\right\rangle_{\nu'\lambda}^{-1} \quad (57b)$$

$$\left\langle S^{\pm}(k,\tau)\right\rangle_{\lambda'\lambda} = \langle\langle A_{\lambda',-k}|\exp(\mp iL\tau)|A_{\lambda',-k}\rangle\rangle \quad (57c)$$

$$\left\langle \dot{S}^{\pm}(k,\tau)\right\rangle_{\nu\lambda'} = \Phi\langle\langle A_{\nu,-k}|L\exp(\mp iL\tau)|A_{\lambda',-k}\rangle\rangle \quad (57d)$$

$$\left\langle S(k)\right\rangle = \left\langle S(k,t=0)\right\rangle \quad (57e)$$

and

$$\exp_{+}\left[-i\int_{0}^{\tau} d\tau_1 A(\tau_1)\right]$$

$$\equiv 1 - i\int_{0}^{\tau} d\tau_1 A(\tau_1) + (-i)^2\int_{0}^{\tau} d\tau_1\int_{0}^{\tau_1} d\tau_2 A(\tau_1)A(\tau_2) + \cdots \quad (58)$$

is the positive time-ordered exponential. Equations (54) with (55) or (56) with (57) when substituted in Eqs. (52) provide us with the COP and the POP representations for the linear response functions, respectively.

4. APPLICATION TO A SINGLE CONSERVED VARIABLE

Suppose that the variable B corresponds to a conserved molecular property such as energy, momentum, or number density; then it obeys the continuity equation

$$\dot{B} = iLB = -\nabla \cdot J \quad (59)$$

where J is the current associated with the quantity B. In k space this yields

$$\dot{B}_k = iLB_k = ikJ_k \quad (60)$$

Often the observable A_k is simply equal to J_k, i.e., we observe the current associated with B. In this case we may use the relations of Appendix C to write $\langle\chi_{JB}(k,\omega)\rangle$ in terms of a single variable which may be chosen to be either B or J. $\chi_{JB}(k,\omega)$ may then be related to $\chi_{BB}(k,\omega)$ or to $\chi_{JJ}(k,\omega)$, respectively:

$$\chi_{JB}(k,\omega) = -\frac{\omega}{k}\chi_{BB}(k,\omega) \quad (61)$$

$$\chi_{JB}(k,\omega) = -\frac{k}{\omega}\left[\chi_{JJ}(k,\omega) - \chi_{JJ}(k,0)\right] \quad (62)$$

Equations (61) or (62) may now be used for the evaluation of $\chi_{JB}(k,\omega)$ using one reduced equation of motion for a single variable ($|B_k\rangle\rangle$ or $|J_k\rangle\rangle$, respectively).

A better method for the evaluation of χ_{JB} which exploits more effectively the symmetry properties of the response functions may be derived as follows: Using Eq. (52b) we have

$$\chi_{JB}(k,\tau) = \sum_{\alpha,\beta} f(\alpha)\left[(J_k)_{\alpha\beta}(B_k^\dagger)_{\beta\alpha}\exp(i\omega_{\alpha\beta}\tau) \right.$$

$$\left. - (B_{-k})_{\alpha\beta}(J_{-k}^\dagger)_{\beta\alpha}\exp(-i\omega_{\alpha\beta}\tau) \right] \qquad (63)$$

where $|\alpha\rangle$, $|\beta\rangle$ are the eigenstates of H [Eq. (35)]. From Eq. (60) we get

$$(B_k)_{\beta\alpha} = \frac{k}{\omega_{\beta\alpha}}(J_k)_{\beta\alpha} \qquad (64)$$

Upon substitution of Eq. (64) in (63) and changing the α and β indexes in the second term, we finally get

$$\chi_{JB}(k,\tau) = k\sum_{\alpha,\beta} \frac{f(\alpha) - f(\beta)}{\omega_{\beta\alpha}}|(J_k)_{\alpha\beta}|^2\exp(i\omega_{\alpha\beta}\tau) \qquad (65)$$

We note that $\chi_{JB}(k,\tau)$ is real and satisfies

$$\chi_{JB}(k,\tau) = \chi_{JB}(-k,-\tau) \qquad (66)$$

It is therefore advantageous to exploit this symmetry and to derive REM which will give $\chi_{JB}(k,\tau)$ directly rather than in the form of a difference of two correlation functions [Eqs. (52)]. To that end we define a new type of scalar product in Liouville space, as follows:

$$\langle\langle A\,|\,B\rangle\rangle_s \equiv -\text{Tr}\left(A^\dagger \frac{F}{L}B\right) \equiv \sum_{\alpha,\beta} \frac{f(\alpha) - f(\beta)}{\omega_{\beta\alpha}}A_{\alpha\beta}^\dagger B_{\beta\alpha} \qquad (67)$$

where

$$F \equiv [f, \ ] \qquad (68a)$$

and

$$L \equiv [H, \ ] \qquad (68b)$$

It is easy to verify that the definition (67) satisfies all the requirements of a scalar product, i.e.,

(a) $$\langle\langle A\,|\,B\rangle\rangle_s^* = \langle\langle B\,|\,A\rangle\rangle_s \qquad (69a)$$

(b) if $|B\rangle\rangle = c_1|B_1\rangle\rangle + c_2|B_2\rangle\rangle$

then $\langle\langle A\,|\,B\rangle\rangle_s = c_1\langle\langle A\,|\,B_1\rangle\rangle_s + c_2\langle\langle A\,|\,B_2\rangle\rangle_s \qquad (69b)$

(c) $\langle\langle A\,|\,A\rangle\rangle_s \geqslant 0$ and the equality sign holds only when $|A\rangle\rangle \equiv 0$.

This holds at least for all distribution functions $f(\alpha)$ which are monotonic, i.e., if $\omega_{\beta\alpha} > 0$ then $f_\beta < f_\alpha$. The scalar product (67) may be alternatively written using the Laplace transform:

$$f(H) = \frac{1}{Z} \int_0^\infty d\lambda \exp(-\lambda H) \tilde{f}(\lambda) \tag{70}$$

so that

$$F \equiv [f, \ ] = \frac{1}{Z} \int_0^\infty d\lambda \, \tilde{f}(\lambda) [\exp(-\lambda H), \ ] \tag{71}$$

Here Z is a normalization factor. We now have

$$\left(\frac{F}{L} B\right)_{\beta\alpha} = \frac{1}{Z} \int_0^\infty d\lambda \, \tilde{f}(\lambda) \exp(-\lambda E_\alpha) \frac{\exp(-\lambda\omega_{\beta\alpha}) - 1}{\omega_{\beta\alpha}} B_{\beta\alpha}$$

$$= -\frac{1}{Z} \int_0^\infty d\lambda \int_0^\lambda d\lambda_1 \, \tilde{f}(\lambda) \exp(-\lambda_1 E_\beta) B_{\beta\alpha} \exp[-(\lambda - \lambda_1)E_\alpha] \tag{72}$$

Upon substitution of Eq. (72) in (67) we get

$$\langle\langle A \mid B \rangle\rangle_s = \frac{1}{Z} \int_0^\infty d\lambda \int_0^\lambda d\lambda_1 \, \tilde{f}(\lambda)$$

$$\times \left\{ \mathrm{Tr} \exp[-(\lambda - \lambda_1)H] A^\dagger \exp(-\lambda_1 H) B \right\} \tag{73}$$

In the special case of a canonical distribution function we have

$$\tilde{f}(\lambda) = \delta(\lambda - \lambda_0) \tag{74}$$

where $\lambda_0 = 1/kT$, $Z(\tau_0)$ is the partition function and we get

$$\langle\langle A \mid B \rangle\rangle_s \rightarrow \frac{1}{Z(\lambda_0)} \int_0^{\lambda_0} d\lambda \, \mathrm{Tr} \exp[-(\lambda_0 - \lambda)H] A^\dagger \exp(-\lambda H) B \tag{75}$$

which is nothing but the Kubo transform,[1] which is often used in the calculation of transport coefficients. Using our new definition of a scalar product (67) or (73), we may express our response function (65) in the form

$$\chi_{JB}(k,\tau) = k\langle\langle J_k(\tau) \mid J_k(0) \rangle\rangle_s \tag{76}$$

Using this scalar product, we may use the formalism of Section 3 with

$$P = |J_k\rangle\rangle\langle\langle J_k| \tag{77}$$

and obtain the following expressions for the transport coefficients: Using the COP formalism we get

$$\chi_{JB}(k,\omega) = -k \frac{1}{\omega - \langle R_{JJ}(k,\omega)\rangle_s} \langle\langle J_k(0) \mid J_k(0)\rangle\rangle_s \tag{78}$$

and when using the POP equations we obtain

$$\chi_{JB}(k,\omega) = ik \int_0^\infty d\tau \exp(i\omega\tau)\exp\left[-\int_0^\tau d\tau_1 (\tau - \tau_1)\langle\psi_{JJ}(k,\tau)\rangle_s\right]$$
$$\times \langle\langle J_k(0) | J_k(0)\rangle\rangle_s \tag{79}$$

where $\langle R \rangle_s$ and $\langle \psi \rangle_s$ are given by Eqs. (55) and (57), respectively, with the projection operator (77) and the scalar product (67). We should reiterate that both expansions (78) and (79) are exact provided the necessary kernels are evaluated to infinite order, but they may yield different results once the kernels are evaluated in an approximate manner. The choice of the appropriate expansion thus depends on the specific problem at hand.[8–10]

5. ELECTRICAL CONDUCTIVITY OF A DISORDERED METAL

We shall now apply the results of Section 4 to the problem of the electrical conductivity of a disordered metal. This problem is of considerable current interest.[13–17] In particular questions such as the nature of the electronic motion in these systems (coherent or diffusive), the existence of a mobility edge (the Mott–Anderson transition), and the effect of dimensionality on these properties are now under active study. The problem was attacked by a variety of methods. We shall therefore use this example in order to demonstrate how the COP and the POP expansions may be used for the explicit evaluation of transport coefficients.

We consider a disordered metal whose conduction electrons are moving in the tight-binding Hamiltonian

$$H = H_0 + \lambda H' \tag{80}$$

where

$$H_0 = \sum_{n,m} V_{nm} c_n^\dagger c_m \tag{80a}$$

and

$$H' = \sum_n U_n c_n^\dagger c_n \tag{80b}$$

Here $c_n^\dagger$ (c_n) are the creation (anihilation) operators for an electron in the nth lattice site, V_{nm} is the exchange interaction, and U_n is the electron energy at the nth site. We assume that V_{nm} are fixed and translationally invariant (i.e., V_{nm} depend only on $|n - m|$). U_n on the other hand are stochastic random variables characterized by the set of moments[13]

$$m^{(1)} \equiv \langle U_n \rangle = 0 \tag{81a}$$

$$m^{(2)}(n) = \langle U_0 U_n \rangle \tag{81b}$$

$$m^{(3)}(n, n') = \langle U_0 U_n U_{n'} \rangle \tag{81c}$$

where $\langle \cdots \rangle$ denotes an ensemble average over the stochastic variable U. λ is a perturbation parameter introduced for bookkeeping purposes and at the end of the calculation we may set $\lambda = 1$. In k space, the Hamiltonian (80) assumes the form[18-20]

$$H_0 = \sum_k \epsilon(k) c_k^\dagger c_k \tag{82a}$$

$$H' = \sum_{kk'} \langle k | U | k' \rangle c_k^\dagger c_{k'} \tag{82b}$$

where

$$c_k = \frac{1}{\sqrt{N}} \sum_n \exp(-ik \cdot r_n) c_n \tag{83a}$$

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_n \exp(ik \cdot r_n) c_n^\dagger \tag{83b}$$

$$\epsilon(k) = \sum_n V_{0,n} \exp(ik \cdot r_n) \tag{84}$$

and

$$\langle k | U | k' \rangle = \frac{1}{N} \sum_n U_n \exp\left[i(k' - k) \cdot r_n \right] \tag{85}$$

where N is the number of lattice sites.

We are interested in calculating the electrical conductivity $\sigma(\omega)$ of this metal. To that end, let us introduce the charge density fluctuation operator $\delta\rho(r)$ and the electric current operator J_k which denotes the coupling of the metal to an external electromagnetic field. These operators are defined as follows[16-19]: The charge density fluctuation operator $\delta\rho(r)$ is given by

$$\delta\rho(r) = \rho(r) - \bar{\rho}(r) = e \sum_j \left[\delta(r - r_j) - \frac{1}{V} \right] \tag{86}$$

$\bar{\rho} = n/V$ is the mean electron density, n being the number of electrons, e is the electronic charge, and V the volume. In k space we have

$$\delta\rho_k = e \sum_j \left[\exp(ik \cdot r_j) - \delta_{k,0} \right] \tag{87}$$

so that

$$\delta\rho(r) = \frac{1}{N} \sum_k \exp(-ikr) \delta\rho_k \tag{88}$$

The electric current operator J_k is given by

$$\delta\dot{\rho}_k = ik \cdot J_k \tag{89}$$

and the coupling operator with an external electromagnetic field is[18]

$$B_k = \frac{\delta\rho_k}{ik} \tag{90}$$

We then have for the electric conductivity[18,19]

$$\sigma(\omega) \equiv \lim_{k \to 0} \sigma(k, \omega) = \lim_{k \to 0} \frac{1}{ik} \chi_{J\rho}(k, \omega)$$

$$= \lim_{k \to 0} \int_0^\infty d\tau \langle\langle J_k(\tau) | J_k(0)\rangle\rangle_s \exp(i\omega\tau) \tag{91}$$

In second quantization we have

$$\delta\rho_k = e \sum_n \exp(ikr_n) c_n^\dagger c_n \tag{92}$$

and

$$|J_k\rangle\rangle = \frac{1}{ik} \delta\dot{\rho}_k = \frac{1}{k} [H, \delta\rho_k] = e \sum_p g(p) c_{p+k/2}^\dagger c_{p-k/2} \tag{93}$$

where

$$g(p) = \frac{\partial\epsilon(p)}{\partial p} \tag{94}$$

Using Eqs. (91) and (93) we get, using the COP reduction scheme,

$$\sigma(k, \omega) = i \frac{1}{\omega - \langle R_{JJ}(k, \omega)\rangle_s} \langle\langle J_k | J_k\rangle\rangle_s \tag{95}$$

where

$$\langle R_{JJ}(k, \omega)\rangle_s = \langle\langle J_k | L \frac{1}{\omega - QLQ} L | J_k\rangle\rangle_s \cdot \langle\langle J_k | J_k\rangle\rangle_s^{-1}$$

$$\equiv \langle D(\omega)\rangle + O(k^2) \tag{95a}$$

and making use of the POP equations we get

$$\sigma(k, \omega) = \int_0^\infty d\tau \exp(i\omega\tau) \exp\left[-\int_0^\tau d\tau_1 (\tau - \tau_1) \langle \psi_{JJ}(k, \tau_1)\rangle_s \right] \cdot \langle\langle J_k | J_k\rangle\rangle_s \tag{96}$$

where

$$\langle \psi_{JJ}(k, \tau)\rangle_s = i \frac{d}{d\tau} \left[\langle\langle J_k | L \exp(-iL\tau) | J_k\rangle\rangle_s \langle\langle J_k | \exp(-iL\tau) | J_k\rangle\rangle_s^{-1} \right]$$

$$\equiv \tilde{D}(\tau) + O(k^2) \tag{96a}$$

Upon substitution of Eq. (95a) in (95) and Eq. (96a) in (96) we finally get

$$\sigma^{\text{COP}}(\omega) = i \frac{1}{\omega - \langle D(\omega) \rangle} \langle |J_0|^2 \rangle_s \tag{97}$$

$$\sigma^{\text{POP}}(\omega) = \int_0^\infty d\tau \exp(i\omega\tau) \exp\left[-\int_0^\tau d\tau_1 (\tau - \tau_1) \langle \tilde{D}(\tau_1) \rangle \right] \langle |J_0|^2 \rangle_s \tag{98}$$

We have thus to evaluate $\langle D(\omega) \rangle$ for the COP and $\langle \tilde{D}(\tau) \rangle$ for the POP. This may be done by expanding these quantities perturbatively in L'. The expansion of $\langle \tilde{D}(\omega) \rangle$ is made using Eqs. (18) and (19) whereas the expansion of $D(\omega)$ may be done using Eq. (34). Using Eqs. (95a) and (96a) we have

$$\langle D(\omega) \rangle = \langle\langle J_0| L' \frac{1}{\omega - L + i\epsilon} L' |J_0\rangle\rangle_s^{-1} \tag{99}$$

$$\langle \tilde{D}(\tau) \rangle = \langle\langle J_0| L' \exp(-iL \cdot \tau) L' |J_0\rangle\rangle_s^{-1} \tag{100}$$

where $|J_0\rangle\rangle$ is given by Eq. (93). Upon comparison of Eqs. (99) and (100) we note that

$$\langle \tilde{D}(\tau) \rangle = -\frac{1}{2\pi i} \int_{-\infty}^\infty d\omega \langle \tilde{D}(\omega) \rangle \exp(-i\omega\tau) \tag{101}$$

We should emphasize that Eq. (101) holds only in our $k \to 0$ calculation and in general $\langle R_{JJ} \rangle$ is not simply the fourier transform of $\langle \psi_{JJ} \rangle$. From Eqs. (99) and (100) we immediately have, to second order in U

$$\langle D(\omega) \rangle = \lambda^2 \sum_{pp'} \frac{f(p) - f(p')}{\omega_{p'p}} |\langle p| U |p'\rangle|^2$$

$$\times |g(p) - g(p')|^2 \frac{1}{\omega - \omega_{pp'} + i\epsilon} + O(\lambda^4) \tag{102}$$

$$\langle \tilde{D}(\tau) \rangle = \lambda^2 \sum_{pp'} \frac{f(p) - f(p')}{\omega_{pp'}} |\langle p| U |p'\rangle|^2$$

$$\times |g(p) - g(p')|^2 \exp(i\omega_{p'p}\tau) + O(\lambda^4) \tag{103}$$

note that $\tilde{D}(\tau)$ is real!

$$\langle |J_0|^2 \rangle \equiv \langle\langle J_0| J_0\rangle\rangle_s = e^2 \sum_{\alpha\beta} \frac{f(\alpha) - f(\beta)}{\omega_{\beta\alpha}} |g(\alpha)|^2 \delta_{\alpha,\beta}$$

$$= -e^2 \sum_\alpha |g(\alpha)|^2 \frac{df(\alpha)}{dE_\alpha} \tag{104}$$

The Anderson model of diagonal disorder implies that

$$\langle U_n U_{n'} \rangle = \langle U^2 \rangle \delta_{nn'} \tag{105}$$

For this model we have

$$|\langle p|U|p'\rangle|^2 = \sum_{nm} \overline{U_n U_m} \exp\left[i(p-p')(r_n - r_m)\right] = \langle U^2 \rangle \tag{106}$$

The higher-order correlation functions $\langle U^4 \rangle$, etc. [Eqs. (81)], will enter only when we calculate $\langle D(\omega) \rangle$ to higher order in λ. It is interesting to note that Eqs. (97) and (98) are in general very different although the input information $[\langle D(\omega) \rangle$ or $\langle \tilde{D}(\tau) \rangle]$ to both is the same. The reason is that the choice of the reduction scheme implicitly assumes properties of the higher correlation functions $\langle U^4 \rangle$ etc.[8–10] There is, however, one limit in which both results coincide. This is the Markovian limit where separation of time scales exists such that $D(\omega)$ is very broad, i.e., we may set

$$D(\omega) = D(0) = -i\Gamma \tag{107a}$$

$$\tilde{D}(\tau) = \Gamma\delta(\tau) \tag{107b}$$

Using these relations in Eqs. (97) and (98) we get

$$\sigma(\omega)^{\text{COP}} = \sigma(\omega)^{\text{POP}} = \frac{i}{\omega + i\Gamma} \langle |J_0|^2 \rangle \tag{108}$$

This is the Drude formula of electrical conductivity[18,19]

$$\operatorname{Re}\sigma(\omega)^{\text{COP}} = \operatorname{Re}\sigma(\omega)^{\text{POP}} = \frac{\Gamma}{\omega^2 + \Gamma^2} \langle |J_0|^2 \rangle \tag{109}$$

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APPENDIX A.   DERIVATION OF THE COP-REM

Suppose we have a set of operators A_ν, $\nu = 1, \ldots, N$ and we are interested in calculating the set of correlation functions

$$C_{\nu\mu}(\tau) \equiv \langle\langle A_\nu(\tau) | A_\mu(0)\rangle\rangle = \operatorname{Tr}\left[A_\nu^+ \exp(-iL\tau)A_\mu f\right] \tag{A.1}$$

where

$$L = [H, \ ] \tag{A.2}$$

and f is the equilibrium distribution function which is a function of the

Hamiltonian H, i.e.,

$$f = f(H) \tag{A.3}$$

so that

$$Lf = 0 \tag{A.4}$$

We now introduce a Mori projection operator P by its action on an ordinary operator $|B\rangle\rangle$

$$P|B\rangle\rangle = \sum_{\nu\mu} |A_\nu\rangle\rangle\langle S^{-1}\rangle_{\nu\mu}\langle\langle A_\mu | B\rangle\rangle \tag{A.5}$$

where

$$\langle S \rangle_{\nu\mu} = \langle\langle A_\nu | A_\mu\rangle\rangle \tag{A.6}$$

P projects onto the subspace spanned by the operators A_ν. We further define

$$Q = 1 - P \tag{A.7}$$

Let us consider now the propagator

$$U(t) \equiv \theta(t)\exp(-iLt) \tag{A.8}$$

which satisfies the equation

$$\dot{U} = -iLU \tag{A.9}$$

Using Eqs. (A.5) and (A.9) we may write

$$P\dot{U} = -iPL(P + Q)U = -iPLPU - iPLQU \tag{A.10a}$$

and

$$Q\dot{U} = -iQLPU - iQLQU \tag{A.10b}$$

When solving Eq. (A.10b) for $Q\dot{U}$ we get

$$QU(t) = QU(0) - i\int_0^t d\tau \exp\left[-iQL(t-\tau)\right] QLPU(\tau) \tag{A.11}$$

Upon substitution of (A.11) in (A.10a) and multiplying by P from the right we get

$$P\dot{U}(t)P = -iPLPU(t)P - \int_0^t d\tau\, PLQ \exp\left[-iQLQ(t-\tau)\right] QLPU(\tau)P \tag{A.12}$$

Multiplying Eq. (A.12) by $A_\nu^\dagger$ from the left and by $A_\mu f$ from the right and taking a trace finally yields Eqs. (20).

APPENDIX B. DERIVATION OF THE POP-REM

We use the notation introduced in Appendix A. Starting from

$$U(t) = \theta(t)\exp(-iLt) \tag{B.1}$$

we have

$$PU(t)P = P\exp(-iLt)P \tag{B.2}$$

and

$$P\dot{U}(t)P = -iPL\exp(-iLt)P \tag{B.3}$$

Equation (B.2) can be rearranged in the form

$$1 = \left[P\exp(-iLt)P \right]^{-1}PU(t)P \tag{B.4}$$

Upon multiplying the right-hand side of Eqs. (B.3) and (B.4) we get

$$P\dot{U}(t)P = -iPM(t)PU(t)P \tag{B.5}$$

$$PM(t)P \equiv \langle M(t)\rangle = \langle PL\exp(-iLt)P\rangle\langle P\exp(-iLt)P\rangle^{-1} \tag{B.6}$$

We now introduce the matrices $\langle\Omega\rangle$ and $\langle\phi\rangle$ defined as follows:

$$\langle \mathsf{M}(t)\rangle \equiv \langle\Omega\rangle - i\int_0^t d\tau\,\langle\phi(\tau)\rangle \tag{B.7}$$

where

$$\langle\Omega\rangle \equiv \langle \mathsf{M}(0)\rangle \tag{B.8}$$

and

$$\langle\phi(\tau)\rangle \equiv i\frac{d}{d\tau}\langle \mathsf{M}(\tau)\rangle \tag{B.9}$$

Using Eqs. (B.5) and (B.7) we have

$$P\dot{U}(t)P = -i\langle\Omega\rangle PU(t)P - \int_0^t d\tau\,\langle\phi(\tau)\rangle PU(t)P \tag{B.10}$$

Upon multiplying Eq. (B.10) by $A_\nu^\dagger$ from the left and $A_\mu f$ from the right and taking a trace we get Eqs. (26).

APPENDIX C. RESPONSE FUNCTION FOR A CONSERVED VARIABLE

Consider an operator B which is a conserved variable for which we have

$$\dot{B}_k \equiv iLB_k = ikJ_k \tag{C.1}$$

where J_k is the current associated with B_k. We take our system to be isotropic so that kJ_k is an ordinary product and not a scalar product. Suppose further than we take our observable A_k to be J_k. In this case, since B_k and J_k are related by the simple relation [Eq. (C.1)], we may express $\chi_{JB}(k, \omega)$ in terms of $\chi_{BB}(k, \omega)$ or $\chi_{JJ}(k, \omega)$. In this way we may evaluate our response function in terms of REM involving a single variable (J or B) instead of considering both variables. This goal is achieved as follows:

We use the relations

$$|A_k\rangle\rangle = |J_k\rangle\rangle = \frac{1}{k} L |B_k\rangle\rangle \tag{C.2}$$

and

$$\langle\langle J_{-k}| = -\langle\langle B_{-k}| L \frac{1}{k} \tag{C.3}$$

to write

$$\langle\langle J_{-k}| G^+(\omega)|B_{-k}\rangle\rangle = -\frac{1}{k}\langle\langle B_{-k}| LG^+(\omega)|B_{-k}\rangle\rangle$$

$$= \frac{1}{k}\left[\langle\langle B_{-k}|B_{-k}\rangle\rangle - \omega\langle\langle B_{-k}|G^+(\omega)|B_{-k}\rangle\rangle\right]$$

$$\tag{C.4}$$

and

$$\langle\langle B_k| G^-(-\omega)|J_k\rangle\rangle = \frac{1}{k}\langle\langle B_k|G^-(-\omega)L|B_k\rangle\rangle$$

$$= \frac{1}{k}\left[-\langle\langle B_k|B_k\rangle\rangle - \omega\langle\langle B_k|G^-(-\omega)|B_k\rangle\rangle\right]$$

$$\tag{C.5}$$

Using Eqs. (52a), (C.4), and (C.5) we get

$$\chi_{JB}(k, \omega) = \frac{\omega}{k}\left[\langle\langle B_{-k}|G^+(\omega)|B_{-k}\rangle\rangle + \langle\langle B_k|G^-(-\omega)|B_k\rangle\rangle\right]$$

$$= -\frac{\omega}{k}\chi_{BB}(k, \omega) \tag{C.6}$$

We have thus expressed χ_{JB} in terms of χ_{BB} (Eq. 61).

Alternatively we may put

$$|B_{-k}\rangle\rangle = \frac{-k}{(L - i\epsilon)}|J_{-k}\rangle\rangle \tag{C.7}$$

$$\langle\langle B_k| = \langle\langle J_k|\frac{k}{L + i\epsilon} \tag{C.8}$$

resulting in

$$\langle\langle J_{-k}|G^+(\omega)|B_{-k}\rangle\rangle = -k\langle\langle J_{-k}|\frac{1}{\omega - L + i\epsilon}\frac{1}{L - i\epsilon}|J_{-k}\rangle\rangle$$

$$= -\frac{k}{\omega}\left[\langle\langle J_{-k}|\frac{1}{\omega - L + i\epsilon}|J_{-k}\rangle\rangle\right.$$

$$\left. - \langle\langle J_{-k}|\frac{1}{-L + i\epsilon}|J_{-k}\rangle\rangle\right]$$

$$= -\frac{k}{\omega}\left[\langle G_{JJ}^+(k,\omega)\rangle - \langle G_{JJ}^+(k,0)\rangle\right] \quad (C.9)$$

Also

$$\langle\langle B_k|G^-(-\omega)|J_k\rangle\rangle = -k\langle\langle J_k|\frac{1}{L + i\epsilon}\frac{1}{\omega + L + i\epsilon}|J_k\rangle\rangle$$

$$= -\frac{k}{\omega}\left\{\langle\langle J_k|\frac{1}{-\omega - L - i\epsilon}|J_k\rangle\rangle\right.$$

$$\left. - \langle\langle J_k|\frac{1}{-L - i\epsilon}|J_k\rangle\rangle\right\}$$

$$= -\frac{k}{\omega}\left\{\langle G_{JJ}^-(-k,-\omega)\rangle - \langle G_{JJ}^-(-k,0)\rangle\right\} \quad (C.10)$$

Using Eqs. (52a), (C.9), and (C.10) we get

$$\chi_{JB}(k,\omega) = \frac{k}{\omega}\left\{\langle G_{JJ}^+(k,\omega)\rangle + \langle G_{JJ}^-(-k,-\omega)\rangle\right.$$

$$\left. - \langle G_{JJ}^+(k,0)\rangle - \langle G_{JJ}^-(-k,0)\rangle\right\}$$

$$= -\frac{k}{\omega}\left[\chi_{JJ}(k,\omega) - \chi_{JJ}(k,0)\right] \quad (C.11)$$

We have thus expressed χ_{JB} in terms of χ_{JJ}, (Eq. 62).

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