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Perturbation theory for classical thermodynamic Green's functions

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A systematic time-dependent perturbation scheme for classical canonical systems is developed based on a Wick's theorem for thermal averages of time-ordered products. The occurrence of the derivatives with respect to the canonical variables noted by Martin, Siggia, and Rose implies that two types of Green's functions have to be considered, the propagator and the response function. The diagrams resulting from Wick's theorem are "double graphs" analogous to those introduced by Dyson and also by Kawasaki, in which the response-function lines form a "tree structure" completed by propagator lines. The implication of a fluctuation-dissipation theorem on the self-energies is analyzed and compared with recent results by Deker and Haake.

I. INTRODUCTION

Recently the need for a systematic classical perturbation theory of thermodynamic Green's functions has become manifest in a variety of different physical problems characterized by nonlinear equations of motion, ranging from dynamical critical phenomena and anharmonic crystal lattices to plasmas and turbulent liquid flows. This need has been eloquently formulated by Martin, Siggia, and Rose (MSR)[1] in a paper which reviews the attempts made in this problem during the last 10 or 15 years and which makes several decisive contributions towards a consistent diagrammatic formulation.

These authors, in fact, recognized the importance of the doubling of dynamical variables occurring naturally in classical perturbation theory. This doubling means that the derivatives with respect to the original variables ψ_ν (the canonical p's and q's) have to be treated on the same footing as the ψ's themselves. It turns out that the natural definitions of the new variables, for which we use the notation $\hat{\psi}_\nu$ of MSR, are linear combinations of the derivatives $\partial/\partial\psi_\nu$ taken with the skew-symmetric matrix D occurring in the canonical equations of motion written in the ψ's. The reason for the importance of these $\hat{\psi}$ variables resides in the fact that the classical time evolution is determined by the Liouville operator, which has a linear form in the derivatives $\partial/\partial\psi_\nu$.

This doubling of dynamical variables gives rise to two types of Green's functions and, as a consequence, to two types of lines in classical diagrams. The structure of classical diagrams is therefore more complex than the Feynman diagrams of quantum systems, and it is natural to seek simplifications.

This was the aim of a recent publication by Deker and Haake,[2] who invoked the existence of a fluctuation dissipation theorem (FDT) to achieve such a simplification and who succeeded to prove a FDT for a large class of classical systems. A FDT gives, in fact, a relation between the two Green's functions occurring in the theory, namely, the propagator or correlation function (which governs the fluctuations) and the response function (whose imaginary part describes dissipation). In their renormalized perturbation theory Deker and Haake[2] propose to eliminate completely one type of Green's function and one type of self-energy by successive partial integrations of the time variables.

While MSR, as well as Deker and Haake, develop a formal renormalized perturbation theory based on Schwinger's functional method, it is the main aim of the present paper to derive a Wick's theorem for time-ordered products and hence to establish an explicit *unrenormalized* perturbation scheme. It is our belief that this Wick's theorem[3] gives the formal procedures of Refs. 1 and 2 a firmer and more transparent basis.

The retarded character of the response function implies that the associated lines form a "tree structure," i.e., a network without closed loops. This tree structure gives rise to "double graphs" analogous to those introduced into quantum field theory by Dyson in 1951 and discussed by Symanzik.[4] A double graph is obtained from a given tree structure by joining the free legs of the vertices by propagator lines.

It is interesting to note that the same double graphs also appear in Kawasaki's perturbation scheme,[5] which was designed to calculate dynamical critical phenomena. This is not surprising, since Kawasaki[5] starts from the same retarded

equation of motion for observables as Dyson[4] (see also Ref. 6). Other perturbation schemes for various correlation functions have been developed and applied in the critical region[7] and in turbulence.[1,3,8]

A well-known difficulty with quantum systems stems from the perturbative expansion of the canonical density matrix. This is because that expansion is identical with the time evolution operator taken at imaginary time $it=-1/k_BT$. Several formalisms have been devised to cope with the dilemma of a simultaneous chronological order along the real and the imaginary time axes (see, e.g., Refs. 9 and 10).

For classical canonical systems the perturbative expansion of the canonical probability density turns out to be much simpler. This is due essentially to Liouville's theorem or, more explicitly, to the skew symmetry of the matrix D occurring in the canonical equations of motion for the ψ variables. In noncanonical classical systems, such as those falling under classes A and B of Ref. 2, the skew symmetry of D and hence Liouville's theorem are lost.[11] In this respect the present paper does not have the generality necessary to cover all classical systems of interest. However, it turns out that the same perturbative expansion remains valid for noncanonical systems, including random forces,[11] so that the present restriction to canonical systems is justified.

We believe indeed that the present paper achieves the goal set by MSR, i.e., to free classical perturbation theory from the guesswork inherent in earlier formulations which made use of quantum-mechanical techniques and, in particular, of the limit $\hbar\to 0$. In fact, this last limit turns out to be very often ambiguous for dynamical calculations. As to the static problem, it is simplified by the absence of the $\hat{\psi}$ variables. And since the free Hamiltonian has a quadratic form in the ψ variables, Wick's theorem for ordinary ψ products is just a consequence of Gaussian integrals.[3,12]

On the other hand, the analogy with quantum theory has been followed as closely as possible in building up the classical perturbation scheme presented here. It is, in fact, useful to consider the set of initial values of the ψ variables as the "state" of the system and the full time evolution of observables as the "Heisenberg representation." The interaction-free evolution from the same state then plays the role of the "interaction representation," and as in the quantum case the key quantity for perturbation theory is the transformation S between the two representations.

As in quantum theory this S transformation also gives the perturbation expansion of the probability density ρ, and it is no surprise that we also need the well-known adiabatic switch-on condition. In its classical form this assumption states that when ρ is traced back to times $t\to-\infty$ along unperturbed orbits it coincides with the probability density ρ_0 of the unperturbed system. For probability densities ρ sufficiently general to describe nonequilibrium situations, which is the scope of this paper, the adiabatic switch-on condition is, of course, a serious physical assumption. While this condition is well known in quantum theory (see, e.g., Ref. 9), it has also been used in the microscopic formulation of kinetic theory (see, e.g., Pomeau and Résibois, Ref. 7).

II. CANONICAL DYNAMICS

We consider systems defined by a Hamiltonian $H(p,q)$ and choose for the canonical variables the notation

$$\psi_j=p_j\,,\quad \psi_{N+j}=q_j\,,\quad j=1,\ldots,N\,. \tag{2.1}$$

Introducing the skew-symmetric $2N\times 2N$ matrix

$$D=-\tilde{D}=-D^{-1}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}, \tag{2.2}$$

the equations of motion can be written in the compact form

$$\dot{\psi}_\nu=\frac{\partial H}{\partial\psi_\mu}D_{\mu\nu}\,,\quad \nu=1,\ldots,2N\,, \tag{2.3}$$

where summation over repeated indices is understood. Furthermore, defining the differential operators[1,2]

$$\hat{\psi}_\nu=D_{\nu\mu}\frac{\partial}{\partial\psi_\mu}, \tag{2.4}$$

the Liouvillian reads

$$\boldsymbol{L}=\frac{\partial H}{\partial\psi_\nu}\hat{\psi}_\nu=\dot{\psi}_\nu\frac{\partial}{\partial\psi_\nu}, \tag{2.5}$$

so that the equation of motion of any dynamical quantity $A(\psi,t)$ is given by

$$\frac{dA}{dt}=[\,\boldsymbol{L},A\,]+\frac{\partial A}{\partial t}, \tag{2.6}$$

where the commutator bracket automatically ensures that $\boldsymbol{L}$ acts only within it.

The above notation is particularly suited for the classical many-body problem, which is known[1,2] to lead to a doubling of the dynamical variables in the sense that Green's functions have to be introduced for pairs of both ψ and $\hat{\psi}$ variables. But in addition this notation also suggests an immediate generalization to noncanonical systems where the matrix D ceases to have the simple form (2.2).[11]

In order to formulate perturbation theory we split the Hamiltonian into a free part H_0 and an

interaction part H_1,

$$H = H_0 + H_1 . \tag{2.7}$$

H_0 is taken as real, positive definite, and of quadratic form, up to a constant,

$$H_0 = \tfrac{1}{2}\psi_\mu E_{\mu\nu}\psi_\nu , \tag{2.8}$$

so that according to (2.3) and (2.5) the free equations of motion are

$$\dot{\psi} = [L_0, \psi] = \psi\Lambda , \tag{2.9}$$

where

$$\Lambda = ED , \tag{2.10}$$

and where

$$L_0 = \psi_\mu \Lambda_{\mu\nu} \frac{\partial}{\partial \psi_\nu} \tag{2.11}$$

is the free Liouvillian.

There exists a nonsingular transformation $\psi \to \psi X$ which diagonalizes Λ according to

$$(X^{-1}\Lambda X)_{\mu\nu} = \lambda_\mu \delta_{\mu\nu} \tag{2.12}$$

(here μ is not summed). Solving (2.9) explicitly in this representation and transforming back, one finds

$$\psi^0_\mu(t) = \psi^0_\nu(t') W_{\nu\mu}(t - t') , \tag{2.13}$$

where

$$W_{\mu\nu}(t) = X_{\mu\rho} e^{\lambda_\rho t} X^{-1}_{\rho\nu} \tag{2.14}$$

is independent of the ψ's and the superscripts indicate free time evolution. From (2.12) and (2.14) we also obtain

$$\dot{W}(t) = W(t)\Lambda . \tag{2.15}$$

It is useful to introduce the time evolution in analogy to quantum mechanics (see, e.g., Ref. 9) by first defining the state of the classical system as the set of initial values at $t = 0$,

$$\psi(0) = \psi^0(0) = \psi . \tag{2.16}$$

Then Eqs. (2.3)–(2.9) are to be understood as the Schrödinger representation and the evolution of an observable from this fixed state,

$$A(\psi(t), t) = U(t) A(\psi, t) U^{-1}(t) , \tag{2.17}$$

is the Heisenberg representation, while the free evolution from the same state,

$$A(\psi^0(t), t) = U_0(t) A(\psi, t) U_0^{-1}(t) , \tag{2.18}$$

defines the interaction representation. It is sometimes of interest to generalize these transformations so as to have the group property, namely,

$$A(\psi(t), t) = U(t, t') A(\psi(t'), t) U(t', t) , \tag{2.19}$$

where

$$U(t, t') \equiv U(t) U^{-1}(t') = U(t, \tau) U(\tau, t') . \tag{2.20}$$

Equation (2.17) may also be generalized to functions of $\hat{\psi}$ by observing that for an arbitrary infinitesimal δ_ν

$$A(\psi + \delta) - A(\psi) = \delta_\nu D_{\nu\mu}[\hat{\psi}_\mu, A(\psi)] \tag{2.21}$$

is also an observable satisfying (2.17). Hence

$$A(\psi(t), \hat{\psi}(t), t) = U(t) A(\psi, \hat{\psi}, t) U^{-1}(t) , \tag{2.22}$$

where $\hat{\psi}(0) = \hat{\psi}$. This generalization will be important later; in particular, it applies to the Liouvillian.

In order to determine this transformation, we differentiate Eq. (2.17), leaving out the parametric time dependence for simplicity. This yields

$$\frac{d}{dt} A(\psi(t)) = U(t) \left(U^{-1}(t) \frac{dU(t)}{dt} A(\psi) + A(\psi) \frac{dU^{-1}(t)}{dt} U(t) \right) U^{-1}(t) , \tag{2.23}$$

or, with the Liouvillian,

$$L(t) \equiv L(\psi, \hat{\psi}, t) = U^{-1}(t) \frac{dU(t)}{dt} = -\frac{dU^{-1}(t)}{dt} U(t) ; \tag{2.24}$$

applying (2.22) to $L(t)$,

$$\frac{d}{dt} A(\psi(t)) = [L(\psi(t), \hat{\psi}(t), t), A(\psi(t))] , \tag{2.25}$$

which gives the precise meaning of Eq. (2.6). Equation (2.24) may also be written

$$\dot{U}(t) = U(t) L(t) = L(\psi(t), \hat{\psi}(t), t) U(t) , \tag{2.26}$$

where we have made use again of (2.22). Without parametric time dependence L is constant and

$$U(t) = e^{Lt} . \tag{2.27}$$

The free Liouvillian, which was assumed to have no parametric time dependence, has the property

$$L_0(\psi^0(t), \hat{\psi}^0(t)) = L_0(\psi, \hat{\psi}) \equiv L_0 , \tag{2.28}$$

which follows from (2.22) and (2.27) applied to the free motion.

In perturbation theory the transformation between the Heisenberg and the interaction representations is of particular interest. It is defined with respect to the initial state (2.16) at $t = 0$ as[13]

$$A(\psi(t), \hat{\psi}(t), t) = S(0, t) A(\psi^0(t), \hat{\psi}^0(t), t) S(t, 0) . \tag{2.29}$$

Application of Eqs. (2.17) and (2.18) immediately gives

$$S(0, t) = S^{-1}(t, 0) = U(t) U_0^{-1}(t) . \tag{2.30}$$

We want this transformation, when applied to a product AB, to have the group property. This is assured by the definition

$$\begin{aligned} S(t,t') &\equiv S(t,0)S(0,t') \\ &= U_0(t)U^{-1}(t)U(t')U_0^{-1}(t') \\ &= S(t,\tau)S(\tau,t') . \end{aligned} \tag{2.31}$$

In order to determine this transformation we take time derivatives of (2.31), making use of Eq. (2.26),

$$\begin{aligned} \frac{\partial}{\partial t}S(t,t') &= -L_1^0(t)S(t,t') , \\ \frac{\partial}{\partial t'}S(t,t') &= S(t,t')L_1^0(t') . \end{aligned} \tag{2.32}$$

Here

$$L_1(\psi,\hat{\psi},t) = \frac{\partial H_1(\psi,t)}{\partial \psi_\nu}\hat{\psi}_\nu \tag{2.33}$$

is the interaction Liouvillian $L(t) - L_0$, and

$$\begin{aligned} L_1^0(t) &\equiv L_1(\psi^0(t),\hat{\psi}^0(t),t) \\ &= e^{L_0 t}L_1(\psi,\hat{\psi},t)e^{-L_0 t} \end{aligned} \tag{2.34}$$

is its interaction representation, in agreement with (2.18). Equations (2.32) may be written in integral equation form,

$$\begin{aligned} S(t,t') &= 1 - \int_{t'}^{t} d\tau\, L_1^0(\tau)S(\tau,t') \\ &= 1 + \int_{t}^{t'} d\tau\, S(t,\tau)L_1^0(\tau) , \end{aligned} \tag{2.35}$$

which by iteration yields the well-known expressions[13]

$$\begin{aligned} S(t,t') &= T\exp\left(-\int_{t'}^{t} d\tau\, L_1^0(\tau)\right) \\ &= \overline{T}\exp\left(+\int_{t}^{t'} d\tau\, L_1^0(\tau)\right) . \end{aligned} \tag{2.36}$$

Here T and $\overline{T}$ are the chronological and antichronological operators which order the factors of a product such that increasing time arguments run from right to left and from left to right, respectively.

From Eq. (2.33) one sees that if

$$H_1 \propto \prod_{i=1}^{n} \psi_{\nu_i} ,$$

that is, if the interaction vertex has n ψ legs, then L_1 has always one $\hat{\psi}$ leg and $(n-1)$ ψ legs. We will distinguish the $\hat{\psi}$ leg graphically by an arrow pointing towards the vertex (see Fig. 1). From the point of view of the doubling of variables $(q,p) \to (\psi,\hat{\psi})$ mentioned earlier, this type of vertex has no analog in conventional many-body quantum theory. In fact, it gives rise to complications which

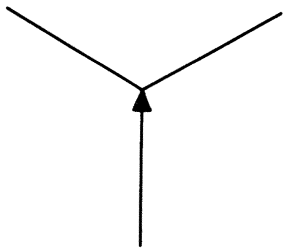

FIG. 1. Graphical representation of a vertex with two ψ legs and one $\hat{\psi}$ leg (with arrow), according to Eq. (2.33).

are typical of classical perturbation theory, as will be seen below. An exception, however, is given by quantum hydrodynamics, where vertices with two p legs occur (see, e.g., Ref. 10).

It is important for the existence of a Wick's theorem (see Sec. IV) that $\hat{\psi}^0$ variables commute with each other for any time arguments and indices,

$$[\hat{\psi}_\mu^0(t),\hat{\psi}_\nu^0(t')] = 0 . \tag{2.37}$$

To prove this, it is sufficient to show that the commutator

$$\left[\frac{\partial}{\partial\psi_\mu^0(t)},\frac{\partial}{\partial\psi_\nu^0(t-\tau)}\right] = e^{L_0 t}[\partial_\mu, e^{-L_0\tau}\partial_\nu e^{+L_0\tau}]e^{-L_0 t}$$

vanishes, where $\partial_\mu = \partial/\partial\psi_\mu$ in the notation of (2.16). First, it follows from (2.11) that

$$[\partial_\nu, e^{L_0\tau}] = e^{L_0\tau}\tau\Lambda_{\nu\lambda}\partial_\lambda ,$$

and hence

$$e^{-L_0\tau}\partial_\nu e^{L_0\tau} = \tau\Lambda_{\nu\lambda}\partial_\lambda + \partial_\nu .$$

But the last expression obviously commutes with ∂_μ. Equation (2.37) is, of course, not true for the perturbed variables $\hat{\psi}(t)$.

III. GREEN'S FUNCTIONS AND SELF-ENERGIES

We are interested in the statistical averages of observables $A(\psi,\hat{\psi})$,

$$\begin{aligned} \langle A\rangle &= \mathrm{Tr}(\rho A) \\ &= \int \prod_\sigma d\psi_\sigma \rho(\psi)A(\psi,\hat{\psi},t) , \end{aligned} \tag{3.1}$$

with an arbitrary density matrix ρ obeying the normalization

$$\mathrm{Tr}\rho = 1 . \tag{3.2}$$

Since we have to allow for both ψ and $\hat{\psi}$ variables the convention adopted in (3.1) that ρ always stands *to the left-hand side* of the observables is very important. This is, in fact, different from the quantum-mechanical trace, which is cyclic with respect to any product.

We want to study the response of the system to a

particular small external field $\delta f_\nu(t)$ which is switched on at t_0 and which we show explicitly by writing, in the Schrödinger representation,

$$H_f(t) = H + \delta H(t), \quad \delta H(t) = \delta f_\nu(t)\psi_\nu . \tag{3.3}$$

The associated Liouvillian is then

$$L_f(t) = L + \delta L(t), \quad \delta L(t) = \delta f_\nu(t)\hat{\psi}_\nu . \tag{3.4}$$

In interaction representation with respect to $\delta f_\nu(t)$ averages are formed with

$$\rho_f(t) = \rho + \delta\rho(t),$$

while ψ_μ evolves as $\psi_\mu(t)$. On the other hand, in Heisenberg representation averages are formed with ρ, while ψ_μ evolves as $\psi^f_\mu(t)$. Hence

$$\langle \psi^f_\mu(t)\rangle = \mathrm{Tr}\rho\psi^f_\mu(t) = \mathrm{Tr}\rho_f(t)\psi(t)$$

or

$$\delta\langle\psi(t)\rangle = \mathrm{Tr}\delta\rho_f(t)\psi(t) = \langle\psi^f(t) - \psi(t)\rangle . \tag{3.5}$$

Now according to (2.29), written for the initial time t_0,

$$\psi^f_\mu(t) = S^f(t_0, t)\psi(t)S^f(t, t_0), \tag{3.6}$$

where $S^f(t, t_0)$ is obtained from (2.35) with the interaction Liouvillian (3.4) in the interaction representation (2.34); to lowest order in $\delta f_\nu(t)$,

$$S^f(t, t_0) = 1 - \int_{t_0}^{t} dt'\, \delta f_\nu(t')\hat{\psi}(t') . \tag{3.7}$$

Insertion into (3.7) yields

$$\psi^f_\mu(t) - \psi_\mu(t) = -\int_{t_0}^{t} dt'\, \delta f_\nu(t')[\psi_\mu(t), \hat{\psi}_\nu(t')]$$

or

$$\delta\langle\psi_\mu(t)\rangle = \int_{t_0}^{t} dt'\, \delta f_\nu(t')D_{\nu\lambda}\left\langle\frac{\partial\psi_\mu(t)}{\partial\psi_\lambda(t')}\right\rangle . \tag{3.8}$$

Taking the switch-on time t_0 to $-\infty$ we arrive at the response function

$$R_{\mu\nu}(t, t') \equiv \frac{\delta\langle\psi_\mu(t)\rangle}{\delta f_\nu(t')} = \theta(t - t')D_{\nu\lambda}\left\langle\frac{\partial\psi_\mu(t)}{\partial\psi_\lambda(t')}\right\rangle . \tag{3.9}$$

We define the Green's functions

$$G_{\phi(t)\phi'(t')} = G_{\phi'(t')\phi(t)} = \langle\overline{T}(\phi(t)\phi'(t'))\rangle , \tag{3.10}$$

where ϕ and ϕ' are any ψ_ν or $\hat{\psi}_\nu$. In particular,

$$G_{\mu\nu}(t, t') \equiv G_{\psi_\mu(t)\psi_\nu(t')} = \langle\psi_\mu(t)\psi_\nu(t')\rangle \tag{3.11}$$

is the propagator which is symmetric in the two variables, while

$$G_{\psi_\mu(t)\hat{\psi}_\nu(t')} = \begin{cases} \langle\psi_\mu(t)\hat{\psi}_\nu(t')\rangle = 0, & \text{for } t < t', \\ \langle\hat{\psi}_\nu(t')\psi_\nu(t)\rangle , & \text{for } t' < t \end{cases}$$

is recognized as the response function (3.9),

$$R_{\mu\nu}(t, t') = G_{\psi_\mu(t)\hat{\psi}_\nu(t')} . \tag{3.12}$$

Indeed, according to (2.23),

$$\hat{\psi}_\nu(t) = U(t)D_{\nu\mu}\frac{\partial}{\partial\psi_\mu}U^{-1}(t),$$

where $\psi(0) = \psi$ are the initial values. But from (2.26) and (2.5) we see that $U^{-1}(t)$ is an exponential of differential operators and hence is unity when it stands completely to the right-hand side. From this argument it also follows that[1,2]

$$G_{\hat{\psi}_\mu(t)\hat{\psi}_\nu(t')} = 0 . \tag{3.13}$$

In the case of *local thermal equilibrium* the Hamiltonian will in general have a parametric time dependence due to external fields, and the density matrix has the canonical form

$$\rho = \exp[F(t) - H(\psi(t), t)] . \tag{3.14}$$

Here the free energy $F(t)$ is determined by the normalization condition (3.2), and we have put $k_B T = 1$ for simplicity.

With (3.14) a useful identity is obtained, for any observable A bounded by a polynomial in ψ and $\hat{\psi}$, by partial integration at an arbitrary time t,[14]

$$\mathrm{Tr}(L\rho A) = -\int\prod_\sigma d\psi_\sigma(t)D_{\mu\nu}\frac{\partial^2 H}{\partial\psi_\nu(t)\partial\psi_\mu(t)}\rho A = 0 . \tag{3.15}$$

Here we have made use of Eqs. (2.4) and (2.5), and the vanishing is due to the skew symmetry (2.2) of D, or, equivalently, to Liouville's theorem.

Specializing to *global equilibrium*, where H has no parametric time dependence and ρ is constant, Eq. (2.6) shows that ρ commutes with L. Equation (3.15) then implies $\langle[L, A]\rangle = 0$, or, in integral form making use of Eqs. (2.22) and (2.27),

$$\langle A(\psi(t), \hat{\psi}(t))\rangle = \langle A(\psi, \hat{\psi})\rangle , \tag{3.16}$$

which expresses time-translation invariance of global equilibrium. In this case it follows with Eqs. (2.19) and (2.20) that the Green's functions (3.10) depend only on the time difference $t - t'$. This is true, in particular, of the free Green's functions

$$G^0_{\phi(t),\phi'(t')} = \langle\overline{T}(\phi^0(t - t')\phi'^0(0))\rangle_0 , \tag{3.17}$$

in which the average is defined with the unperturbed density matrix

$$\rho_0 = e^{F_0 - H_0(\psi)} . \tag{3.18}$$

From (2.13) we obtain with the initial condition (2.16)

$$G^0_{\mu\nu}(t) = \langle\psi_\lambda\psi_\nu\rangle_0 W_{\lambda\mu}(t) . \tag{3.19}$$

In view of Eq. (2.8) the average $\langle\psi_\lambda\psi_\nu\rangle_0$ may be evaluated by making use of the properties of Gaussian integrals. With the help of the identity[12]

$$\langle e^{\xi_\nu\psi_\nu}\rangle_0 = \exp[\tfrac{1}{2}\xi_\mu(E^{-1})_{\mu\nu}\xi_\nu]\,, \tag{3.20}$$

we immediately obtain

$$\langle\psi_\alpha\psi_\beta\rangle_0 = \frac{\partial^2}{\partial\xi_\alpha\,\partial\xi_\beta}\langle e^{\xi_\nu\psi_\nu}\rangle_0\Big|_{\xi=0} = (E^{-1})_{\alpha\beta}\,, \tag{3.21}$$

so that (3.19) becomes

$$G^0_{\mu\nu}(t) = \tilde{W}_{\mu\lambda}(t)(E^{-1})_{\lambda\nu}\,. \tag{3.22}$$

The free-response function follows immediately from (3.9) and (2.13),

$$R^0_{\mu\nu}(t) = -\theta(t)\tilde{W}_{\mu\lambda}(t)D_{\lambda\nu}\,. \tag{3.23}$$

The occurrence, for classical systems, of two types of Green's functions is analogous to the situation with quantum systems without particle conservation, such as the quasiparticles in superconductors or superfluids[9] or the phonons in quantum fluids[15] or dielectric crystals.[16] As in these theories a 2×2 matrix form for the Green's functions is indicated and was actually introduced by MSR.[1] Here we find it convenient to introduce a $4N\times4N$ matrix notation,

$$\underline{G} = \begin{pmatrix} G_{\psi_\mu\psi_\nu} & G_{\psi_\mu\hat{\psi}_\nu} \\ G_{\hat{\psi}_\mu\psi_\nu} & G_{\hat{\psi}_\mu\hat{\psi}_\nu} \end{pmatrix}. \tag{3.24}$$

Similarly we introduce a matrix

$$\underline{\Sigma} = \begin{pmatrix} \Sigma_{\psi_\mu\psi_\nu} & \Sigma_{\psi_\mu\hat{\psi}_\nu} \\ \Sigma_{\hat{\psi}_\mu\psi_\nu} & \Sigma_{\hat{\psi}_\mu\hat{\psi}_\nu} \end{pmatrix} \tag{3.25}$$

for the self-energies which are defined through the Dyson equation

$$\underline{G} = \underline{G}^0 + \underline{G}^0\underline{\Sigma}\underline{G}\,, \tag{3.26}$$

or formally by

$$\underline{\Sigma} = \underline{G}^{0-1} - \underline{G}^{-1}\,. \tag{3.27}$$

Note that in Eq. (3.26) matrix multiplication also includes the time-convolution integrals.

Defining the transposed response function as

$$(R^T)_{\mu\nu}(t,t') = R_{\nu\mu}(t',t)\,, \tag{3.28}$$

Eqs. (3.11)–(3.13) lead to the following form of the matrix (3.24):

$$\underline{G} = \begin{pmatrix} G & R \\ R^T & 0 \end{pmatrix}, \tag{3.29}$$

whose inverse is, formally,

$$\underline{G}^{-1} = \begin{pmatrix} 0 & (R^T)^{-1} \\ R^{-1} & -R^{-1}G(R^T)^{-1} \end{pmatrix}. \tag{3.30}$$

By comparison with Eqs. (3.25) and (3.27) it then follows immediately that[1,2]

$$\Sigma_{\psi\psi} = 0\,. \tag{3.31}$$

Introducing for the remaining self-energies a notation analogous to the one chosen for the Green's functions,

$$\begin{aligned} &\Sigma_{\mu\nu}(t,t') = \Sigma_{\hat{\psi}_\mu(t)\hat{\psi}_\nu(t')}\,, \\ &\Pi_{\mu\nu}(t,t') = \Sigma_{\psi_\mu(t)\hat{\psi}_\nu(t')}\,, \\ &(\Pi^T)_{\mu\nu}(t,t') = \Pi_{\nu\mu}(t',t) = \Sigma_{\hat{\psi}_\mu(t)\psi_\nu(t')}\,, \end{aligned} \tag{3.32}$$

we have

$$\underline{\Sigma} = \begin{pmatrix} 0 & \Pi \\ \Pi^T & \Sigma \end{pmatrix}. \tag{3.33}$$

In terms of the $2N\times2N$ submatrices introduced in Eqs. (3.29) and (3.33) the Dyson equation (3.26) has the following content:

$$\begin{aligned} &G - G^0 = G^0\Pi R^T + R^0\Pi^T G + R^0\Sigma R^T\,, \\ &R - R^0 = R^0\Pi^T R\,. \end{aligned} \tag{3.34}$$

These relations are also readily verified starting from Eqs. (3.27) and (3.30).

IV. WICK'S THEOREM. DIAGRAMS

In Sec. II we have reduced the full time evolution of observables to the free one with the help of the operator $S(t,t')$ [see Eqs. (2.29), (2.31), and (2.36)]. In order to arrive at a perturbation scheme in the form of a systematic diagrammatic analysis we also need the reduction of the general density matrix ρ to the free matrix ρ_0 of Eq. (3.18).

Liouville's theorem states that

$$\frac{d\rho}{dt} = 0 = [L,\rho] + \frac{\partial\rho}{\partial t}\,,$$

or, in integrated form, in the notation of (2.16),

$$\rho(\psi(t),t) = \rho(\psi,0) \equiv \rho = \text{const.} \tag{4.1}$$

On the other hand, Eq. (2.29), applied to the function $\rho(\psi(t),t)$, reads

$$\rho(\psi(t),t) = S(0,t)\rho(\psi^0(t),t)S(t,0)\,. \tag{4.2}$$

Now the adiabatic switch-on condition states that

$$\lim_{t\to-\infty}\rho(\psi^0(t),t) = \lim_{t\to-\infty}\rho_0(\psi^0(t)) = \rho_0\,, \tag{4.3}$$

where ρ_0 is given by (3.18). After taking the limit $t\to-\infty$ in Eq. (4.2), insertion of (4.3) leads to the desired result,

$$\rho = S(0,-\infty)\rho_0 S(-\infty,0)\,. \tag{4.4}$$

Here we have, of course, assumed the existence of the limit $t\to-\infty$ on both sides of Eq. (4.2). Since we want our theory to be sufficiently general to describe nonequilibrium situations, ρ must be left

quite general. In this case the switch-on condition (4.3) is a serious physical assumption which, however, is currently and successfully made in the literature.

With Eqs. (2.26) and (4.4) it is now possible to reduce an arbitrary $\overline{T}$ product of polynomials $A(\psi, \hat{\psi})$ to the interaction representation. Making use of the group property (2.31) and of the anti-time-ordering action of the operator $\overline{T}$ we get

$$\langle \overline{T}(A_1(t_1)\cdots A_n(t_n))\rangle = \int \prod_\sigma d\psi_\sigma [S(0,-\infty)\rho_0 \overline{T}(S(-\infty,+\infty)A_1^0(t_1)\cdots A_n^0(t_n))], \tag{4.5}$$

where we have introduced a factor $S(t_n, +\infty) = 1$ at the far right-hand side.

In order to get rid of the factor $S(0,-\infty)$ to the left-hand side of ρ_0 in Eq. (4.5), we write

$$S(0,-\infty) = 1 - \int_{-\infty}^{0} d\tau \frac{\partial H_1(\psi^0(\tau),\tau)}{\partial \psi_\mu^0(\tau)} D_{\mu\nu} \times \frac{\partial}{\partial \psi_\nu^0(\tau)} S(\tau,-\infty),$$

where we have made use of (2.35), (2.34), (2.33), and (2.4). Transforming the integration variables in Eq. (4.5) to $\psi^0(\tau)$, we perform a partial integration over $\psi_\nu^0(\tau)$ of the term proportional to $S(0,-\infty) - 1$. Provided that the exponential decay of ρ_0 is strong enough to annihilate the boundary terms of this partial integration, we end up with a factor

$$D_{\mu\nu} \frac{\partial^2 H_1(\psi^0(\tau),\tau)}{\partial \psi_\mu^0(\tau)\, \partial \psi_\nu^0(\tau)}$$

which, as in Eq. (3.15), vanishes because of the skew symmetry of the D matrix, or, equivalently, because of Liouville's theorem. Hence $S(0,-\infty)$ can be replaced by unity in Eq. (4.5), so that

$$\langle \overline{T}(A_1(t_1)\cdots A_n(t_n))\rangle = \langle \overline{T}(S(-\infty,+\infty)A_1^0(t_1)\cdots A_n^0(t_n))\rangle_0 . \tag{4.6}$$

Taking a fixed term in the Taylor expansion (2.36) of $S(-\infty,+\infty)$, the last expression reduces to a sum of new $\overline{T}$-products,

$$\tau^0(\phi_1\cdots\phi_m) \equiv \langle \overline{T}(\phi_1^0(t_1)\cdots\phi_m^0(t_m))\rangle_0 , \tag{4.7}$$

multiplied with the vertex functions contained in the interaction Liouvillian L_1. As in Eqs. (3.10) and (3.17) we want the ϕ's in (4.7) to stand for ψ or $\hat{\psi}$ variables. This requires, however, that some of the time arguments may coincide, first, because L_1 contains more than one factor ψ, and, second, because we allowed the A's in the product (4.5) to be arbitrary polynomials.

Our next task is the factorization of the products (4.7), or, in other words, the establishment of a Wick's theorem for $\overline{T}$ products. The first step is to eliminate a given $\hat{\psi}_\nu^0(t')$ by commuting it successively with all factors standing to its right-hand side in the anti-time-order. This we do until $\hat{\psi}_\nu^0(t')$ arrives at the right-hand end of the product, where it annihilates.

According to (2.37) commutation with another factor $\hat{\psi}$ has no effect, while commutation with a ψ introduces a ψ-independent term

$$[\hat{\psi}_\nu^0(t'), \psi_\mu^0(t)] = D_{\nu\lambda} \frac{\partial \psi_\mu^0(t)}{\partial \psi_\lambda^0(t')} = D_{\nu\lambda} W_{\lambda\mu}(t-t') . \tag{4.8}$$

This is true if $\psi_\mu^0(t)$ stands to the right-hand of $\hat{\psi}_\nu^0(t')$ in the anti-time-order, that is, if $t > t'$. We may extend (4.8) to $t < t'$ with the help of a factor $\theta(t-t')$ by defining the contraction (denoted by dots to the right of the symbols)

$$\langle \overline{T}(\cdots \hat{\psi}_\nu^{0\bullet}(t')\cdots\psi_\mu^{0\bullet}(t)\cdots)\rangle_0 = \langle \overline{T}(\cdots\times\cdots\times\cdots)\rangle_0 \langle \overline{T}(\hat{\psi}_\nu^0(t')\psi_\mu^0(t))\rangle_0 , \tag{4.9}$$

where a cross means omission of the corresponding factor. From Eqs. (3.9), (3.10), and (3.12) applied to the free Green's functions it is readily seen that for $t > t'$ the contraction in (4.9) is identical with (4.8).

Thus we arrive at the first result,

$$\langle \overline{T}(\cdots\hat{\psi}^0\cdots)\rangle_0 = \sum \langle \overline{T}(\cdots\hat{\psi}^{0\bullet}\cdots\psi^{0\bullet}\cdots)\rangle_0 , \tag{4.10}$$

where the sum runs over all ψ factors in the product. Since according to (4.9) contraction eliminates a $\hat{\psi}$, ψ pair in $\tau^0(\phi_1\cdots\phi_m)$, all $\hat{\psi}$'s may be eliminated in favor of free-response functions by a sufficient number of contractions. Obviously, a $\tau^0(\phi_1\cdots\phi_m)$ which contains more $\hat{\psi}$'s than ψ's is zero.

We are thus left with products $\tau^0(\psi_{\mu_1}\cdots\psi_{\mu_m})$ of commuting factors which, according to (2.13) and (2.16), may be put into the form

$$\tau^0(\psi_{\mu_1}\cdots\psi_{\mu_m}) = \langle \psi_{\nu_1}\cdots\psi_{\nu_m}\rangle_0 W_{\nu_1\mu_1}(t_1)\cdots W_{\nu_m\mu_m}(t_m) . \tag{4.11}$$

The products $\langle \psi_{\nu_1}\cdots\psi_{\nu_m}\rangle_0$ may be generated from the identity (3.20) by differentiation with respect to $\xi_{\nu_1}\cdots\xi_{\nu_m}$ and then putting $\xi = 0$. It immediately follows that $\langle \psi_{\nu_1}\cdots\psi_{\nu_m}\rangle_0 = 0$ for odd m. For $m = 2n$ we may write

$$\langle \psi_{\nu_1}\cdots\psi_{\nu_{2n}}\rangle_0 = \frac{1}{2^n n!} (E^{-1})_{\sigma_1\tau_1}\cdots(E^{-1})_{\sigma_n\tau_n} \times \partial_{\nu_1}\cdots\partial_{\nu_{2n}}(\xi_{\sigma_1}\xi_{\tau_1}\cdots\xi_{\sigma_n}\xi_{\tau_n}), \tag{4.12}$$

where $\partial_\nu = \partial/\partial\xi_\nu$. Now we select an arbitrary pair of indices α, β out of $\nu_1\cdots\nu_{2n}$ such that $\partial_\alpha\partial_\beta$ acts

on the last pair $\xi_{\sigma_n}\xi_{\tau_n}$. Because of the freedom in the labelings and the symmetry of E this can be done in $2n$ ways; the result is

$$(E^{-1})_{\alpha\beta}\Big(\frac{1}{2^{n-1}(n-1)!}(E^{-1})_{\sigma_1\tau_1}\cdots(E^{-1})_{\sigma_{n-1}\tau_{n-1}} \times\cdots\not\partial_\alpha\cdots\not\partial_\beta\cdots \times(\xi_{\sigma_1}\xi_{\tau_1}\cdots\xi_{\sigma_{n-1}}\xi_{\tau_{n-1}})\Big),$$

where the barred derivatives are to be omitted. This can be written in the form of a contraction,

$$\langle\cdots\dot{\psi}_\alpha\cdots\dot{\psi}_\beta\cdots\rangle_0=\langle\cdots\times\cdots\times\cdots\rangle_0(E^{-1})_{\alpha\beta}. \tag{4.13}$$

Now the selection of pairs of indices $\alpha\beta$ on the right-hand side of (4.12) can be done in $n(2n-1)$ ways; hence

$$\langle\psi_{\nu_1}\cdots\psi_{\nu_{2n}}\rangle_0=\sum\langle\cdots\dot{\psi}\cdots\dot{\psi}\cdots\rangle_0, \tag{4.14}$$

where the sum extends over all pairs.

Reinstating the time dependence we may use Eqs. (3.17) and (3.22) to define the contraction

$$\langle\overline{T}(\cdots\psi^0_\alpha{}^{\bullet}(t)\cdots\psi^0_\beta{}^{\bullet}(t')\cdots)\rangle_0 =\langle\overline{T}(\cdots\times\cdots\times\cdots)\rangle_0\langle\overline{T}(\psi^0_\alpha(t)\psi^0_\beta(t'))\rangle_0, \tag{4.15}$$

which is written in the same form as (4.9). Making use of (4.14) and (4.15) in (4.11) we obtain

$$\langle\overline{T}(\cdots\psi^0\cdots\psi^0\cdots)\rangle_0=\sum\langle\overline{T}(\cdots\psi^{0\bullet}\cdots\psi^{0\bullet}\cdots)\rangle_0. \tag{4.16}$$

By successive application of this reduction we finally arrive at a complete factorization of any $\overline{T}$ product. This is Wick's theorem, which now may be stated in the following form:

$$\langle\overline{T}(\phi^0_1(t_1)\cdots\phi^0_{2n}(t_{2n}))\rangle_0 =\sum_{(\nu_i,\bar{\nu}_i)}\prod_{i=1}^{n}\langle\overline{T}(\phi^0_{\nu_i}(t_{\nu_i})\phi^0_{\bar{\nu}_i}(t_{\bar{\nu}_i}))\rangle_0, \tag{4.17}$$

where the sum is over all pairings $(\nu_i,\bar{\nu}_i)$.

This derivation of Wick's theorem is very similar to the one given for imaginary-time-ordered products by one of us[17] where also three types of contractions occurred due to the nonvanishing of normally ordered products. Here the $\hat{\psi}$ variables behave like absorption operators and the shifting to the right-hand side corresponds to the standard derivation of Wick's theorem for normally ordered products in quantum field theory.[18] However, the ψ variables are not analogous to creation operators, and this gives rise to the complication analogous to those encountered with thermodynamic Green's functions.[17]

We now are in a position to introduce diagrams. In accord with the diagrammatic definition of vertices introduced in Fig. 1 we associate a simple line to the propagator G^0 and a simple line with an outward arrow pointing towards the past for the response function R^0, and similarly with double lines for G and R (Fig. 2). It follows immediately from these definitions that closed loops of R lines vanish. This leads to a *tree structure* of R lines which is defined such that exactly one R line is incident at every vertex, while the number of emerging R lines may vary between zero and the number of legs of the vertex. The procedure to construct diagrams of given vertex structure (fixed number of legs), given order (fixed number of vertices), and given external lines (fixed number and type) now is as follows: Insert all possible tree diagrams into the given structure such that each vertex has exactly one arrow, and then fill in all possible propagator lines.

Thus the diagrams have the structure of *double graphs* similar to those introduced in quantum field theory by Dyson in 1951 for retarded products.[4] As in our case Dyson's tree structure is formed by retarded Green's functions, and the number of tree lines emerging at every vertex is exactly unity, while the number of incident lines may vary between zero and the number of legs of the vertex [see Fig. 4 of Ref. 4(b)]. Note that our arrows have direction opposite to those of Symanzik. The reason is that we introduced arrows as a property of the interaction vertex (see Fig. 1), which here is the natural thing to do. It is interesting to note also that Kawasaki's diagrams are exactly the same double graphs, the only difference being that instead of drawing arrows Kawasaki assigns a definite time direction to his diagrams.[5] This similarity is not surprising, since Kawasaki starts from the same retarded equation of motion as Dyson and Symanzik.

As an application let us now discuss the diagrammatic content of the Dyson equation for vertices with three legs. In Fig. 3 the property (3.31)

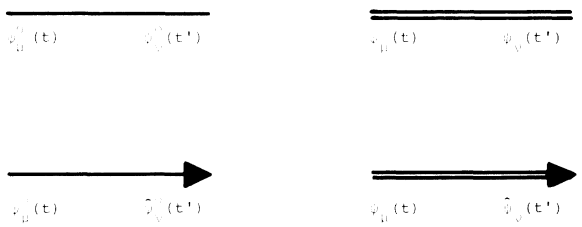

FIG. 2. Graphical representation of the free propagator $G^0_{\mu\nu}(t-t')$ (single line), the free response function $R^0_{\mu\nu}(t-t')$ (single line with arrow), the full propagator $G_{\mu\nu}(t-t')$ (double line), and the full response function $R_{\mu\nu}(t-t')$ (double line with arrow). Arrows point towards the past.

is seen from the diagrams for $\Sigma_{\psi\psi}$, which all vanish (closed loops). Figure 4 shows the lowest-order contributions to Π and Σ. Note that the second Eq. (3.34) is exactly represented by Fig. 4(a) of Ref. 1(a), whereas Fig. 4(b) of Ref. 1(a) may be obtained from the first Eq. (3.34) only under special requirements pertaining to the Navier-Stokes equation.

V. FLUCTUATION-DISSIPATION THEOREM. DISCUSSION

As observed by MSR[1] and by Deker and Haake[2] the complication of two types of diagrams may be reduced in part by exploiting the connection between propagators and response functions known as the fluctuation-dissipation theorem (FDT). The derivation of a FDT for classical canonical systems has been given independently in Refs. 2 and 14. The purpose of the present rederivation is to show the extent of its validity. It turns out, in fact, that the key property needed is the canonical form (3.14) of the density matrix.

Starting from Eq. (3.9), we transform the integration variables of the average to $\psi(t')$ and perform a partial integration of $\psi_\lambda(t')$. The result is

$$R_{\mu\nu}(t,t') = \theta(t-t')D_{\nu\lambda}\lim_{\psi_\lambda\to\infty}\left(\rho\psi_\mu(t)\Big|_{-\psi_\lambda}^{+\psi_\lambda} - \int_{-\psi_\lambda}^{+\psi_\lambda}\prod_\sigma\psi_\sigma(t')\frac{\partial\rho}{\partial\psi_\lambda(t')}\psi_\mu(t)\right), \tag{5.1}$$

where, according to (4.1), $\rho=\rho(\psi(t'),t')$. If ρ is of the local equilibrium form (3.14), where H may still depend on external fields, then the boundary terms vanish, and, in view of (2.3),

$$D_{\nu\lambda}\frac{\partial\rho}{\partial\psi_\lambda(t')} = \rho\dot{\psi}_\nu(t') . \tag{5.2}$$

Thus (5.1) becomes

$$R_{\mu\nu}(t,t') = -\theta(t-t')\frac{\partial G_{\mu\nu}(t,t')}{\partial t'}, \tag{5.3}$$

which is the FDT. It is obvious from this derivation that the FDT will not be true for general non-equilibrium situations.

For the transposed response function as defined in (3.28) the FDT reads

$$R^T_{\mu\nu}(t,t') = -\theta(t'-t)\frac{\partial G_{\mu\nu}(t,t')}{\partial t} . \tag{5.4}$$

In the special case of global equilibrium where the Green's functions depend only on the time difference, Eqs. (5.3) and (5.4) may be combined into the simple matrix relation [cf. Eq. (2.45) of Ma and Mazenko, Ref. 6]

$$R(t) - R^T(t) = \dot{G}(t) . \tag{5.5}$$

As was emphasized by Deker and Haake,[2] the existence of a FDT can be used to eliminate one of the two self-energies Σ and Π introduced in Sec. III. This is true *provided that global equilibrium holds*, so that Eq. (5.5) is applicable; indeed we have not been able to derive this relation between Σ and Π for *local* equilibrium.

We start from Eqs. (3.34) by projecting out G^0

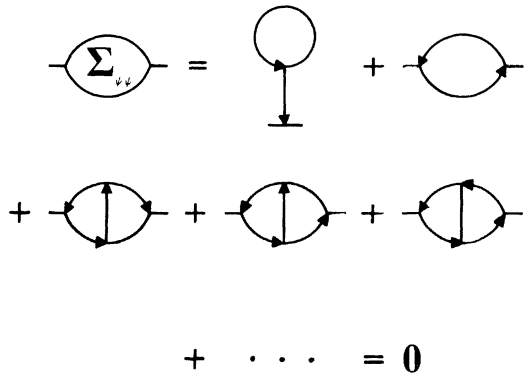

FIG. 3. Lowest-order diagrams contributing to Eq. (3.31). All diagrams vanish because of closed response function loops .

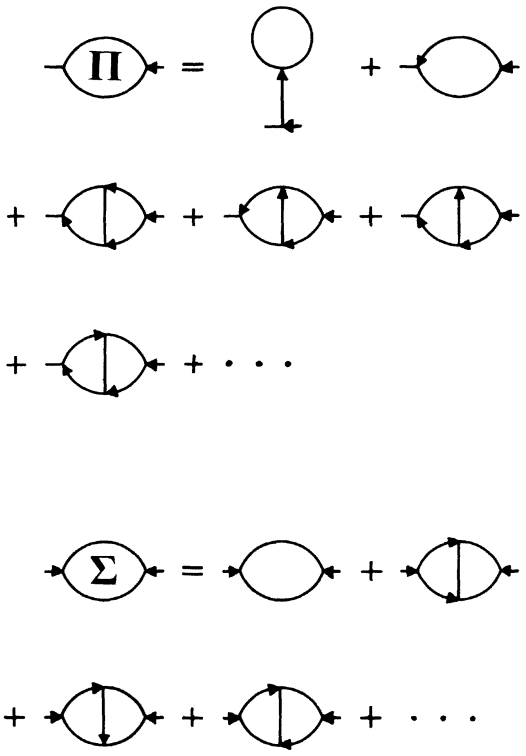

FIG. 4. Lowest-order diagrams contributing to the self-energies Π and Σ according to Eqs. (3.34).

with the help of the relation

$$\left(\frac{d}{dt}-\tilde{\Lambda}\right)G^0(t)=0\,, \tag{5.6}$$

which follows immediately from Eqs. (3.22) and (2.15). Since according to (3.23), (2.14), and (2.15)

$$\left(\frac{d}{dt}-\tilde{\Lambda}\right)R^0(t)=-\delta(t)D\,, \tag{5.7}$$

this projection yields

$$\left(\frac{d}{dt}-\tilde{\Lambda}\right)G=-D(\Pi^T G+\Sigma R^T)\,, \tag{5.8}$$

$$\left(\frac{d}{dt}-\tilde{\Lambda}\right)R=-D(\underline{1}+\Pi^T R)\,, \tag{5.9}$$

where matrix multiplication and time integration are understood. We now take the time derivative of Eq. (5.8). This step requires some precautions because of the step functions contained on the right-hand side.

Indeed, causality of $R(t)$ implies analyticity of its Fourier transform

$$R(\omega)=\int_0^\infty dt\,R(t)e^{i\omega t}$$

in the upper half-plane $\mathrm{Im}\omega>0$. Then $R^{-1}(\omega)$ exists and is analytical (up to poles) in the same domain. Therefore $R^{-1}(t)$ also exists and is causal, while for $R^T(t)$ and $(R^T)^{-1}(t)$ anticausality holds, i.e.,

$$\begin{aligned}&R(t),R^{-1}(t),\Pi^T(t)\propto\theta(t)\,,\\ &R^T(t),(R^T)^{-1}(t),\Pi(t)\propto\theta(-t)\,.\end{aligned} \tag{5.10}$$

These relations, together with time-translation invariance, imply that

$$\begin{aligned}\Pi^T G&=\int_{-\infty}^{t}dt'\,\Pi^T(t-t')G(t')\\ &=\int_{-\infty}^{0}dt'\,\Pi^T(-t')G(t'-t)\,,\\ \Sigma R^T&=\int_{-\infty}^{0}dt'\,\Sigma(t-t')R^T(t')\,,\end{aligned} \tag{5.11}$$

from which follows that

$$\frac{d}{dt}\,(\Pi^T G+\Sigma R^T)=\Pi^T\dot{G}+\dot{\Sigma}R^T\,. \tag{5.12}$$

Inserting this result together with the FDT (5.5) into the time derivative of Eq. (5.8), we find

$$\left(\frac{d}{dt}-\tilde{\Lambda}\right)(R-R^T)=-D[\Pi^T(R-R^T)+\dot{\Sigma}R^T]\,. \tag{5.13}$$

After substitution of Eq. (5.9) and multiplication from the left-hand side with $D=-D^{-1}$ and from the right-hand side with $(R^T)^{-1}$, Eq. (5.13) leads to

$$\dot{\Sigma}(t)=(R^T)^{-1}(t)+\Pi^T(t)-D\left(\frac{d}{dt}-\tilde{\Lambda}\right)\delta(t)\,. \tag{5.14}$$

But here the last term is just the reciprocal,

$$(R^0)^{-1}(t)=D\left(\frac{d}{dt}-\tilde{\Lambda}\right)\delta(t)\,, \tag{5.15}$$

as can be verified from Eq. (5.7), either by multiplication with R^0 or through Fourier transforms. Since from the second Eq. (3.34) there follows, after taking the T transpose defined in Eqs. (3.28) and (3.32),

$$\Pi=(R^{0T})^{-1}-(R^T)^{-1}\,, \tag{5.16}$$

we obtain the final result

$$\dot{\Sigma}(t)=\Pi^T(t)-\Pi(t)\,, \tag{5.17}$$

or applying the relations (5.10),

$$\dot{\Sigma}(t)=\begin{cases}\Pi^T(t), & \text{for } t>0\,,\\ -\Pi(t), & \text{for } t<0\,.\end{cases} \tag{5.18}$$

Here the first equality is the same as Eq. (7.1) of Deker and Haake,[2] while the second is a consequence of the first. This is because, quite generally,

$$\Sigma^T=\Sigma\,, \tag{5.19}$$

which follows from Eqs. (3.27), (3.30), and (3.33), since according to Eq. (3.11)

$$G^T=G\,. \tag{5.20}$$

This symmetry (5.19) also follows from Eqs. (3.23), (3.14), and (3.17) of Ref. 2, and in this sense Deker and Haake's result (7.1) is complete. Note also the analogy of the T transposition with time reversal in Eqs. (5.18).

In closing, we wish to comment on the shifting procedure for time derivatives used by Deker and Haake[2] to prove diagrammatically their Eq. (5.5). The fact is that at each response function line a boundary term is picked up by differentiation of the θ function. This can be seen by using as an example Eq. (5.11), which by differentiation becomes

$$\dot{\Pi}^T G+\Pi^T(0^+)G=\Pi^T\dot{G}\,.$$

Here the boundary term $-\Pi^T(0^+)G$ is picked up by shifting the time derivative from Π^T to G. Deker and Haake avoid such boundary terms by keeping time-integration limits formally at $-\infty$ and $+\infty$. In this formal sense the diagrammatical proof of their Eq. (5.5) is, of course, correct, and may in principle be used to simplify diagrams by eliminating one of the Green's functions G or R.

ACKNOWLEDGMENTS

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