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Response Function of the Second Kind in Many-Body Systems

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We analyze a new type of response function which portrays the properties of a system perturbed by an external field in terms of the perturbed two-point correlations of density fluctuations rather than in terms of perturbed averages of physical quantities. This "response function of the second kind" satisfies both fluctuation-dissipation-like theorems, relating it to three-point equilibrium functions, and hierarchical relationship linking it to conventional quadratic (rather than linear) response functions. In the equal-time limit, when the two density fluctuations are observed at the same time, the response function of the second kind is intimately connected to the two-particle correlation function of kinetic theory. This linkage opens an avenue for developing novel approximation techniques for correlated many-body systems.

KEY WORDS: Response function; correlations; dynamical structure function; quadratic response function; fluctuation-dissipation theorem; plasma; electron gas; many-body systems.

1. INTRODUCTION

Since the introduction of the linear response functions as an important tool in many-body theory, mainly through the pioneering work of Pines, Nozieres, Silin, and Rukhadze,[1] the frequency- and wave-number-dependent dielectric function and related response functions have become quantities of central interest in the portrayal of the physical behavior of many-body systems. The relationship between the response function and equilibrium two-point correlations, known as the fluctuation-dissipation

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theorem (FDT),[2] cast in its modern form by Kubo, has been one of the main ingredients in the success of the formalism.

It is evident, however, that the conventional linear response functions constitute only a restricted group in the more extended family of generalized response functions. One direction along which the generalization can be pursued is to consider higher than linear terms in the generally nonlinear response of the system to an external perturbation. Quadratic and higher-order response functions have traditionally been used in nonlinear optics, but their importance in many-body physics has been realized only more recently.[3–5] Similarly to the linear case, where the Kubo relationships provide the important link to equilibrium quantities, a quadratic fluctuation-dissipation theorem (QFDT)[6–8] plays a pivotal part in exploiting the information inherent in the quadratic response functions.

The second direction along which the notion of the conventional response function can be expanded is arrived at by focusing on averages of products of several physical quantities, rather than on the average of a single physical quantity, to characterize the response of the system to the external perturbation. To be more specific, we can concentrate on the particle density fluctuations $n(\mathbf{x}t)$. While the conventional density response function χ relates to the response, as given by the first-order perturbed average $\langle n(\mathbf{x}t)\rangle^{(1)}$, the generalization to two density fluctuations, taken at two different space-time points, results in considering $\langle n(\mathbf{x}_1 t_1)\, n(\mathbf{x}_2 t_2)\rangle^{(1)}$. This latter certainly both differs from its equilibrium value $\langle n(\mathbf{x}_1 t_1)\, n(\mathbf{x}_2 t_2)\rangle^{(0)}$, the familiar two-point function [related to the dynamical structure function $S(\mathbf{k}\omega)$] and contains significant information not available from the analysis of $\langle n(\mathbf{x}t)\rangle^{(1)}$. Thus, one is led to the introduction of a density response function "of the second kind," say Ξ, which now connects the perturbed two-point function with the external perturbation.

This novel response function appears naturally in the analysis of the kinetics of correlated many-body systems. Its significance lies in the wealth of relationships it satisfies, partly as fluctuation-dissipation theorems (i.e., in relation to equilibrium quantities), partly as hierarchical relationships, linking it to conventional quadratic response functions.

The concept of the response function of the second kind (or, more briefly, "double response functions") was explicity introduced first by Golden and Kalman,[9] although the concept was already implicit in ref. 3. The notion of "responding correlations" in a different context was explored by Stanton and Nelkin.[10] The concept was also used more recently, in connection with the derivation of the QFDT[6] and in establishing a new approximation technique for highly correlated plasmas and electron liquids.[4] A systematic study of its properties and in particular of the FDT and related relationships it satisfies, has, however not been undertaken. It is the purpose of the present paper to do this. In Section 2, after providing a precise definition for the function Ξ, we establish the FDT that links it to the equilibrium three-point function. In Section 3 we combine the FDT of Section 2 with the statements of the QFDT[6] in order to obtain the hierarchical relations between Ξ and quadratic response functions. Section 4 is devoted to the important equal-time (fluctuations taken at two different points in space, but at identical times), which has the most direct applications in many-body theory.

Earlier discussions on the double response function were restricted to the classical case. The present treatment is based on the correct dynamics of the density operators and is quite general. As a consequence, the ordering of the density operators in their product is of relevance and any particular choice implies a certain arbitrariness. We choose $\langle n(\mathbf{x}_1 t_1)\, n(\mathbf{x}_2 t_2)\rangle$ (in this order) as the fundamental quantity, but other choices (e.g., symmeterized products) would be equally reasonable. We pay special attention to the evaluation of the classical and zero-temperature limits: especially compact and useful relationships emerge in these cases from response function hierarchies.

2. FLUCTUATION-DISSIPATION THEOREM

The linear density response functions of the second kind $\hat{\Xi}(\xi_1 \tau; \xi_2 \tau_2)$ is defined through the space-time integral that connects the averages of products of the density fluctuation operator $n(\mathbf{x}t)$ with the external perturbing potential energy $\hat{\Phi}(\mathbf{x}t)$; this latter is regarded as a classical quantity (c-number):

$$\langle n(\mathbf{x}_1 t_1)\, n(\mathbf{x}_2 t_2)\rangle^{(1)} = \int d^3x \int dt\, \hat{\Xi}(\mathbf{x}_1 - \mathbf{x}, t_1 - t; \mathbf{x}_2 - \mathbf{x}, t_2 - t)\, \hat{\Phi}(\mathbf{x}t) \qquad (1)$$

or, in Fourier representation

$$\begin{gathered}\langle n_{\mathbf{k}_1}(\omega_1)\, n_{\mathbf{k}_2}(\omega_2)\rangle^{(1)} = \hat{\Xi}(\mathbf{k}_1 \omega_1; \mathbf{k}_2 \omega_2)\, \hat{\Phi}(\mathbf{k}\omega) \\ \mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2 \\ \omega = \omega_1 + \omega_2\end{gathered} \qquad (2)$$

Here and in the sequel the superscript denotes the order in the perturbing potential; the superscript (1) refers to the average taken over the first-order perturbed ensemble. Similar relationships hold for $\Xi(\xi_1 t_1; \xi_2 t_2)$, which connects to the total (external plus induced) average potential $\Phi(\mathbf{x}t)$

$$\Phi = \hat{\Phi} + \Phi^{\text{ind}}$$

Φ^{ind} is related to the first-order average density perturbation; if $\varphi(k)$ is the Fourier transform of the interaction potential in the system [$\varphi(k) = 4\pi e^2/k^2$ for a Coulomb system],

$$\Phi^{\text{ind}}(\mathbf{k}\omega) = \varphi(k)\langle n(\mathbf{k}\omega)\rangle^{(1)}$$

and thus

$$\hat{\Xi}(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2) = \frac{1}{\varepsilon(\mathbf{k}\omega)}\Xi(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2) \tag{3}$$

where $\varepsilon(\mathbf{k}\omega)$ is the customary longitudinal linear dielectric response function. The functions $\hat{\Xi}$ and Ξ are the "external" and "total" response functions, analogous to the conventional external $\hat{\chi}$ and total χ (also referred to, in a different parlance, as χ and χ_{screened}).

The perturbing potential generates a term H^1 in the Hamiltonian, additional to the equilibrium part H^0:

$$H = H^0 + H^1(t)$$

$$H^1(t) = \int n(\mathbf{x})\,\hat{\Phi}(\mathbf{x}t)\,d^3x$$

$$= \frac{1}{V}\sum_{\mathbf{k}} n_{-\mathbf{k}}\hat{\Phi}(\mathbf{k}, t) \tag{4}$$

$n(\mathbf{x})$ and $n_{\mathbf{k}}$ are the operators of the density fluctuation (with $n_{\mathbf{k}=0} = 0$).

Since we are concerned now with the time evolution of two dynamical quantities at two different time points in a nonstationary system, the appropriate approach to evaluate the correlation $\langle n_{\mathbf{k}_1}(t_1)\,n_{\mathbf{k}_2}(t_2)\rangle^{(1)}$ is a description in terms of the Heisenberg picture operators averaged over the equilibrium statistical operator $\Omega^{(0)}$, according to

$$\langle n_{\mathbf{k}_1}(t_1)\,n_{\mathbf{k}_2}(t_2)\rangle^{(1)} = \operatorname{Tr}\{\Omega^{(0)}[n^{(1)}_{\mathbf{k}_1}(t_1)\,n^{(0)}_{\mathbf{k}_2}(t_2) + n^{(0)}_{\mathbf{k}_1}(t_1)\,n^{(1)}_{\mathbf{k}_2}(t_2)]\} \tag{5}$$

The choice of the ordering of the n-operators is arbitrary: studying the symmetric and antisymmetric projections would be equally reasonable. In the Heisenberg picture, the density operator $n_{\mathbf{q}}(t)$ satisfies the equation of motion

$$\frac{d}{dt}n^{(1)}_{\mathbf{q}} = \frac{i}{\hbar}\{[H^0, n^{(1)}_{\mathbf{q}}] + [H^1, \mathbf{n}^{(0)}_{\mathbf{q}}]\} \tag{6}$$

The formal solution of Eq. (6) is

$$n^{(1)}_{\mathbf{q}}(t) = \frac{i}{\hbar V}\sum_{\mathbf{k}}\int_{-\infty}^{t} dt'\,\hat{\Phi}(\mathbf{k}t')[n^{(0)}_{-\mathbf{k}}(t'), n^{(0)}_{\mathbf{q}}(t)] \tag{7}$$

Now Eq. (7) can be employed to derive a general expression for the first-order two-point function $\langle n_{\mathbf{k}_1}(t_1)\, n_{\mathbf{k}_2}(t_2)\rangle^{(1)}$. By substituting it into Eq. (5), one obtains

$$\begin{aligned}\langle n_{\mathbf{k}_1}(t_1)\, n_{\mathbf{k}_2}(t_2)\rangle^{(1)} = \frac{i}{\hbar V}\int d\tau\, [\Theta(t_1-\tau)\{\langle n_{-\mathbf{k}}(0)\, n_{\mathbf{k}_1}(t_1-\tau)\, n_{\mathbf{k}_2}(t_2-\tau)\rangle^{(0)} \\ - \langle n_{\mathbf{k}_1}(t_1-\tau)\, n_{-\mathbf{k}}(0)\, n_{\mathbf{k}_2}(t_2-\tau)\rangle^{(0)}\} \\ + \Theta(t_2-\tau)\{\langle n_{\mathbf{k}_1}(t_1-\tau)\, n_{-\mathbf{k}}(0)\, n_{\mathbf{k}_2}(t_2-\tau)\rangle^{(0)} \\ - \langle n_{\mathbf{k}_1}(t_1-\tau)\, n_{-\mathbf{k}_2}(t_2-\tau)\, n_{-\mathbf{k}}(0)\rangle^{(0)}\}]\, \hat{\Phi}(\mathbf{k},\tau) \qquad (8)\end{aligned}$$

$\Theta(\tau)$ is the step function.

Following ref. 6, we now introduce the equilibrium dynamical three-point functions

$$\begin{aligned}S(\mathbf{q}_1, t_1; \mathbf{q}_2, t_2; \mathbf{q}_3, t_3) = \frac{1}{N}\langle n_{\mathbf{q}_1}(t_1)\, n_{\mathbf{q}_2}(t_2)\, n_{\mathbf{q}_3}(t_3)\rangle^{(0)} \\ \mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3=0\end{aligned} \qquad (9)$$

The ordering of density operators in S is of obvious relevance: there are six different S-functions, which fall into two cycles. Equation (8) now helps one to identify the function $\hat{\Xi}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)$ in terms of the S-functions:

$$\begin{aligned}&\hat{\Xi}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \\ &= -\frac{in}{\hbar}\{\Theta(\tau_1)[S(\mathbf{k}_1, \tau_1; -\mathbf{k}, 0; \mathbf{k}_2, \tau_2) - S(-\mathbf{k}, 0; \mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)] \\ &\quad + \Theta(\tau_2)[S(\mathbf{k}_1\tau_1; \mathbf{k}_2, \tau_2; -\mathbf{k}, 0) - S(\mathbf{k}_1, \tau_1; -\mathbf{k}, 0; \mathbf{k}_2, \tau_2)]\} \qquad (10)\end{aligned}$$

In deriving (10), we have exploited the invariance of the average under time translation. In Fourier representation Eq. (10) is equivalent to

$$\begin{aligned}\hat{\Xi}(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2) = \frac{-in}{\hbar}\int d\nu\, \delta_+(\nu)[S(\mathbf{k}_1, \omega_1-\nu; -\mathbf{k}, \nu-\omega; \mathbf{k}_2, \omega_2) \\ - S(-\mathbf{k}, \nu-\omega; \mathbf{k}_1, \omega_1-\nu; \mathbf{k}_2, \omega_2) \\ + S(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2-\nu; -\mathbf{k}, \nu-\omega) \\ - S(\mathbf{k}_1, \omega_1; -\mathbf{k}, \nu-\omega; \mathbf{k}_2, \omega_2-\nu)] \qquad (11) \\ \omega = \omega_1+\omega_2 \\ \mathbf{k} = \mathbf{k}_1+\mathbf{k}_2\end{aligned}$$

Here

$$\delta_{\pm}(\nu)=\frac{1}{2}\,\delta(\nu)\pm\frac{i}{2\pi}\,P\,\frac{1}{\nu}$$

is the projection operator for generating a plus (minus) function (a reminder: a plus (minus) function is analytic on the upper (lower) half-plane).

Taking the imaginary part of both sides of Eq. (11) and exploiting the fact that the S-functions in Fourier representation are real[6] and that the different S-functions within a cycle are related[6] to each other by

$$S(bca)=e^{-\beta\hbar\omega_a}S(abc) \tag{12}$$

(the abbreviated notation is rather self-explanatory, except for the convention $\mathbf{k}_0, \omega_0 \equiv -\mathbf{k}, -\omega$), one arrives at the rather simple relationship (with the notation $\hat{\Xi}=\hat{\Xi}'+i\hat{\Xi}''$, etc.)

$$\begin{aligned}\hat{\Xi}''(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)&=\frac{n}{\hbar}\,\{S(012)-S(120)\}\\&=\frac{n}{\hbar}\,(1-e^{-\beta\hbar\omega})\,S(012)\end{aligned} \tag{13}$$

The similarity between Eq. (13) and the conventional Kubo relationship[2] for the ordinary linear response function $\chi(\mathbf{k}\omega)$ is rather striking. Nevertheless, it would be erroneous to identify (13) as the fundamental relationship for $\hat{\Xi}$. It can be easily established from (10) that $\hat{\Xi}$ is not a plus-function of its frequency arguments. As a result, the full frequency dependence of $\hat{\Xi}''(\omega_1\omega_2)$ or of $\Xi(\omega_1\omega_2)$ cannot be reconstituted from the mere knowledge of their imaginary parts $\hat{\Xi}''(\omega_1\omega_2)$ or $\Xi''(\omega_1\omega_2)$. This is of, course, in contrast to the case of $\chi(\omega)$, whose frequency behavior is fully determined by $\chi''(\omega)$. Thus we are led to regard Eq. (11) rather than Eq. (13) as the fundamental relationship constituting the FDT for the response function of the second kind.

It is interesting to note that the FDT, Eq. (11), does not have an easily tractable classical limit. The $\hbar\to 0$ limit of (11) leads to the appearance of rather unwieldy Poisson brackets and therefore it is of limited usefulness. In this respect the situation is rather similar to what happens in relation to the quadratic FDT for the ordinary quadratic response function (see next section),[6,7] where in the "primitive" from of the FDT one encounters[7] the same problem.

3. RESPONSE FUNCTION OF THE SECOND KIND AND QUADRATIC RESPONSE FUNCTIONS

The quadratic density response function $\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$ and $\hat{\chi}(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$ are defined by

$$\langle n_{\mathbf{k}}(\omega)\rangle^{(2)}=\frac{1}{V}\sum_{\mathbf{k}_1\mathbf{k}_2}\int\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)\,\Phi(\mathbf{k}_1\omega_1)\,\Phi(\mathbf{k}_2\omega_2)$$

$$=\frac{1}{V}\sum_{\mathbf{k}_1\mathbf{k}_2}\int\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\hat{\chi}(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)\,\hat{\Phi}(\mathbf{k}_1\omega_1)\,\hat{\Phi}(\mathbf{k}_2\omega_2) \tag{14}$$

$$\mathbf{k}=\mathbf{k}_1+\mathbf{k}_2$$

$$\omega=\omega_1+\omega_2$$

χ and $\hat{\chi}$ are related to each other through

$$\hat{\chi}(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)=\frac{\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)}{\varepsilon(\mathbf{k}_1\omega_1)\,\varepsilon(\mathbf{k}_2\omega_2)\,\varepsilon(\mathbf{k}\omega)} \tag{15}$$

The quadratic fluctuation-dissipation theorem (QFDT)[6,7] links the three-point functions to the quadratic response functions. The QFDT, combined with the results of the previous section, allows one to relate the linear response function of the second kind $\Xi(\mathbf{k}\omega)$ to combinations of ordinary quadratic functions $\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$. We will refer to these relationships as response function hierarchies (RFH). Such hierarchical relationships are of considerable practical interest, since they can serve as starting points to nonperturbative approximation schemes for strongly coupled many-body systems.[3,4]

The derivation is premised on expressions derived from Eqs. (42a) and (42b) of ref. 6; written again in a rather obvious abbreviated notation, they are as follows:

$$S(120)=\frac{4\hbar^2}{n}\frac{1}{D(012)}\left[(1-e^{+\beta\hbar\omega})\,\hat{\chi}'(12)+(e^{+\beta\hbar\omega}-e^{+\beta\hbar\omega_1})\,\hat{\chi}'(01)-(1-e^{+\beta\hbar\omega_1})\,\hat{\chi}'(20)\right]$$

$$S(102)=\frac{4\hbar^2}{n}\frac{1}{D(012)}\left[(e^{-\beta\hbar\omega_2}-e^{+\beta\hbar\omega_1})\,\hat{\chi}'(12)+(1-e^{-\beta\hbar\omega_2})\,\hat{\chi}'(01)-(1-e^{+\beta\hbar\omega_1})\,\hat{\chi}'(20)\right] \tag{16}$$

$$S(012)=\frac{4\hbar^2}{n}\frac{1}{D(012)}\left[-(1-e^{-\beta\hbar\omega})\,\hat{\chi}'(12)+(1-e^{-\beta\hbar\omega_2})\,\hat{\chi}'(01)-(e^{-\beta\hbar\omega}-e^{-\beta\hbar\omega_2})\,\hat{\chi}'(20)\right]$$

with

$$D(012) = 2[\sinh(\beta\hbar\omega) - \sinh(\beta\hbar\omega_1) - \sinh(\beta\hbar\omega_2)]$$

Combination of Eq. (16) with Eq. (11) provides the desired result:

$$\hat{\Xi}(12) = -2i\hbar \int dv\, \delta_+(v) \left\{ \left[1 - \operatorname{cth}\left(\beta\hbar \frac{\omega_2}{2}\right)\right] [\hat{\chi}'(\bar{1}2) - \hat{\chi}'(2\bar{0})] - \left[1 + \operatorname{cth}\left(\beta\hbar \frac{\omega_1}{2}\right)\right] [\hat{\chi}'(1\bar{2}) - \hat{\chi}'(\bar{0}1)] \right\} \tag{17}$$

Again, the abbreviated notation has been used; the meaning of the barred variables is

$$\bar{1} = \mathbf{k}_1, \omega_1 - v$$
$$\bar{2} = \mathbf{k}_2, \omega_2 - v$$
$$\bar{0} = -\mathbf{k}, v - \omega$$

The expression is obtained by using the identity

$$\frac{1 + \cosh(x) - \cosh(y) - \cosh(x+y)}{\sinh(x+y) - \sinh(x) - \sinh(y)} = -\operatorname{cth}\left(\frac{x}{2}\right) \tag{18}$$

By exploiting the analytic properties of $\chi(\omega_1, \omega_2)$, one can further reduce Eq. (17) to

$$\hat{\Xi}(12) = -i\hbar \left\{ \left[1 - \operatorname{cth}\left(\beta\hbar \frac{\omega_2}{2}\right)\right] [\hat{\chi}(12) - \hat{\chi}^*(20)] - \left[1 + \operatorname{cth}\left(\beta\hbar \frac{\omega_1}{2}\right)\right] [\hat{\chi}(12) - \hat{\chi}^*(01)] \right\} \tag{19}$$

While in Section 2 we noted the problematic structures of the classical limits of the FDT relationships, both between $\hat{\Xi}(12)$ and S-functions on the one hand, and between $\hat{\chi}(12)$ and the S-functions on the other, here there is no difficulty in establishing the classical limit of the RFH relation. The straightforward result is

$$\hat{\Xi}(12) = \frac{2i}{\beta} \left\{ \frac{1}{\omega_2} [\hat{\chi}(12) - \hat{\chi}^*(20)] + \frac{1}{\omega_1} [\hat{\chi}(12) - \hat{\chi}^*(01)] \right\} \tag{20}$$

The expression is now manifestly symmetric in its arguments 1 and 2, as it should be.

It is also of interest to consider the zero-temperature limit. It is obvious from (19) that for the two terms in (19), respectively, only the $\omega_2 < 0$ and $\omega_1 > 0$ domains survive. This could also be inferred from the original definition, Eq. (5), since all intermediate states have energies higher than the ground state. Thus one is led to

$$\hat{\Xi}(12) = -2i\hbar\{\Theta(-\omega_2)[\hat{\chi}(12) - \hat{\chi}^*(20)] - \Theta(\omega_1)[\hat{\chi}(12) - \hat{\chi}^*(01)]\} \quad (21)$$

4. EQUAL-TIME LIMIT

Of special interest is the situation where the operators $n_{\mathbf{k}_1}$ and $n_{\mathbf{k}_2}$ are taken at the same time, $\tau_1 = \tau_2 = \tau$. This is the only case of interest in applications to kinetic theory.[3,4] We now consider in some detail the relevent relationships under this condition.

We note first that in the equal-time limit the two density operators commute and thus $\hat{\Xi}(12)$ is a symmetric function of its arguments. Second, $\hat{\Xi}(\omega)$ now indeed is, in contrast to $\hat{\Xi}(\omega_1, \omega_2)$ a genuine plus-function. In Fourier representation the equal-time limit corresponds to projecting out to the $\omega = \omega_1 + \omega_2$ line by applying the projection operator $(1/2\pi) \int d\omega_1 \int d\omega_2\, \delta(\omega_1 + \omega_2 - \omega)$:

$$\hat{\Xi}(\mathbf{k}_1, \mathbf{k}_2, \omega) = -\frac{i}{2\pi\hbar} n \int d\nu \int d\mu\, \delta_+(\nu)[S(\mathbf{k}_1, \omega - \mu; \mathbf{k}_2, \mu - \nu; -\mathbf{k}, \nu - \omega) - S(-\mathbf{k}, \nu - \omega; \mathbf{k}_1, \omega - \mu; \mathbf{k}_2, \mu - \nu)] \quad (22)$$

and

$$\hat{\Xi}''(\mathbf{k}_1, \mathbf{k}_2, \omega) = -\frac{1}{4\pi\hbar} n \int d\mu\, [S(\mathbf{k}_1, \omega - \mu; \mathbf{k}_2, \mu; -\mathbf{k}, -\omega) - S(-\mathbf{k}, -\omega; \mathbf{k}_1, \omega - \mu; \mathbf{k}_2, \mu)] \quad (23)$$

Equation (23) can now be regarded as the equal-time FDT for the response function of the second kind.

Both Eqs. (22) and (23) have simple classical limits:

$$\hat{\Xi}(\mathbf{k}_1, \mathbf{k}_2, \omega) = -\frac{i}{2\pi} \omega\beta n \int d\nu \int d\mu\, \delta_+(\nu)\, S(\mathbf{k}_1, \omega - \mu; \mathbf{k}_2, \mu - \nu; -\mathbf{k}, \nu - \omega) - \frac{1}{4\pi^2} \beta n \int d\mu \int d\nu\, S(\mathbf{k}_1, \omega - \mu; \mathbf{k}_2, \mu - \nu; -\mathbf{k}, \omega - \nu) \quad (24)$$

and

$$\hat{\Xi}''(\mathbf{k}_1, \mathbf{k}_2, \omega) = -\frac{1}{4\pi} \omega\beta n \int d\mu\, S(\mathbf{k}_1, \omega - \mu; \mathbf{k}_2, \mu; -\mathbf{k}, -\omega) \quad (25)$$

The time domain equivalent of Eq. (24),

$$\hat{\Xi}(\mathbf{k}_1, \mathbf{k}_2; \tau) = \beta n \frac{\partial}{\partial \tau} \{\Theta(\tau)\, S(\mathbf{k}_1, 0; \mathbf{k}_2, 0; -\mathbf{k}, -\tau)\} \tag{26}$$

was already implied by a result given by Golden and Kalman.[3]

Further relationships are obtained in terms of the quadratic response functions by taking the equal-time projection of Eq. (19):

$$\begin{aligned} &\hat{\Xi}(\mathbf{k}_1, \mathbf{k}_2, \omega) \\ &\quad = \frac{i\hbar}{2\pi} \int d\mu \,\mathrm{cth}\left(\beta\hbar \frac{\mu}{2}\right) [\hat{\chi}(\mathbf{k}_1, \omega-\mu; \mathbf{k}_2, \mu) - \hat{\chi}^*(\mathbf{k}_2, \mu; -\mathbf{k}, -\omega) \\ &\qquad + \hat{\chi}(\mathbf{k}_1, \mu; \mathbf{k}_2, \omega-\mu) - \hat{\chi}^*(-\mathbf{k}, -\omega; \mathbf{k}_1, \mu)] \end{aligned} \tag{27}$$

Here we have exploited the fact that integrals such as $\int d\mu\, \hat{\chi}(\mathbf{k}_2, \mu; -\mathbf{k}, -\omega)$ vanish because of the plus-function character of the integrand. We also note the explicit $\mathbf{k}_1 \leftrightarrow \mathbf{k}_2$ symmetry of (27), which is indeed required since the equal-time n-operators commute.

The classical limits of (27) can be cast in an appealingly simple form. Making use of the Kramers–Kronig relations for $\hat{\chi}(20)$ and $\hat{\chi}(01)$, one obtains

$$\begin{aligned} \hat{\Xi}(\mathbf{k}_1, \mathbf{k}_2, \omega) = &\frac{1}{\pi\beta} \int d\mu \frac{1}{\mu} [\hat{\chi}(\mathbf{k}_1, \omega-\mu; \mathbf{k}_2, \mu) + \hat{\chi}(\mathbf{k}_1, \mu; \mathbf{k}_2, \omega-\mu)] \\ &+ \frac{1}{\beta} [\hat{\chi}^*(\mathbf{k}_2, 0; -\mathbf{k}, -\omega) + \hat{\chi}^*(-\mathbf{k}, -\omega; \mathbf{k}_1, 0)] \end{aligned} \tag{28}$$

Further employing the symmetry relations[3] obeyed by $\hat{\chi}$,

$$\begin{aligned} \chi(\mathbf{k}_2, 0; -\mathbf{k}, -\omega_1) &= \chi^*(\mathbf{k}_1, \omega_1; \mathbf{k}_2, 0) \\ \chi(-\mathbf{k}, -\omega_1; \mathbf{k}_1, 0) &= \chi^*(\mathbf{k}_1, 0; \mathbf{k}_2, \omega_2) \end{aligned} \tag{29}$$

one can identify the rhs of Eq. (28) as the δ_- projection of a symmetrized kernel. Thus the classical RFH expression assumes the extremely useful form

$$\hat{\Xi}(\mathbf{k}_1, \mathbf{k}_2, \omega) = -\frac{2}{\beta} \int d\mu\, \delta_-(\mu) [\chi(\mathbf{k}_1, \mu; \mathbf{k}_2, \omega-\mu) + \chi(\mathbf{k}_2; \mu; \mathbf{k}_1, \omega-\mu)] \tag{30}$$

This relationship was already reported and used[4] in establishing a dynamical mean field theory formalism for strongly coupled Coulomb systems. An essentially identical result, in a somewhat different language, was first obtained by Golden and Kalman.[3]

Finally, one can consider the zero-temperature limit of (27), with obvious relevance to the problem of the strongly correlated degenerate electron liquid. One finds

$$\hat{\Xi}(\mathbf{k}_1, \mathbf{k}_2, \omega) = -\frac{i\hbar}{\pi}\left\{\int_{-\infty}^{0} d\mu\, [\hat{\chi}(\mathbf{k}_1, \omega-\mu; \mathbf{k}_2, \mu) - \hat{\chi}^*(\mathbf{k}_2, \mu; -\mathbf{k}, -\omega)] - \int_{0}^{\infty} d\mu\, [\hat{\chi}(\mathbf{k}_1, \mu; \mathbf{k}_2, \omega-\mu) - \hat{\chi}^*(-\mathbf{k}, -\omega; \mathbf{k}_1, \mu)]\right\}$$

5. CONCLUSIONS

In this paper we have introduced a new type of response function which portrays the response of a many-body system to an external perturbation in terms of the perturbation-induced modified averages of two physical quantities taken at two different space-time points, rather than in terms of perturbed averages of one single physical variable, as customary in the theory of conventional response functions.

Although the paradigm we had in mind in the present discussion was that of a system with Coulomb interaction, the derivation and the results are not contingent upon the assumption of any particular kind of interaction. Neither is the premise that the perturbed physical quantity is the density an important restriction: the "second kind" equivalents of the conventional spin, etc., response functions can be worked out, although it would require the appropriate generalization of the QFDT.

These newly introduced "response functions of the second kind" (or "double response functions") exhibit a rich analytic structure which links them both to equilibrium three-point correlations and to conventional quadratic (rather than linear) response functions. The first set of relationships are analogous to the Kubo-type fluctuation-dissipation (FD) theorems, while the latter constitute a new type of response function hierarchy (RFH).

We have focused on the density–density response $\hat{\Xi}(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2)$ to an external potential. We have established the FD relations linking $\hat{\Xi}(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2)$ and its counterpart $\Xi(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2)$ to three-point density correlations $S(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2; -\mathbf{k}-\omega)$ and the RFH connecting $\hat{\Xi}(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2)$ with the quadratic response function $\hat{\chi}(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2)$. It is primarily through the latter that approximation techniques can be worked out for the calculation of $\Xi(\mathbf{k}_1\omega_1; \mathbf{k}_2\omega_2)$. Of special importance is the equal-time limit, where the density fluctuations are observed at identical times. The importance stems from the intimate relationship that Ξ in this limit maintains with the perturbed two-particle correlations which emerge in the analysis of kinetic equations. This linkage provides a powerful tool in the analysis of correlated many-body systems; the usefulness of this line of attack has already been demonstrated with regard to strongly coupled classical plasmas. The general approach developed in this paper opens the way to further exploit the formalism, especially in relation to the problem of the strongly correlated electron liquid.

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