

CONTRIBUTION TO THE QUANTUM NONLINEAR THEORY OF THERMAL FLUCTUATIONS

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Submitted June 12, 1969

Zh. Eksp. Teor. Fiz. 58, 1612–1622 (May, 1970)

The derivation of the three-index (quadratic) fluctuation-dissipation theorem is improved by applying a theorem which permits one to interchange the operators in the equilibrium moment functions. Analogous relations are obtained for the four-index (cubic) theory and the arbitrariness which remains in the theory in expressing the fluctuation characteristics (nonlinear susceptibilities) is investigated.

1. INTRODUCTION

THERE is no need to discuss the great role played in contemporary statistical physics by linear fluctuation-dissipation thermodynamics (the results of Nyquist, Callen, Welton, and Onsager^[1-3]). The number of papers in which it is applied to electric and other systems is extremely large. Meanwhile, fluctuation-dissipation and non-equilibrium thermodynamics is not yet exhausted. An important and even more voluminous part is concerned with nonlinear theory. The number of papers touching upon the latter is very much smaller (cf.^[4-7]). Interest in nonlinear theory is warranted from the point of view of both theory and application, since nonlinear systems and effects are playing a large and expanding role at the present time.

Linear thermodynamics is applicable also to nonlinear systems, but is inadequate for a more or less complete account of them. For a more exhaustive analysis of the fluctuations in nonlinear systems it is advisable to use additional relations from nonlinear theory, which have (e.g., in the framework of the three-index theory) the same degree of generality as the relations from the linear theory, and also, possibly, to use other relations with a lesser degree of generality.

Different variants of the unified (linear-nonlinear) theory are possible: Markovian and non-Markovian, quantum and non-quantum; transitions from one variant to another are possible. In this article only one problem will be considered: the derivation of relations of the fluctuation-dissipation theorem type (^[2] Sec. 127) for the three- and four-index cases in the quantum non-Markovian variant. In this variant, as in the other variants investigated by the author, the three-index theory displays complete similarity to the two-index theory, i.e., to the usual linear theory. The results concerning this case given in the article have a close bearing on the results obtained by Efremov^[7]. The formulas (3.9), (3.10) and (3.18), absent in^[7], reinforce Efremov's results. The method of derivation is also improved.

In the four-index theory, the position is more complicated; in it we can establish a number of general thermodynamic relations, of which, however, there are not enough to establish completely the fluctuation characteristics from the dissipation characteristics

(without additional reasoning which reduces the extent of the generality). In the variant of the theory under consideration, generalized admittance functions are taken as the dissipation characteristics and correlation functions are established in terms of them. Thus, the result of the investigation has a partly negative character. In Sec. 4, the degree of arbitrariness which remains in establishing the theory in the framework of the four-index quantum non-Markovian theory is studied.

In this paper, the following simple and useful theorem (cf.^[8], p. 18) concerning the interchange of operators in equilibrium moment functions is used. It states that, if the averaging corresponds to the equilibrium Gibbs density matrix $\exp(\beta F - \beta \mathcal{H})$ (\mathcal{H} is the time-independent Hamiltonian), then

$$\langle B(t)D \rangle = \langle DB(t + i\beta\hbar) \rangle \equiv e^{i\beta\mathcal{H}} \langle DB(t) \rangle \quad (1.1)$$

for arbitrary D and $B(t)$ (the subscript B in $p_B = \partial/\partial t$ denotes that the time-differentiation refers to B).

This theorem enables us to improve the derivation of the basic results. This improvement is especially important in the nonlinear theory, where the calculations are of necessity more cumbersome than in the linear theory. Application of an analogous method to the linear (two-index) case gives an extremely simple derivation of the usual fluctuation-dissipation theorem, which in our notation (explained below) is written as:

$$\langle F^i F^h + F^h F^i \rangle = -i\hbar \frac{L+1}{L-1} (G^{ih} - G^{hi}), \quad (1.2)$$

$$L = e^{i\beta\mathcal{H}} p_i.$$

The object of this article is to obtain nonlinear generalizations of this theorem.

2. THE CONNECTION BETWEEN THE COMMUTATOR FUNCTIONS AND THE ADMITTANCE FUNCTIONS OF THE NONLINEAR THEORY

The goal we shall set ourselves is the derivation of relations between the fluctuation characteristics of an equilibrium process, i.e., moments of the internal parameters, of the type $\langle F_{\alpha_n}(t_n) \dots F_{\alpha_1}(t_1) \rangle$, and the dissipation characteristics of a non-equilibrium process, i.e., the generalized admittance functions

$$G_{\alpha\beta_n \dots \beta_1}(t; t_n, \dots, t_1).$$

First (in the present section), the question of the connection between the commutator functions and the generalized admittance functions will be considered. Admittance functions are introduced in connection with the study of the response (in the general case, nonlinear) of a system to varying external forces $h_\alpha(t)$ (cf., e.g.,^[1,7,9]). Let the external forces $h_\alpha(t)$ act on the generalized coordinates, i.e., on the internal thermodynamic parameters F_α , $\alpha = 1, 2, \dots$. This means that the system is described by the perturbed Hamiltonian:

$$\mathcal{H}_{\text{per}} = \mathcal{H} - \sum_{\alpha} h_{\alpha}(t) F_{\alpha} \equiv \mathcal{H} - h(t) F, \quad (2.1)$$

where \mathcal{H} is the unperturbed Hamiltonian.

The presence of the perturbing forces $h_\alpha(t)$ leads to the fact that the average perturbed values $A_\alpha(t) = \langle F_{\alpha \text{ per}}(t) \rangle$ of the internal parameters, (the response of the system) differ from the corresponding unperturbed values $\langle F_\alpha(t) \rangle$, which are constant because of the stationarity of the system and which, without loss of generality, can be assumed to be equal to zero. Representing the response in the form of an expansion

$$\langle F_\alpha(t)_{\text{per}} \rangle = \sum_{n=1}^{\infty} \frac{1}{n!} \int \dots \int G_{\alpha, \beta_1 \dots \beta_n}(t; t_n, \dots, t_1) \times h_{\beta_1}(t_n) \dots h_{\beta_n}(t_1) dt_n \dots dt_1, \quad (2.2)$$

we introduce the admittance functions G , satisfying the causality condition

$$G_{\alpha \beta_1 \dots \beta_n}(t, t_n, \dots, t_1) = 0 \quad \text{for } t < \max(t_1, \dots, t_n). \quad (2.3)$$

Below we shall denote the pair (β_1, t_1) by one index k_1 , with similar notation for other pairs. Since the admittance $G^{k_1 k_2 \dots k_n}$ is equal to the variational derivative of $\langle F_{\text{per}}^k \rangle$ with respect to h^{k_1}, \dots, h^{k_n} at the zero-point $h \equiv 0$, it is a symmetric function of k_1, \dots, k_n .

As is known, (cf., e.g.,^[1,7,9]), application of nonstationary perturbation theory gives the following expression for the admittance functions:

$$G^{h_{k_1} \dots h_{k_n}} = (i/\hbar)^n P_n \langle [\dots [F^k, F^{k_n}], \dots] F^{k_1} \rangle \times \eta(t - t_n) \eta(t_n - t_{n-1}) \dots \eta(t_2 - t_1), \quad (2.4)$$

where the averaging is performed over the equilibrium state;

$$\eta(\tau) = 1 \text{ for } \tau > 0, \quad \eta(\tau) = 0 \text{ for } \tau < 0,$$

P_n indicates summation over the permutations of the indices $1, \dots, n$ ($n!$ terms). We introduce the notation

$$V^{h_{k_1} \dots h_{k_n}} = \langle [\dots [F^{h_{k_1}}, F^{h_{k_{n-1}}}], \dots] F^{h_{k_n}} \rangle, \quad (2.5)$$

in which the equalities (2.4) take the form

$$G^{h_{k_1}} = (i/\hbar) V^{h_{k_1}} \eta(t - t_1), \\ G^{h_{k_1} h_{k_2}} = (i/\hbar)^2 [V^{h_{k_1} h_{k_2}} \eta(t - t_2) \eta(t_2 - t_1) + V^{h_{k_1} h_2} \eta(t - t_1) \eta(t_1 - t_2)], \\ G^{h_{k_1} h_{k_2} h_{k_3}} = (i/\hbar)^3 P_3 V^{h_{k_1} h_{k_2} h_{k_3}} \eta(t - t_3) \eta(t_3 - t_2) \eta(t_2 - t_1). \quad (2.6)$$

We do not need other values of n .

Below it will be useful to use the symmetry conditions for the functions (2.5) with respect to time reversal $t \rightarrow -t$. We shall assume that the quantum variables $F_\beta(t)$ are eigenfunctions of the time-reversal operator, i.e., they transform to $\epsilon_\beta F_\beta(-t)$, where $\epsilon_\beta = 1$ for quantities which are even in the time and $\epsilon_\beta = -1$ for quantities odd in the time. The equi-

ilibrium moment $\langle F_{\beta m}(t_m) \dots F_{\beta 1}(t_1) \rangle$ is assumed to be invariant on time reversal in the following sense:

$$\langle F_{\beta m}(t_m) \dots F_{\beta 1}(t_1) \rangle = \epsilon_{\beta m} \dots \epsilon_{\beta 1} \langle F_{\beta m}(-t_m) \dots F_{\beta 1}(-t_1) \rangle^*. \quad (2.7)$$

For this it is necessary that the unperturbed Hamiltonian possess the property of invariance. It follows from (2.7) and (2.5) that the function $V^{k_m \dots k_1}$ has an analogous property:

$$V_{\beta m} \dots \beta_1(t_m, \dots, t_1) = \epsilon_{\beta m} \dots \epsilon_{\beta 1} V_{\beta m}^* \dots \beta_1(-t_m, \dots, -t_1). \quad (2.8)$$

Consequently, if the behavior of the function $V^{k_m \dots k_1}$ is known, say, in the region $t_m > \dots > t_1$, it is not difficult to find its behavior in the region $t_1 > \dots > t_m$ also.

The complex-conjugation operation occurring in (2.7) and (2.8) is a specifically quantum effect. The transformations corresponding to time reversal were studied in^[9].

3. RELATIONS IN THREE-INDEX FLUCTUATION-DISSIPATION THEORY

By direct inspection it is not difficult to see that the function

$$V^{mlk} = \langle [[F^m, F^l], F^k] \rangle = \langle F^m F^l F^k - F^l F^m F^k - F^k F^m F^l + F^k F^l F^m \rangle \quad (3.1)$$

has the obvious properties:

$$V^{mlk} = -V^{lmk}, \quad (3.2)$$

$$V^{mlk} + V^{lkm} + V^{kml} = 0. \quad (3.3)$$

Hence it is clear that there are only two independent functions V .

We shall relate the above commutator functions to correlation functions. Applying formula (1.1), we have

$$\langle F^k F^l F^m \rangle = e^{i\beta \hbar p_k} \langle F^l F^m F^k \rangle. \quad (3.4)$$

Using (3.4), we write (3.1) in the form

$$V^{mlk} = (1 - K) \langle F^m F^l F^k - F^l F^m F^k \rangle. \quad (3.5)$$

Here and below we use for brevity the notation

$$K = e^{i\beta \hbar p_k}, \quad L = e^{i\beta \hbar p_l}, \quad M = e^{i\beta \hbar p_m}. \quad (3.6)$$

By virtue of the stationarity of the fluctuations, the relations

$$p_k + p_l + p_m = 0, \quad KLM = 1. \quad (3.7)$$

are fulfilled. From (3.5), by cyclic permutation of the indices, we obtain

$$V^{hml} = (1 - L) \langle F^h F^m F^l - F^m F^h F^l \rangle$$

or, if we use relations of the type (3.4), but with permuted indices,

$$V^{hml} = (1 - L) [K \langle F^m F^l F^h \rangle - L^{-1} \langle F^l F^m F^h \rangle]. \quad (3.8)$$

We shall regard the equalities (3.5) and (3.8) (divided by $1 - K$ and $1 - M$) as a system of equations for the two unknowns $\langle F^m F^l F^k \rangle$ and $\langle F^l F^m F^k \rangle$. Solving it, after a series of transformations performed using (3.6) and (3.3), we shall have

$$\langle F^m F^l F^k \rangle = (1 - M^{-1})^{-1} [(1 - K)^{-1} V^{mlk} + (1 - L^{-1})^{-1} V^{hml}] \\ = (M - 1)^{-1} (L - 1)^{-1} (K - 1)^{-1} [M V^{mlk} + V^{hml} + K^{-1} V^{lkm}]. \quad (3.9)$$

Using this basic result, it is not difficult to find the

symmetrized correlation functions also, e.g., the cyclically symmetrized function

$$R^{mlk} = \langle F^m F^l F^k \rangle + \langle F^k F^m F^l \rangle + \langle F^l F^k F^m \rangle = (1 - K + M^{-1}) \langle F^m F^l F^k \rangle.$$

For it we obtain

$$R^{mlk} = (M - 1)^{-1} (L - 1)^{-1} (K - 1)^{-1} \sum_{(3)} P(M + L^{-1}) V^{mlk}, \quad (3.10)$$

where the sum extends over the cyclic permutations P and contains three terms. Further, the symmetrization $R^{mlk} + R^{lmk}$ gives a completely symmetrized correlation function. It is also easy to obtain some partially symmetrized correlation functions, e.g., the function $\langle [F^m, [F^l, F^k]_+]_+ \rangle$, calculated in^[7], and also the commutator function $\langle [F^m, [F^l, F^k]_-]_+ \rangle$, in terms of which the variational derivative

$$\delta \langle [F^m, F^l]_+ \rangle / \delta h^k \quad (3.11)$$

at the zero-point is expressed; this function was also found in^[7].

In order to obtain the three-index analog of the fluctuation-dissipation theorem (1.2), it remains to express the functions V^{mlk} occurring in the right hand side of the derived formulas (3.9), (3.10), etc., in terms of the admittance function G^{mlk} , using the second of the formulas (2.6).

We shall introduce the functions $g^{mlk}, a^{lkm}, b^{kml}, \dots$, each of which possesses the property: $f^{mlk} = 0$ outside the region $t_m > t_l > t_k$; the functions are taken to be equal to $-V^{mlk}/\hbar^2$ inside the region in which they are non-zero. Then, obviously, the function $-V^{mlk}/\hbar^2$ is written in the form of a sum with six terms:

$$-\hbar^{-2} V^{mlk} = g^{mlk} + a^{lkm} + b^{kml} + c^{lmk} + d^{klm} + e^{mkl}.$$

Using the symmetry property (3.2), half the functions introduced can be eliminated from this expression by expressing them in terms of the remaining ones

$$-\hbar^{-2} V^{mlk} = g^{mlk} + a^{lkm} + b^{kml} - g^{imk} - a^{mkl} - b^{klm}. \quad (3.12)$$

Further, because of (3.3) the equality $g^{mlk} + a^{mlk} + b^{mlk} = 0$ is fulfilled, i.e., (3.12) takes the form

$$-\hbar^{-2} V^{mlk} = g^{mlk} + a^{lkm} - g^{kml} - a^{kml} - g^{lmk} - a^{lmk} + g^{klm} + a^{klm}. \quad (3.13)$$

We now use the time-symmetry property (2.8). Introducing the time-conjugation operation

$$\hat{V}_{\beta_m \dots \beta_l (t_m, \dots, t_l)} = V_{\beta_m \dots \beta_l}^* (-t_m, \dots, -t_l), \quad (3.14)$$

we can write the equality (2.8) for $m = 3$ thus:

$$V^{mlk} = \hat{V}^{mlk}.$$

Putting (3.13) into this, we obtain

$$g^{klm} + a^{klm} = \hat{g}^{mlk}, \quad -a^{mkl} = \hat{a}^{lkm}.$$

Consequently, (3.13) is transformed into the equality

$$V^{mlk} = -\hbar^2 (g^{mlk} - g^{lkm} + \hat{g}^{mkl} - \hat{g}^{imk} - g^{lmk} + g^{mkl} - \hat{g}^{lkm} + \hat{g}^{mkl}). \quad (3.15)$$

Putting this expression into the second of the equalities (2.6) and taking into account only those terms which are non-zero in the region considered $t > \max(t_1, t_2)$, we have

$$G^{mlk} = g^{mlk} + g^{mkl} \quad (3.16)$$

for any relationship between the times. Therefore, (3.15) takes the form

$$V^{mlk} = -\hbar^2 (G^{mlk} - G^{lkm} + \text{time conj.}). \quad (3.17)$$

Putting (3.17) into (3.10), we obtain

$$\langle F^m F^l F^k \rangle = -\hbar^2 \left[M \frac{G^{lkm} + \hat{G}^{lkm}}{(K-1)(M-1)} + \frac{G^{mlk} + \hat{G}^{mlk}}{(L-1)(K-1)} + K^{-1} \frac{G^{kml} + \hat{G}^{kml}}{(M-1)(L-1)} \right]. \quad (3.18)$$

In an analogous way, we can express other correlation functions and also the function (3.11), in terms of G^{mlk} . In this way, the results of^[7] are easily derived from the more general formulas given above, but not vice versa.

In the formulas obtained one can of course transform to the spectral representation. In this the operators p_m, p_l , and p_k occurring in (3.4)–(3.10) are replaced by $i\omega_m, i\omega_l$ and $i\omega_k$. Because of the stationarity, the relation $\omega_m + \omega_l + \omega_k = 0$ is fulfilled, so that we can write out only two independent frequencies.

Thus, all the three-index fluctuation characteristics can be completely expressed in terms of a dissipation characteristic such as the three-index admittance function. Consequently, the same program as in the usual (two-index) fluctuation-dissipation theorem is carried through completely in the framework of the three-index theory.

4. THE FOUR-INDEX RELATIONS

We shall try to fulfil the above program in the four-index theory. We shall consider the function (2.5) for $m = 4$:

$$V^{nmik} = \langle [[F^n, F^m], F^l], F^k \rangle. \quad (4.1)$$

It is not difficult to see by direct inspection that the following symmetry relations are fulfilled

$$V^{nmik} + V^{mnik} = 0, \quad (4.2)$$

$$V^{nmik} + V^{mnlk} + V^{lnmk} = 0, \quad (4.3)$$

$$V^{nmik} + V^{mnikl} + V^{lknm} + V^{klmn} = 0. \quad (4.4)$$

If we take the set of 24 functions V obtained by all the possible permutations of the indices, the relation (4.2) reduces the number of independent functions to 12, then (4.3) reduces it to 8, and (4.4) reduces it to 6.

Because of (1.1), the operator $e^{i\beta \hbar p_k}$ leads to a cyclic permutation of the indices:

$$\langle F^k F^n F^m F^l \rangle = e^{i\beta \hbar p_k} \langle F^n F^m F^l F^k \rangle. \quad (4.5)$$

As a result of this we have

$$[[F^n, F^m], F^l], F^k = (1 - K) [[F^n, F^m], F^l] F^k$$

(we are using the notation (3.6)). Writing out $[[F^n, F^m], F^l]$ in detail and using the notation

$$(1 - K)^{-1} V^{nmik} = W^{nmik}, \quad Q^{nmik} = \langle F^n F^m F^l F^k \rangle, \quad (4.6)$$

consequently we shall have

$$W^{nmik} = Q^{nmik} + Q^{lmnk} - Q^{mnlk} - Q^{lnmk}. \quad (4.7)$$

As a consequence of relations of the type (4.5), the number of linearly independent functions Q is reduced

to 6, which is the same as the number of independent functions V or W. The equality (4.7) establishes the correspondence $Q \rightarrow W$. It is clear from the following treatment that the correspondence between the independent functions Q and W is nondegenerate and it is possible to establish inverse formulas for the transformation $W \rightarrow Q$, i.e., to solve (4.7) for the functions W, i.e., for V also. To do this, we add to (4.7) the following equations, obtained from (4.7) by the interchange (n, m) (l, k) and the interchange (n, l) (m, k):

$$\begin{aligned} W^{mnlk} &= Q^{mnlk} + Q^{knlm} - Q^{nmkl} - Q^{klnm}, \\ W^{lknm} &= Q^{lknm} + Q^{nklm} - Q^{klnm} - Q^{nlkm} \end{aligned} \quad (4.8)$$

(the remaining interchange (n, k), (m, l) of the normal divisor of the group because of (4.4) does not give an independent equation.) Going over to the cyclic factor group of three permutations, corresponding to the symmetry (4.3), to (4.7) and (4.8) we add the analogous equations, obtained, say, by the permutations (nml) and having the form

$$\begin{aligned} W^{mlnk} &= Q^{mlnk} + Q^{nbnk} - Q^{lmbk} - Q^{nmkl}, \\ W^{lmkn} &= Q^{lmkn} + Q^{kmln} - Q^{mknl} - Q^{klmn}, \\ W^{nkm}l &= Q^{nkm}l + Q^{mkn}l - Q^{knlm} - Q^{mnlk}. \end{aligned} \quad (4.9)$$

The remaining permutation of the above three indices, because of (4.3), gives nothing new. By using permutation relations of the type (4.5), all the functions Q occurring in (4.7)–(4.9) can be converted to the unknown functions

$$\begin{aligned} x &= Q^{mnlk}, \bar{x} = Q^{lmbk}, y = Q^{lmkn}, \bar{y} = Q^{mnlk}, \\ z &= Q^{mlnk}, \bar{z} = Q^{nlmk}. \end{aligned} \quad (4.10)$$

After this the above equations take the form of a system of equations

$$\begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ K & L^{-1} & -L^{-1} & -K & 0 & 0 \\ LK & NK & -K & -M^{-1} & 0 & 0 \\ -1 & -1 & 0 & 0 & 1 & 1 \\ -N^{-1} & -K & 0 & 0 & K & N^{-1} \\ -K & -L^{-1} & 0 & 0 & NK & MK \end{pmatrix} \begin{pmatrix} x \\ \bar{x} \\ y \\ \bar{y} \\ z \\ \bar{z} \end{pmatrix} = \begin{pmatrix} W^{mnlk} \\ W^{mnlk} \\ W^{lknm} \\ W^{lknm} \\ W^{lmkn} \\ W^{lmkn} \end{pmatrix}, \quad (4.11)$$

(NMLK = 1).

This is found to be nondegenerate and permits us to express $x = \langle F^{\mathbf{n}} F^{\mathbf{m}} F^{\mathbf{l}} F^{\mathbf{k}} \rangle$ in terms of W or V. The solution of this system is given in the Appendix. It is obvious that the result obtained there enables us also to calculate the symmetrized correlation functions.

We recall now that our basic problem is to express the correlation functions in terms of the admittance functions. For this it is necessary to use the third of the formulas (2.6), which takes the form

$$G^{hh_3h_2h_1} = P_3 g^{hh_3h_2h_1},$$

with the notation

$$g^{hh_3h_2h_1} = (i/\hbar)^3 V^{hh_3h_2h_1} \eta(t-t_3) \eta(t_3-t_2) \eta(t_2-t_1). \quad (4.12)$$

It is consequently not difficult to see that the function $G^{kk_3k_2k_1}$ uniquely determines the function (4.12) and vice versa.

To express the function $V^{nm}lk$ in terms of $G^{nm}lk$ or $g^{nm}lk$ we shall introduce certain (so far undetermined) functions $a^{nm}lk, b^{nm}lk, \dots$, each of which goes to zero outside the region $t_n > t_m > t_l > t_k$, like $f^{m}lk$.

Using the symmetry properties (4.2) and (4.3), we shall have

$$\begin{aligned} (i/\hbar)^3 V^{nm}lk &= a^{nm}lk - a^{mnlk} + b^{m}lnk - b^{n}lmk \\ &- (a^{lnmk} + b^{lnmk}) + (a^{lmnk} + b^{lmnk}) + c^{nmkl} - c^{mnlk} \\ &+ d^{m}lkn - d^{n}lkm - (c^{lnkm} + d^{lnkm}) + (c^{lknm} + d^{lknm}) \\ &+ e^{n}kml - e^{m}knl + f^{m}kln - f^{n}klm - (e^{lknm} + f^{lknm}) \\ &+ (e^{lkmn} + f^{lkmn}) + h^{k}nml - h^{k}mnl + q^{kmln} - q^{knlm} \\ &- (h^{klnm} + q^{klnm}) + (h^{klmn} + q^{klmn}). \end{aligned} \quad (4.13)$$

Here eight undetermined functions appear. The properties (4.4) establish two additional relations between them

$$b + c + d + e - q = 0, \quad a + b + d - f + h = 0. \quad (4.14)$$

Using the time-symmetry property (2.8), we obtain the relations:

$$e = \bar{c} + \bar{d}, \quad f = -\bar{d}, \quad h = \bar{a} + \bar{b}, \quad q = -\bar{b} \quad (4.15)$$

(the time-conjugation notation (3.14) is used), which enable us to write (4.14) in the form

$$a + b + d + \bar{a} + \bar{b} + \bar{d} = 0, \quad a + \bar{a} = c + \bar{c}. \quad (4.16)$$

It remains to use the relation (4.12), which determines a, and consequently also \bar{a} ($a = g$).

Now all the available relations have been exhausted and the arbitrary functions introduced remain incompletely determined. After (4.15) and (4.12) have been used, there remain three arbitrary functions, say, b, c and d. The relations (4.16) connect their time-even parts, determining, as it were, one more function (a half plus a half). In all, two functions remain undetermined and the function $V^{nm}lk$ can be set arbitrarily in two regions out of 24. This arbitrariness is not fortuitous and has its analog in the non-quantum Markovian theory. It is possible to remove this arbitrariness only by going beyond the bounds of the theory described and using some additional assumptions which reduce the degree of generality. We recall that, up to now, the generality of the treatment has been exactly the same as in the usual fluctuation-dissipation theorem.

From the results given it is possible to obtain various consequences, e.g., (making $\hbar \rightarrow 0$) the formulas of non-quantum fluctuation-dissipation thermodynamics.

Thus, in the four-index theory we have found a linear transformation $V \rightarrow Q$ of the commutator functions V into the correlation functions Q which is inverse to the transformation $Q \rightarrow V$. In contrast to the transformation $Q \rightarrow V$, the transformation $V \rightarrow g$ of the commutator functions into the admittance functions $g^{nm}lk$ cannot be inverted since it is found to be degenerate. Therefore, arbitrariness remains in seeking a transformation $g \rightarrow V$; as the investigation has shown, the correlation functions were, roughly speaking, one-sixth undetermined.

The negative answer to the question of the existence of a linear transformation form g to V is not fortuitous. To be convinced of this, it is useful to apply the theory to the particular case of a linear system, for which all the admittance functions g, apart from the two-index one, are equal to zero. If a linear transformation $g \rightarrow V$ existed, the vanishing of g would imply the vanishing of V, and then, because of the proven transformation $V \rightarrow Q$, the fourth moments Q would consequently also disappear, which is absurd.

It is of interest to seek nonlinear formulas by which

the moment $Q^{nm}lk$ would be expressed not only in terms of $g^{nm}lk$ but also in terms of other admittance functions, say, two-index functions. In favour of such formulas is the fact that for a purely linear system (in which the fluctuations are Gaussian), the moment $Q^{nm}lk$ is expressed bilinearly in terms of g^{lk} . It is easy to see this if we use the usual (two-index) fluctuation-dissipation theorem and the simple formulas for the Gaussian case, which in the non-quantum variant have the form $Q^{nm}lk = Q^{nm}Q^{lk} + Q^{nl}Q^{mk} + Q^{nk}Q^{ml}$.

In conclusion, however, we shall give another solution of the problem of surmounting the arbitrariness remaining in the four-index theory. We shall express the function $Y^{nm}lk$ in terms of $g^{nm}lk$ and the function

$$Y^{nm}lk = \frac{\hbar}{i} \frac{\delta \langle [F_{\text{per}}^n, F_{\text{per}}^m], F_{\text{per}}^l \rangle}{\delta h^k} \text{ for } h(t) \equiv 0. \quad (4.17)$$

Using in the differentiation the usual methods which led to (2.4), we obtain

$$Y^{nm}lk = \langle [[U^{nk}, F^m], F^l] + [[F^n, U^{mk}], F^l] + [[F^n, F^m], U^{lk}] \rangle, \quad (4.18)$$

$$U^{nk} = [F^n, F^k] \eta(t_n - t_k).$$

Transforming the last term by means of the formula

$$[[A, B], C] + [[B, C], A] + [[C, A], B] = 0,$$

and putting in it $A = F^n$, $B = F^m$, and $C = U^{lk}$, we write (4.18) in the form

$$Y^{nm}lk = V^{nkm} \eta(t_n - t_k) - V^{mkn} \eta(t_m - t_k) + (V^{lkmn} - V^{lknm}) \eta(t_l - t_k).$$

If into this we substitute (4.13), we shall have

$$(i/\hbar)^3 Y^{nm}lk = (c + e + f - h - q)^{nm}lk - (c + e + d - q)^{mlnk} + (d - f + h)^{lnmk} + a^{nmkl} - (a + b + e + h)^{mlkn} + (b + e + h)^{lnkm} + a^{nkm}l - c^{mkl}n - (a - c)^{lknm} - \text{inter}.$$

(where "inter" denotes the analogous expression with the indices n and m interchanged) or

$$(i/\hbar)^3 Y^{nm}lk = g^{nm}lk + b^{mlnk} - (g + b)^{lnmk} + g^{nmkl} + (d - \tilde{c})^{mlkn} - (g + d - \tilde{c})^{lnkm} + g^{nkm}l - c^{mkl}n - (g - c)^{lknm} - \text{inter}.$$

by virtue of (4.12) and (4.14)–(4.16). Hence it is clear that, knowing the behavior of the function $Y^{nm}lk$ in the regions $t_m > t_l > t_n > t_k$, $t_m > t_k > t_l > t_n$ and $t_m > t_l > t_k > t_n$, we can uniquely determine the functions b , c and d , i.e., completely remove all the arbitrariness.

APPENDIX

Writing Eq. (4.11) in the form

$$D\xi \equiv [D_{61}, D_{65}]\xi = W,$$

where D_{65} is a 6×5 matrix, we have

$$x = \det [WD_{65}] / \det D.$$

To calculate the determinants in this expression it is convenient to transform them by combining columns. Adding the third column to the first and subtracting it from the fourth, then adding the fifth column to the second and subtracting it from the sixth, and, for the determinant D , first adding the fourth and sixth columns to the first, we shall have, after factoring out K^3

$$\Delta' = \begin{vmatrix} W_1 & 0 & 1 & 0 & 0 & 0 \\ W_2 & 0 & L^{-1} & MN-1 & 0 & 0 \\ W_3 & N-1 & K & 1-LN & 0 & 0 \\ W_4 & 0 & 0 & 0 & 1 & 0 \\ W_5 & 0 & 0 & 0 & K & LM-1 \\ W_6 & N(1-M) & 0 & 0 & NK & M-N \end{vmatrix},$$

$$\Delta = K \begin{vmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & L^{-1} & MN-1 & 0 & 0 \\ L(1-N) & N-1 & K & 1-LN & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & K & LM-1 \\ M-1 & N(1-M) & 0 & 0 & NK & M-N \end{vmatrix}.$$

We shall represent the first column as a sum of two columns, the first of which has three zero lower elements and the second three zero upper elements. After this Δ' and Δ are decomposed into a sum of two determinants, each of which is equal to a product of two simple third-order determinants. In this way we obtain easily

$$\Delta' = N(1-M)(LM-1)[(K-N)W_1 + (LN-1)W_2 + (MN-1)W_3] - (N-1)(MN-1)[(KM-1)W_4 + (N-M)W_5 + (LM-1)W_6];$$

$$\Delta = K(1-M)(1-N)(LM-1)(MN-1)(LN-1).$$

Introducing the expression

$$\Gamma^2 = -(1-N)^2(1-M)^2(1-L)^2(1-K)^2(NM-1)(ML-1)(LK-1) \times (KN-1)(NL-1)(MK-1) = [(1-N)(1-M)(1-L)(1-K)]^2 K^2 \times (NM-1)^2(ML-1)^2(NL-1)^2,$$

i.e., $\Gamma = (1-L)(1-K)\Delta$, which is invariant with respect to the cyclic permutations (N, M, L, K) and taking the first of the formulas (4.6) into account we have, consequently,

$$\Gamma x = N(1-L)(1-M)(LM-1)(K-N)V^{nm}lk + N(1-K)(1-M)(LM-1)(LN-1)V^{mnlk} + N(1-K)(1-L)(LM-1)(MN-1)V^{lnkm} + (1-L)(1-N)(MN-1)(KM-1)V^{mlnk} + (1-L)(1-K)(MN-1) \times (N-M)V^{lknm} + (1-K)(1-N)(MN-1)(LM-1)W^{nkm}l.$$

Because of the relations (4.2)–(4.4), we can put our result into a different and, in particular, more symmetric form. Thus, subtracting the expression

$$^{1/2}N(LM-1)(1-K)(1-M)(LN-1)(V^{nm}lk + V^{lknm} + V^{mnlk} + V^{hlmn}) + ^{1/2}(1-L)(1-N)(MN-1) \times (KM-1)(V^{mlnk} + V^{nkm}l + V^{lknm} + V^{hnm}l),$$

which vanishes by virtue of (4.4), and taking (4.2) into account we obtain

$$\Gamma \langle F^n F^m F^l F^k \rangle = [K^{-1}(1-M)(KN-1)(N+LK)V^{nm}lk + (1-L)(MN-1)(M+KN)V^{mlkn} + N(1-K)(LM-1) \times (L+NM)V^{lknm} + MN(1-N)(KL-1)(K+ML)V^{knml}] - ^{1/2}[K^{-1}(1-M)(NK-1)(1+K)(1+NL)V^{nm}lk + (1-L)(MN-1)(1+N)(1+MK)V^{mlkn} + N(1-K)(LM-1) \times (1+M)(1+LN)V^{lknm} + MN(1-N)(KL-1)(1+L) \times (1+KM)V^{lknm}] + ^{1/2}[N(1-M)(1-K)(ML-1)(NL-1) \times (V^{mnlk} - V^{hlmn}) + MN(1-L)(1-N)(LK-1)(MK-1) \times (V^{lknm} - V^{hnm}l)].$$

Here, each expression in square brackets is constructed in a cyclically symmetric way and has a property of the type (4.5).

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Translated by P. J. Shepherd

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