TIME CORRELATIONS OF QUANTITIES DESCRIBED BY THE KINETIC EQUATIONS

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Submitted to JETP editor November 6, 1962

J. Exptl. Theoret. Phys. (U.S.S.R.) **44**, 1915-1919 (June, 1963)

Relations are derived which make it possible, with the aid of the kinetic equations, to find the correlation function of quantities at various instants of time. In a number of cases, it is sufficient to know the equations which the mean values of the quantities obey in order to find their correlations.

1. A theory of equilibrium fluctuations of quantities described by macroscopic equations has been developed by Rytov[1] and Landau and Lifshitz[2,3]. A generalization of the theory of equilibrium fluctuations to the case of quantities described by the kinetic equations has been carried out in the works of Abrikosov and Khalatnikov[4] and Gor'kov, Dzyaloshinskiĭ, and Pitaevskiĭ.[5] The method used in these researches consisted of introducing into the corresponding equation of additional random terms whose correlations are determined by means of the Callen-Welton fluctuation-dissipation theorem[6,7,2]. In the present note, we set forth for finding the correlation functions a method that does not use the Callen-Welton theorem and is suitable, in particular, for finding correlation functions in non-equilibrium and non-stationary processes. This method is essentially a generalization of the method applied by Leontovich[8] for the calculation of stationary correlations of quantities whose mean values obey linear equations (see also [9], Secs. 117, 120).

2. We shall establish a series of general relations which make it possible to find the time correlations of quantities by means of the kinetic equations. We recall that the kinetic equations are derived for a certain projection

$$\mathscr{P}\hat{\rho} = \hat{\sigma} \qquad (1)$$

of the density matrix $\hat{\rho}$ of the entire system which, generally speaking, possesses an infinite number of degrees of freedom (see, for example, the works of Zwanzig[10] and of the author[11]).[1] With the aid of the matrix σ the average values of the quantities A and B of interest to us are found according to the well-known rule

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[1] In the case of Bogolyubov's chains[12] the operator $\mathscr{P}$ makes possible the transition from the N-th distribution function f_N (where N is the total number of particles) to f_1.

$$\langle A(t) \rangle = \mathrm{Sp}\,\hat{\sigma}(t)\,\hat{A}/\mathrm{Sp}\,\hat{\sigma}(t); \quad \langle B(t') \rangle = \mathrm{Sp}\,\hat{\sigma}(t')\,\hat{B}/\mathrm{Sp}\,\hat{\sigma}(t'). \quad (2)$$

We shall show how to find the mean value of quantities of the type

$$\eta_{AB}(t, t') = \langle \hat{A}(t)\,\hat{B}(t') \rangle \qquad (3)$$

by means of the density matrix $\hat{\sigma}(t)$.

We express in terms of the quantity $\eta_{AB}(t, t')$ the correlation functions

$$\psi_{AB}(t, t') = \tfrac{1}{2}\eta_{AB}(t, t') + \tfrac{1}{2}\eta_{BA}(t', t) \qquad (4)$$

and the response functions (see the work of Kubo[13]),

$$\varphi_{AB}(t, t') = i\hbar^{-1}\langle[\hat{A}(t), \hat{B}(t')]\rangle$$
$$= i\hbar^{-1}\{\eta_{AB}(t, t') - \eta_{BA}(t', t)\}. \qquad (5)$$

By means of the density matrix $\hat{\rho}$ and the operators $\hat{A}(t)$ and $\hat{B}(t')$ we find in the Heisenberg representation

$$\eta_{AB}(t, t') = \mathrm{Sp}\,\hat{\rho}\hat{A}(t)\,\hat{B}(t')/\mathrm{Sp}\,\hat{\rho}. \qquad (6)$$

(We recall that the matrix $\hat{\rho}$ does not depend on the time.) By using Eq. (6), we prove the following assertions:

a) Let $\langle A(t) \rangle \neq 0$; then, dividing and multiplying the right hand side of (6) by $\mathrm{Sp}\,\hat{\rho}\hat{A}(t)$, we get

$$\langle \hat{A}(t)\,\hat{B}(t') \rangle = \langle A(t) \rangle \langle B'(t') \rangle, \qquad (7)$$

$$\langle B'(t') \rangle = \mathrm{Sp}\,\hat{\rho}_t'\hat{B}(t')/\mathrm{Sp}\,\hat{\rho}_t', \quad \hat{\rho}_t' = \hat{\rho}\hat{A}(t). \qquad (8)$$

In a similar way we can represent

$$\langle \hat{A}(t)\,\hat{B}(t') \rangle = \langle A''(t) \rangle \langle B(t') \rangle, \qquad (9)$$

$$\langle A''(t) \rangle = \mathrm{Sp}\,\hat{\rho}_{t'}''\hat{A}(t)/\mathrm{Sp}\,\hat{\rho}_{t'}'', \quad \hat{\rho}_{t'}'' = \hat{B}(t')\hat{\rho}, \qquad (10)$$

where it is assumed that $\mathrm{Sp}\,\hat{\rho}_{t'}'' = \mathrm{Sp}\,\hat{B}(t')\hat{\rho} \neq 0$. It follows from (8) and (10) that the quantities $\langle B'(t') \rangle$ and $\langle A''(t) \rangle$ have the meaning of the average values of $\hat{B}(t')$ (for fixed value of t), and of $\hat{A}(t)$ (for

fixed value of t'), respectively, in the states ρ'_t and $\rho''_{t'}$.

b) Let $\langle \hat{A}(t) \rangle = \langle \hat{B}(t) \rangle = 0$; then, using (6), we obtain the following relations without difficulty:

$$\langle \hat{A}(t)\hat{B}(t') \rangle = \mathrm{Sp}\,\hat{\rho}_1 \hat{B}(t')/\mathrm{Sp}\,\hat{\rho}_1 \equiv \langle B_1(t') \rangle$$

$$= \mathrm{Sp}\,\hat{\rho}_2 \hat{A}(t)/\mathrm{Sp}\,\hat{\rho}_2 \equiv \langle A_2(t) \rangle, \qquad (11)$$

$$\hat{\rho}_1 = \hat{\rho} + \hat{\rho}\hat{A}(t), \qquad \hat{\rho}_2 = \hat{\rho} + \hat{B}(t')\hat{\rho}. \qquad (12)$$

The meaning of relations (7), (9), and (11) is that the quantity $\eta_{AB}(t, t')$ behaves for fixed $t(t')$ like a certain mean value of $B(t')(A(t))$ [multiplied by $\langle A(t) \rangle$ ($\langle B(t') \rangle$) in the case a)].

In order to find the average values of $B(t')$ [or $A(t)$], one must make use of the kinetic equation for the quantity $\hat{\sigma}$. As an initial condition for the solution of the kinetic equation, it is necessary to take

$$\hat{\sigma}'(0) = \mathscr{P}\hat{\rho}'_t = \hat{\sigma}(0)\hat{A}(t) \qquad (13)$$

in case a) for fixed t [see (8)] or

$$\hat{\sigma}''(0) = \mathscr{P}\hat{\rho}''_{t'} = \hat{B}(t')\hat{\sigma}(0) \qquad (14)$$

for fixed t' [the same case a), Eq. (10)]. In the case b) it is necessary to take the initial condition in the form

$$\hat{\sigma}_1(0) = \mathscr{P}\hat{\rho}_1 = \hat{\sigma}(0) + \hat{\sigma}(0)\hat{A}(t) \qquad (15)$$

for fixed t, and

$$\hat{\sigma}_2(0) = \mathscr{P}\hat{\rho}_2 = \hat{\sigma}(0) + \hat{B}(t')\hat{\sigma}(0) \qquad (16)$$

for fixed t'.

We recall that the closed equation for $\mathscr{P}\hat{\rho}$-$\hat{\sigma}$ holds only for a certain class of initial conditions [14,15,10,11]. Therefore, generally speaking, it is necessary in concrete cases to establish the fact that the transition from $\hat{\rho}$ to $\hat{\rho}'$ does not take the density matrix out of this class.

Let us consider the case of the stationary process

$$[\hat{H}, \hat{\rho}] = 0,$$

where $\hat{H}$ is the Hamiltonian of the entire system. In this case, for $\langle A \rangle = \langle B \rangle = 0$, the following relations hold:

$$\eta_{AB}(t, t') = \eta_{AB}(t - t') = \langle A_2(t - t') \rangle = \langle B_1(t' - t) \rangle, \qquad (17)$$

where $\langle B_1(\tau) \rangle$ and $\langle A_2(\tau) \rangle$ are found from the kinetic equation as the mean values of the quantities B and A, by means of the respective density matrices $\hat{\sigma}_1(\tau)$ and $\hat{\sigma}_2(\tau)$, which satisfy the initial conditions

$$\hat{\sigma}_1(0) = \hat{\sigma}(0) + \hat{\sigma}(0)\hat{A}; \qquad \hat{\sigma}_2(0) = \hat{\sigma}(0) + \hat{B}\hat{\sigma}(0). \qquad (18)$$

3. Let us consider the particular case in which the average values of the quantities A, B, ... obey the linear equations

$$\dot{x}_i = -\alpha_{ik}x_k \qquad (19)$$

(here and in what follows, summation over all repeated indices is implied).

It follows from what has been said above that the equations for the quantities $\psi_{ik}(\tau)$ and $\varphi_{ik}(\tau)$ in the stationary case (for $\tau > 0$) have the form

$$\dot{\psi}_{ji} = -\alpha_{jl}\psi_{li}; \qquad \dot{\varphi}_{ji} = -\alpha_{jl}\varphi_{li}. \qquad (20)$$

Bearing in mind that $\psi_{ji}(\tau) = \psi_{ij}(-\tau)$ (see, for example, [9]), it is not difficult to find an equation for the Fourier components of the correlation functions (which give the spectrum of fluctuations of the corresponding quantities).

For this purpose, it is necessary to multiply the first equation of (20) by $e^{i\omega\tau}$ and integrate from 0 to ∞:

$$\psi_{ji}(0) + i\omega \int_0^\infty \psi_{ji}(\tau)e^{i\omega\tau}\,d\tau = \alpha_{jl}\int_0^\infty \psi_{li}(\tau)e^{i\omega\tau}\,d\tau,$$

$$\psi_{ij}(0) - i\omega \int_{-\infty}^0 \psi_{ij}(\tau)e^{i\omega\tau}\,d\tau = \alpha_{il}\int_{-\infty}^0 \psi_{jl}(\tau)e^{i\omega\tau}\,d\tau. \qquad (21)$$

Solving this set of equations, and making use of the fact that

$$\psi_{ji}(0) = \tfrac{1}{2}\langle \hat{x}_j\hat{x}_i \rangle + \tfrac{1}{2}\langle \hat{x}_i\hat{x}_j \rangle,$$

we can find the fluctuation spectrum

$$(x_jx_i)_\omega = \frac{1}{2\pi}\int_{-\infty}^\infty \psi_{ji}(\tau)e^{i\omega\tau}\,d\tau. \qquad (22)$$

The relations (21) are identical with those obtained in the paper of Leontovich [8].

In addition to the fluctuation spectrum, we can find the complex susceptibility (admittance) from the second system of (20). This is equal to (see [13])

$$\chi_{ik}(\omega) = \int_0^\infty \varphi_{ik}(\tau)e^{i\omega\tau}\,d\tau. \qquad (23)$$

In a fashion similar to (21), we find

$$i\omega\chi_{ji}(\omega) - \alpha_{jl}\chi_{li}(\omega) = -\varphi_{ji}(0) = -i\hbar^{-1}\langle [\hat{x}_j, \hat{x}_{ji}] \rangle. \qquad (24)$$

Solving this set of equations, we find the susceptibility of the system.

In the special case of a harmonic oscillator with friction, Eqs. (19) have the form

$$\dot{Q} = P, \qquad \dot{P} = -\omega_0^2 Q - \gamma P, \qquad (25)$$

where $x_1 = Q$, $x_2 = P$, $\alpha_{11} = 0$, $\alpha_{12} = -1$, $\alpha_{21} = \omega_0^2$, $\alpha_{22} = \gamma$. In this case, we find from (21), (22), and

(24) (keeping it in mind that $[Q, P] = i\hbar$, and assuming $\langle \hat{Q}\hat{P} + \hat{P}\hat{Q} \rangle = 0$)

$$(x_1^2)_\omega = \frac{1}{\pi} \frac{\omega_0^2 \gamma \langle x_1^2 \rangle}{(\omega_0^2 - \omega^2)^2 + \omega^2 \gamma^2} , \tag{26}$$

$$\chi_{11}(\omega) = \frac{\omega_0^2 - \omega^2 + i\omega\gamma}{(\omega_0^2 - \omega^2)^2 + \omega^2 \gamma^2} . \tag{27}$$

The initial equations (25) are approximate. In particular, they do not describe the behavior of the harmonic oscillator after a very short interval of time, comparable with the correlation time τ_C of the surroundings of the oscillator (thermostat). We note that this surrounding (the dissipative system in the terminology of the author[16,11]) is indeed responsible for the relaxation process of the oscillator. The degree of accuracy of Eqs. (25) can be tested, in particular, with the aid of the Callen-Welton theorem,[6] in accord with which we have

$$(x_1^2)_\omega = \chi_{11}''(\omega) \frac{\hbar}{\pi} \left\{ \frac{1}{2} + \frac{1}{e^{\hbar\omega/kT} - 1} \right\} , \tag{28}$$

where $\chi_{11}''(\omega)$ is the imaginary part of the susceptibility. On the other hand, we have from Eqs. (26) and (27):

$$(x_1^2)_\omega = (\omega_0^2/\pi\omega) \langle x_1^2 \rangle \chi_{11}''(\omega). \tag{29}$$

A comparison of (28) and (29) shows that the susceptibility and the fluctuation spectrum of the harmonic oscillator located in a state of thermodynamic equilibrium satisfy the Callen-Welton theorem[6] if the frequency interval $\Delta\omega = \omega - \omega_0$, in which $\chi_{11}''(\omega)$ differs appreciably from zero, satisfies the inequalities

$$|\Delta\omega| \ll kT/\hbar \quad \text{for } \omega_0 \ll kT/\hbar, \tag{30}$$

$$\Delta\omega \ll \omega_0 \quad \text{for } \omega_0 \gg kT/\hbar. \tag{31}$$

Thus (29) satisfies the Callen-Welton theorem in the classical region for any relation between $\Delta\omega \approx \gamma$ and ω_0, if $\omega_0^2 \langle x_1^2 \rangle = kT$. We note that this is in accord with the conclusion by V. L. Ginzburg[17] that the theorem of equipartition over the degrees of freedom is satisfied in the classical region for arbitrary γ for resistances that are independent of the frequency (in our case, γ).

On the other hand, in the quantum region, the accuracy of Eq. (25) is limited by the condition that the damping be small. In this case, as is well known,[2]

$$\omega_0^2 \langle x_1^2 \rangle = \frac{\hbar\omega_0}{2} + \frac{\hbar\omega_0}{e^{\hbar\omega_0/kT} - 1} . \tag{32}$$

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[2]In the analysis that has been given we have not made use of Eq. (32), since this expression cannot hold in the quantum region for strong damping.[17] On the other hand, we have not assumed small damping beforehand.

If we substitute this expression in (29), then it is easy to see that (29) will approximately coincide with (28) under the condition

$$\Delta\omega \approx \gamma \ll max\,(\omega_0, kT/\hbar).$$

One can then draw the conclusion that the role of the correlation time τ_C of a dissipative system is assumed by $\hbar/kT$ for high temperatures and by ω_0^{-1} for low ones (see [11]).

In conclusion, the author thanks V. I. Bespalov for valuable discussion of the results of the research.

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