General theory of thermal fluctuations in nonlinear systems

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A method is proposed for investigating the thermal fluctuations in an arbitrary system subjected to the influence of a dynamic perturbation (and in contact with a thermostat). An exact formula is obtained for the characteristic functional of the fluctuations of the macroscopic variables. The formula contains all the most general consequences of the basic postulates of statistical mechanics regarding the macroscopic variables. An infinite set of relations between the moment and cumulant functions of the equilibrium and nonequilibrium fluctuations (in particular, the Onsager reciprocity relations and the fluctuation-dissipation theorems) follows from the formula. The consequences of the additional assumption that the macroscopic variables are Markovian are also considered.

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1. Theorems that stem from the following general assumptions about the character of the macroscopic motion are of great importance in statistical thermodynamics: 1) the microscopic motion obeys the laws of mechanics and is, therefore, reversible in time; 2) a system in thermodynamic equilibrium with a thermostat has a Gibbs distribution function (density matrix, in the quantum case); 3) the influence of mechanical external perturbations is described by an interaction Hamiltonian (linear in the external forces). From the reversibility in time follow the Onsager reciprocity relations, from the second and third assumptions follow the fluctuation-dissipation theorems, and from the combination of all three assumptions follow the multi-index relations of nonlinear fluctuation thermodynamics.[1–6,10] To derive these one uses perturbation theory, expanding the moments of the nonequilibrium fluctuations in series in powers of the external forces.

Efremov,[1,2] by the perturbation method, was the first to obtain three-index relations between the third-order moments of equilibrium fluctuations and the quadratic response of a system to an external perturbation. The analysis of the four-index relations,[4,6,10] however, has turned out to be extremely cumbersome, and it is impossible in practice to investigate the relations of higher order by the perturbation method. How to present the entire aggregate of information contained in all possible multi-index relations in a closed and visible form has, therefore, remained unclear. The answer to this question is given in the present paper.

We show that the set of relations of different orders can be replaced by a single exact generating formula for the characteristic functional of the stochastic thermodynamic variables or for the corresponding probability functional. The derivation, given in Sec. 2, of the fundamental generating formula (4) from a classical mechanical model and from the three aforementioned assumptions does not require the use of perturbation theory; it is an exact theorem, of which all the multi-index relations obtained previously and a large number of new relations are consequences. When formulated in terms of the probability functional (7) this theorem acquires greater simplicity and clarity. In Sec. 4 the consequences of the additional assumption that the set of macrovariables under consideration is Markovian are analyzed. Section 5 is devoted to a generalization of the generating formula (4) to the quantum case.

2. We shall consider a classical mechanical system with Hamiltonian $H_0=H_0(\alpha,\beta)$, where α is the set of generalized coordinates and β is the set of momenta canonically conjugate to them. We suppose that before the time $t=0$ the system was in thermodynamic equilibrium with the surroundings at temperature T and conformed with the Gibbs distribution[1)]

$$D(\alpha,\beta)=q^{-1}\exp\{-H_0(\alpha,\beta)/T\},$$

where q is the normalization constant. We assume that at time $t=0$ external forces $x_k(t)$ began to act on the system, and the Hamiltonian took the form

$$H(t)=H_0-h(t),\quad h(t)=\sum_k x_k(t)Q_k(\alpha,\beta)\equiv x(t)Q(\alpha^t,\beta^t).$$

Here the macroscopic variables $Q(t)\equiv Q(\alpha^t,\beta^t)$ are conjugate to the external forces; the values of the microscopic coordinates and momenta at time t are denoted by α^t and β^t. We express $Q(t)$ in terms of the initial values α^0 and β^0 of the microvariables:

$$Q(t)=Q_t[\alpha^0,\beta^0;x(\theta)],\ t>0,$$

where $Q_t[\alpha^0,\beta^0;x(\theta)]$ is a certain functional of the realization $x(\theta)$ for $t\geqslant\theta\geqslant 0$, determined by the equations of motion.

In the following we shall use the symmetry of the equations of motion under change of sign of the time. Under time reversal the momenta change sign. If the equilibrium Hamiltonian H_0 does not contain a constant magnetic field (or other time-odd parameters), then $H_0(\alpha,-\beta)=H_0(\alpha,\beta)$. Otherwise, it is necessary to reverse the direction of the magnetic field at the same time. We shall assume that the macrovariables $Q(t)$ possess a definite parity under time reversal, i.e., $Q_k(\alpha,-\beta)$, $=\varepsilon_k Q_k(\alpha,\beta)$, where $\varepsilon_k=\pm 1$. The time reversibility of the mechanical motion implies that, for $t\geqslant\tau\geqslant 0$,

$$Q(\tau)=Q_\tau[\alpha^0,\beta^0;x(\theta)]=\varepsilon Q_{t-\tau}[\alpha^t,-\beta^t;\varepsilon x(t-\theta)].\qquad(1)$$

Here ε is a diagonal matrix with elements ε_k.

The evolution and fluctuations of the variables $Q(\tau)$ for $t\geqslant\tau\geqslant 0$ are determined by the characteristic functional

$$\left\langle \exp\left\{\int_0^t u(\tau)Q(\tau)d\tau\right\}\right\rangle_{x(\theta)}$$
$$=\int d\alpha^0 d\beta^0 \exp\left\{\int_0^t u(\tau)Q_\tau[\alpha^0,\beta^0,x(\theta)]d\tau\right\}D(\alpha^0,\beta^0),$$

where $u_k(\tau)$ are arbitrary trial functions, and $\int d\alpha^0 d\beta^0$ is an integral over the whole phase space (the subscript $x(\theta)$ on the averaging symbol indicates for which realization of the external forces the nonequilibrium average is taken).

We shall elucidate which properties of the characteristic functional stem from the time-reversibility formulas (1). We introduce the quantity

$$E=\int_0^t x(\tau)\dot{Q}(\tau)d\tau,$$

which, as follows from the Hamiltonian equations of motion, gives the change in the internal energy of the system under the action of the external forces, i.e.,

$$H_0(\alpha^0,\beta^0)+E=H_0(\alpha^t,\beta^t). \tag{2}$$

Next we consider the average

$$\left\langle \exp\left\{\int_0^t u(\tau)Q(\tau)d\tau\right\}e^{-E/T}\right\rangle_{x(\tau)}$$
$$=\int d\alpha^0 d\beta^0 \exp\left\{\int_0^t u(\tau)Q_\tau[\alpha^0,\beta^0;x(\theta)]d\tau\right\}\frac{1}{q}\exp\left\{-\frac{H_0+E}{T}\right\}. \tag{3}$$

We substitute the equality (2) into this and then change to new integration variables α^t, β^t, using the fact that the Jacobian of the transformation from α^0, β^0 to α^t, β^t is equal to unity. Transforming also the exponent of the first exponential in the right-hand side of (3) by means of formula (1), we obtain

$$\left\langle \exp\left\{\int_0^t u(\tau)Q(\tau)d\tau\right\}e^{-E/T}\right\rangle_{x(\tau)}$$
$$=\int d\alpha^t d\beta^t \exp\left\{\int_0^t u(\tau)\varepsilon Q_{t-\tau}[\alpha^t,-\beta^t;\varepsilon x(t-\theta)]d\tau\right\}D(\alpha^t,\beta^t)$$
$$=\int d\alpha^t d\beta^t \exp\left\{\int_0^t u(t-\tau)\varepsilon Q_\tau[\alpha^t,\beta^t;\varepsilon x(t-\theta)]d\tau\right\}D(\alpha^t,-\beta^t)$$
$$=\left\langle \exp\left\{\int_0^t u(t-\tau)\varepsilon Q(\tau)d\tau\right\}\right\rangle_{\varepsilon x(t-\theta)}.$$

Here we have taken into account that (in the absence of a magnetic field) $D(\alpha,-\beta)=D(\alpha,\beta)$.

Since the times $t=0$ and t are in no way special, we can take $-\infty$ as the start of the action of the external force and put the upper limit of all the integrals equal to $+\infty$. Then, using the time-translation invariance of the unperturbed motion of the system, we arrive at the principal formula of this paper:

$$\left\langle \exp\left\{\int_{-\infty}^{\infty} u(\tau)Q(\tau)d\tau\right\}e^{-E/T}\right\rangle_{x(\theta)}=\left\langle \exp\left\{\int_{-\infty}^{\infty} u(-\tau)\varepsilon Q(\tau)d\tau\right\}\right\rangle_{\varepsilon x(-\theta)}, \tag{4}$$

$$E=\int_{-\infty}^{\infty} x(\tau)\dot{Q}(\tau)d\tau. \tag{5}$$

Formula (4) relates the characteristic functionals of stochastic processes $Q(t)$ for the forward and time-reversed motions of the system. Inasmuch as, in its derivation, the Hamiltonian of the system was in no way made concrete, it contains all the most general consequences of the microscopic reversibility in respect of the macrovariables $Q(t)$. It is not difficult to obtain a completely analogous formula for the characteristic functional of the variables $J(t)\equiv\dot{Q}(t)$, which we shall call the currents:

$$B[u;x]\equiv\ln\left\langle \exp\left\{\int_{-\infty}^{\infty} u(\tau)J(\tau)d\tau\right\}\right\rangle_{x(\theta)},$$
$$B[u-x/T;\,x]=B[-\varepsilon\tilde{u};\,\varepsilon\tilde{x}]. \tag{6}$$

Here we have introduced the notation $\tilde{u}(\tau)\equiv u(-\tau)$, $\tilde{x}(\tau)\equiv x(-\tau)$.

The results obtained can be given a physically intuitive form if we write them not in terms of the characteristic functionals but in terms of the density of the probability measure in the space of the macroscopic trajectories of the system. Thus, being interested in the variables $Q(t)$, we shall denote the probability-measure density in the space of the trajectories $Q(t)$ (for given realizations of the external forces) by the symbol $P[Q;x]$. Then formula (4) is equivalent to the equality

$$P[Q;\,x]e^{-E/T}=P[\varepsilon\tilde{Q};\,\varepsilon\tilde{x}]. \tag{7}$$

When $x\equiv 0$, $E\equiv 0$ and this formula states simply that the probabilities of the forward and time-reserved trajectories $Q(t)$ and $\varepsilon Q(-t)$ are the same. We integrate both sides of (7) over all trajectories $Q(t)$. The integral of the right-hand side should be equal to unity, and we arrive at the interesting relation

$$\langle e^{-E/T}\rangle=1, \tag{8}$$

which holds for an arbitrary realization of the external forces. We also obtain this result from (4), when we put $u(\tau)\equiv 0$.

If we take into account that

$$\langle e^{-E/T}\rangle\geqslant e^{-\langle E\rangle/T},$$

it follows from this and from (8), since the temperature is positive, that $\langle E\rangle\geqslant 0$. Thus, for an arbitrary mechanical external perturbation a system always absorbs energy, on the average, if it was originally in thermodynamic equilibrium.

We shall discuss briefly the meaning of the results obtained, which can be interpreted in two ways. Inasmuch as the interaction with the thermostat was switched off simultaneously with the switching-on of the perturbation, formulas (4) and (6)–(8) characterize those properties of the mechanical evolution of the system that stem from the reversibility and the special Gibbs form of the initial condition for the distribution function. The temperature T here is simply a parameter of the initial distribution and pertains to the remote past, if the external forces act for a long time. It is possible, however, to assume that: 1) the external forces act only on a small part A of the whole system $A+B$ under consideration, and the variables $Q(t)$ also pertain to the system A; 2) the whole system $A+B$ is in contact with the thermostat, but the energy of interaction with the thermostat is relatively very small and the role of the thermostat reduces to just the forming of the Gibbs equilibrium distribution in the absence of the external perturbations. Then, when the perturbation is switched on, in relation to the small subsystem A the large subsystem B will play the role of a thermostat maintaining the temperature T. In this case the parameter T in all our formulas has the meaning of the constant temperature of a thermostat and pertains to the actual moment of time. In either of these two interpretations, the formulas (4), (7) and (8) characterize the excitation of the system from the state of thermodynamic equilibrium.

We note that all the formulas can be extended to the case when the Hamiltonian of the perturbation is nonlinear in the external forces and internal parameters:

$$H(t)=H_0-h[x(t);\,Q],\quad h(\varepsilon x;\,\varepsilon Q)=h(x;\,Q).$$

As follows from Hamilton's equations, in this case the functional of the absorbed energy E in formulas (4), (7) and (8) must be specified (in place of (5)) by the more general expression

$$E=\int_{-\infty}^{\infty}\left\{\frac{d}{dt}-\dot{x}(t)\frac{\partial}{\partial x(t)}\right\}h[x(t);\,Q(t)]dt.$$

We shall consider next certain consequences of the basic formulas (4), (6) and (7).

3. We shall obtain various relations between the equilibrium and nonequilibrium moment functions of the variables $Q(t)$ and $J(t)$ by applying functional differentiation with respect to $u(t)$, $x(t)$ to (4), (6) and (7) and then putting $u(t)=x(t)=0$. Here it is necessary to invoke the principle of causality, according to which an arbitrary moment function with time arguments t_k does not depend on $x(t)$ if $t>t_k$. It is obvious that to any relation between the moment functions of the stochastic processes $Q(t)$, $J(t)$ there corresponds a relation, completely identical in form, between the cumulant functions.

We shall give an example of the calculations. We multiply both sides of (7) by $Q(t)$ and integrate over the trajectories:

$$\langle Q(t)e^{-E/T}\rangle_x=\varepsilon\langle\tilde{Q}(t)\rangle_{\varepsilon\tilde{x}},\quad \tilde{Q}(t)=Q(-t).$$

We differentiate this equality with respect to $x(t_1)$ and put $x(t)\equiv 0$:

$$\left[\frac{\delta}{\delta x(t_1)}\langle Q(t)\rangle_x\right]_{x=0}-\frac{1}{T}\langle Q(t)\dot{Q}(t_1)\rangle_0=\left[\varepsilon\frac{\delta}{\delta x(t_1)}\langle\tilde{Q}(t)\rangle_{\varepsilon\tilde{x}}\right]_{x=0}=\varepsilon^2\left[\frac{\delta}{\delta\tilde{x}(t_1)}\langle\tilde{Q}(t)\rangle\right]_{x=0},$$

where $\langle\ldots\rangle_0$ denotes an equilibrium average (in the absence of external forces) and the factor ε^2 has an obvious tensor meaning. Let $t>t_1$; then $-t<-t_1$ and, by virtue of causality, the right-hand side should be equal to zero. As a result we obtain the two-index fluctuation-dissipation formula

$$\left[\frac{\delta}{\delta x(t_1)}\langle Q(t)\rangle\right]_{x=0}=\frac{1}{T}\langle Q(t)\dot{Q}(t_1)\rangle_0,\quad t>t_1. \tag{9}$$

(Here and below we omit the subscript x from the nonequilibrium averages.)

Completely analogously we can obtain the multi-index relations, which are written most simply in terms of the currents $J(t)=\dot{Q}(t)$. Without concerning ourselves with the calculations, we give here only the three- and four-index relations. We first introduce abbreviated notation, clarifying it by examples:

$$Y_{12}(\tau)\equiv\langle J_1(t)J_2(t-\tau)\rangle_0,\quad Y_{12|}(\tau)\equiv\left[\frac{\delta}{\delta x_2(t-\tau)}\langle J_1(t)\rangle\right]_{x=0},$$

$$Y_{123|4}(\tau_1\tau_2\tau_3)\equiv\left[\frac{\delta}{\delta x_3(t-\tau_1-\tau_2)}\langle J_1(t)J_2(t-\tau_1)J_4(t-\tau_1-\tau_2-\tau_3)\rangle\right]_{x=0}$$

etc., where all the $\tau_k\geqslant 0$ and by $\langle J\ldots J\rangle$ we mean either the moment or the cumulant functions of the currents. In this notation, after it has been differentiated with respect to t formula (9) takes the form

$$Y_{12|}(\tau)=T^{-1}Y_{12}(\tau). \tag{10}$$

Putting $x=0$ in (6), we obtain the following symmetry relations for the equilibrium moment functions of the currents:

$$Y_{12\ldots n}(\tau_1\tau_2\ldots\tau_{n-1})=(-1)^n\varepsilon_1\ldots\varepsilon_n Y_{n\ldots 21}(\tau_{n-1}\ldots\tau_2\tau_1). \tag{11}$$

In particular, for $\tau_k=0$ we have

$$\langle J^n\rangle=(-\varepsilon)^n\langle J^n\rangle.$$

Consequently, if Q_k is an even variable ($\varepsilon_k=I$), the equilibrium one-dimensional distribution of the current J_k is symmetric, i.e., opposite directions of the current are equally probable. From (10) and (11) for $n=1$, making the tensor notation explicit we obtain the Onsager reciprocity relations:

$$\left[\frac{\delta}{\delta x_m(0)}\langle J_k(\tau)\rangle\right]_{x=0}=\varepsilon_k\varepsilon_m\left[\frac{\delta}{\delta x_k(0)}\langle J_m(\tau)\rangle\right]_{x=0}.$$

We write out the three-index relations:

$$\begin{gathered}Y_{123}(\tau_1\tau_2)=-\varepsilon_1\varepsilon_2\varepsilon_3Y_{321}(\tau_2\tau_1)\\ Y_{123|}(\tau_1\tau_2)=T^{-1}Y_{123}(\tau_1\tau_2),\\ Y_{12|3|}(\tau_1\tau_2)=T^{-1}Y_{12|3}(\tau_1\tau_2),\\ T^{-2}Y_{123}(\tau_1\tau_2)=Y_{12|3|}(\tau_1\tau_2)-\varepsilon_1\varepsilon_2\varepsilon_3Y_{32|1|}(\tau_2\tau_1).\end{gathered} \tag{12}$$

The complete independent four-index relations have the form

$$\begin{gathered}Y_{1234}(\tau_1\tau_2\tau_3)=\varepsilon_1\varepsilon_2\varepsilon_3\varepsilon_4Y_{4321}(\tau_3\tau_2\tau_1),\\ Y_{12|3|4|}(\tau_1\tau_2\tau_3)=T^{-1}Y_{12|3|4}(\tau_1\tau_2\tau_3),\\ Y_{123|4|}(\tau_1\tau_2\tau_3)=T^{-1}Y_{123|4}(\tau_1\tau_2\tau_3),\\ Y_{12|34|}(\tau_1\tau_2\tau_3)=T^{-1}Y_{12|34}(\tau_1\tau_2\tau_3),\\ Y_{1234|}(\tau_1\tau_2\tau_3)=T^{-1}Y_{1234}(\tau_1\tau_2\tau_3),\\ Y_{12|3|4}(\tau_1\tau_2\tau_3)-\varepsilon_1\varepsilon_2\varepsilon_3\varepsilon_4Y_{43|2|1}(\tau_3\tau_2\tau_1)\\ =Y_{12|34|}(\tau_1\tau_2\tau_3)-\varepsilon_1\varepsilon_2\varepsilon_3\varepsilon_4Y_{43|21|}(\tau_3\tau_2\tau_1),\\ T^{-2}Y_{1234}(\tau_1\tau_2\tau_3)=Y_{123|4|}(\tau_1\tau_2\tau_3)+\varepsilon_1\varepsilon_2\varepsilon_3\varepsilon_4Y_{43|21|}(\tau_3\tau_2\tau_1).\end{gathered} \tag{13}$$

Formula (12) expresses the third equilibrium cumulant function in terms of the second variation of the nonequilibrium average $\langle J \rangle$ with respect to the external forces; the first variation of the nonequilibrium correlation function can also be expressed in terms of this variation. The four-index relations do not enable us to relate the equilibrium fourth cumulant to the nonequilibrium averages. However, according to (13), the fourth equilibrium cumulant is determined by the second variation of the nonequilibrium correlation function with respect to the forces. These are the well-known results obtained in[1-4,6,10] for the quantum case by the method of perturbation theory and presented there in a (much more complicated) spectral form. Our method does not require the use of perturbation theory and makes it possible to obtain multi-index relations from the exact generating formulas (4), (6) and (7) by a comparatively simple route. As a straightforward analysis of formula (6) shows, the equilibrium cumulant functions of orders $2N$ and $2N+1$ can be expressed in terms of the variations of the N-th and lower nonequilibrium cumulant functions with respect to the forces. We remark also that the formula derived by Stratonovich[5] that relates the two-dimensional equilibrium and one-dimensional nonequilibrium distributions of $Q(t)$ follows from (4).

4. We shall assume that the macrovariables $Q(t)$ form a complete set, i.e., they uniquely determine their future. In this case it is natural to assume their fluctuations to be Markovian. We shall consider what information about the kinetic operator of a Markovian process $Q(t)$ can be extracted from the general formula (7). We shall denote the probability density of the stationary nonequilibrium distribution for $x(t)=x=\text{const}$ by $W_x(Q)$, and the probability density of the equilibrium fluctuations by $W_0(Q)$. We put $Q(t_k)\equiv Q_k$ and stipulate that $t_1 \geqslant t_2 \ldots \geqslant t_n$. We take the trajectory of the external forces to be piecewise-constant: $x(t)=x_k=\text{const}$ for $t_k > t > t_{k+1}$. We denote by the symbol $V_{\tau k}(Q_k \mid Q_{k+1};\ x_k, x_{k+1}\ldots)$ the probability density of a transition from Q_{k+1} to Q_k in the time $\tau_k \equiv t_k - t_{k+1}$ (and if $x_m = 0$ we shall not include x_m among the arguments).

We now put $x_k = 0$ for $k \neq 1$, $\tau_1 = \tau$, and $x_1 = x$. Formula (7) takes the form

$$P[Q;\ x] \exp\{-x(Q_1-Q_2)/T\} = P[\varepsilon\tilde{Q}_1;\ \varepsilon\tilde{x}].$$

Integrating this equality over all trajectories with the two fixed points $Q(t_1)=Q_1$ and $Q(t_2)=Q_2$, we obtain

$$V_\tau(Q_1|Q_2;\ x)\, W_0(Q_2) \exp\{-x(Q_1-Q_2)/T\} = V_\tau(\varepsilon Q_2|\varepsilon Q_1;\ \varepsilon x)\, W_0(\varepsilon Q_1). \tag{14}$$

In the limit as $\tau \to \infty$, Q_1 and Q_2 should become statistically independent, and therefore (14) becomes

$$W_x(Q_1)\, W_0(Q_2) \exp\{-x(Q_1-Q_2)/T\} = W_{\varepsilon x}(\varepsilon Q_2)\, W_0(\varepsilon Q_1).$$

From this it follows that

$$W_x(Q) \sim W_0(Q)\, e^{xQ/T}, \quad W_0(Q) = W_0(\varepsilon Q). \tag{15}$$

Next, let $x_k = 0$ for $k \neq 1, 2$. From (7), by the previous method, we obtain

$$V_{\tau_1}(Q_1|Q_2;\ x_1, x_2)\, V_{\tau_2}(Q_2|Q_3;\ x_2)\, W_0(Q_3) \times \exp\{-[x_1(Q_1-Q_2)+x_2(Q_2-Q_3)]/T\}$$
$$= V_{\tau_2}(\varepsilon Q_3|\varepsilon Q_2;\ \varepsilon x_2, \varepsilon x_1)\, V_{\tau_1}(\varepsilon Q_2|\varepsilon Q_1;\ \varepsilon x_1)\, W_0(\varepsilon Q_1).$$

From this and from (14), (15), it is not difficult to obtain the equality

$$V_{\tau_1}(Q_1|Q_2;\ x_1, x_2)\, V_{\tau_2}(\varepsilon Q_3|\varepsilon Q_2;\ \varepsilon x_2)\, W_0(Q_2) \exp\{-x_1(Q_1-Q_2)/T\}$$
$$= V_{\tau_2}(\varepsilon Q_3|\varepsilon Q_2;\ \varepsilon x_2, \varepsilon x_1)\, V_{\tau_1}(\varepsilon Q_2|\varepsilon Q_1;\ \varepsilon x_1)\, W_0(Q_1),$$

integration of which over Q_3 gives

$$V_{\tau_1}(Q_1|Q_2;\ x_1, x_2)\, W_0(Q_2) \exp\{-x_1(Q_1-Q_2)/T\}$$
$$= V_{\tau_1}(\varepsilon Q_2|\varepsilon Q_1;\ \varepsilon x_1)\, W_0(Q_1).$$

The right-hand side of this equality does not depend on x_2, and, therefore, the left-hand side, i.e., V_{τ_1}, also does not, in fact, depend on x_2.

Thus, in combination with the Markovian assumption, the time symmetry of the motion leads to the following important result: the probability density of a transition from $Q(t_2)$ and $Q(t_1)$ depends only on $x(t)$ for $t_1 > t > t_2$ and does not depend on that part of the realization of the external forces that precedes the time t_2. This means that the kinetic operator of the Markovian stochastic process $Q(t)$ should depend in an instantaneous manner on the external forces. At the same time, we have obtained a symmetry property for the transition-probability density:

$$V_\tau(Q_1|Q_2;\ x)\, W_x(Q_2) = V_\tau(\varepsilon Q_2|\varepsilon Q_1;\ \varepsilon x)\, W_x(Q_1). \tag{16}$$

The latter formula is equivalent to the following relations between the kinetic coefficients $K_n(x, Q)$:

$$W_0(Q)\,(-\varepsilon)^n K_n(\varepsilon x, \varepsilon Q) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} \left(\frac{d}{dQ} + \frac{x}{T}\right)^m K_{n+m}(x, Q)\, W_0(Q).$$

These restrictions, following from formulas (15) and (16), on the kinetic coefficients have been analyzed by Stratonovich.[7-9] However, in his papers,[7-9] the relations (15) and (16) appear as initial postulates, and the external forces are assumed to be constant. First, we have derived (15) and (16) from the more general nonmarkovian relation (7), and, secondly, we have shown that it is necessary to extend the results of Stratonovich[7-9] to the case of time-dependent external forces (in this case the kinetic coefficients are determined by the instantaneous value of $x(t)$).

5. In conclusion we shall derive the quantum equivalent of the classical time-symmetry formula (4). Inasmuch as a quantum system does not have a trajectory, we cannot introduce for it a characteristic or probability functional, and it is necessary to consider the quantum moment functions directly. We denote by

$$\rho = q^{-1} e^{-H_0/T}$$

the equilibrium density matrix, and by $Q(t)$, $A_k(t)$ the Hermitian operators of the physical variables in the Heisenberg picture, which are related to the operators Q, A_k in the Schrödinger picture by the formulas

$$Q(t) = S^+(t, 0)\, Q S(t, 0), \quad A_k(t) = S^+(t, 0)\, A_k S(t, 0),$$
$$S(t, \tau) \equiv \overleftarrow{\exp}\left\{-\frac{i}{\hbar}\int_\tau^t H(t')\, dt'\right\}, \quad H(t) = H_0 - x(t)\, Q.$$

Here and below the symbols $\overrightarrow{\exp}$ and $\overleftarrow{\exp}$ will denote, respectively, the chronological and antichronological ordering of the exponential, and the cross denotes the Hermitian conjugate. The nonequilibrium quantum moment functions are determined by the formulas

$$\langle A_1(t_1)A_2(t_2)\dots A_n(t_n)\rangle_{x(\tau)}\equiv \mathrm{Sp}\,\{A_1(t_1)A_2(t_2)\dots A_n(t_n)\rho\}.$$

In order to find the time-symmetry relations for them, we shall consider the average

$$\mathrm{Sp}\,\{A_1(t_1)\dots A_n(t_n)S^+(t,\,0)\rho S(t,\,0)\}\equiv a, \tag{17}$$

assuming first, as in Sec. 2, that the external forces $x(\tau)=0$ for $\tau<0$ and that $t>t_k\geqslant 0$. Using the properties of the trace $\mathrm{Sp}\{\dots\}$ and the formula

$$S(\tau,\,0)=S^+(t,\,\tau)S(t,\,0),$$

it is not difficult to bring (17) to the form

$$a=\mathrm{Sp}\,\{S(t,\,t_1)A_1S^+(t,\,t_1)\dots S(t,\,t_n)A_nS^+(t,\,t_n)\rho\}. \tag{18}$$

The values of (18) is not changed when the operator under the trace is replaced by its transpose. Therefore, denoting the transpose by a bar above, we can write, in place of (18),

$$a=\mathrm{Sp}\,\{\bar S^+(t,\,t_n)\bar A_n\bar S(t,\,t_n)\dots \bar S^+(t,\,t_1)\bar A_1\bar S(t,\,t_1)\bar\rho\}. \tag{19}$$

We now recall that under time reversal any Hermitian operator (in the Schrödinger picture) goes over into its transpose. If all the physical quantities under consideration possess a definite parity under time reversal, then $\bar A_k=\varepsilon_k A_k$ and $\bar Q=\varepsilon Q$, where $\varepsilon_k=\pm 1$ and $\varepsilon=\pm 1$. (Generally speaking, the relations $\bar A_k=\varepsilon_k U^+A_kU$ and $\bar Q=\varepsilon U^+QU$ hold, where U is a certain unitary operator. However, the values of $\mathrm{Sp}\{\dots\}$ and of the moment functions remain unchanged under any unitary transformation U, so that we can assume $U=I$.) Furthermore, if the equilibrium Hamiltonian H_0 does not contain time-odd parameters, e.g., a constant magnetic field, then $\bar H_0=H_0$. Otherwise, taking the transpose of H_0 is equivalent to reversing the direction of the magnetic field. Assuming that $\bar H_0=H_0$ and $\bar\rho=\rho$, we obtain from (19)

$$a=\varepsilon_1\dots\varepsilon_n\,\mathrm{Sp}\,\{\bar S^+(t,\,t_n)A_n\bar S(t,\,t_n)\dots \bar S^+(t,\,t_1)A_1\bar S(t,\,t_1)\rho\}, \tag{20}$$

$$\bar S(t,\,t)=\overrightarrow{\exp}\left\{-\frac{i}{\hbar}\int_\tau^t\bar H(t')\,dt'\right\}=\overleftarrow{\exp}\left\{-\frac{i}{\hbar}\int_0^{t-\tau}\bar H(t-t')\,dt'\right\}$$
$$=\overleftarrow{\exp}\left\{-\frac{i}{\hbar}\int_0^{t-\tau}[H_0-\varepsilon x(t-t')\,Q]\,dt'\right\}. \tag{21}$$

In the latter formula we have used the well-known rule for going over from a chronologically ordered exponential to an antichronologically ordered one.

It is easy to see from formulas (20) and (21) that $\mathrm{Sp}\{\dots\}$ in (20) coincides with the moment function with the time-reversed external force $\varepsilon x(t-\tau)$:

$$a=\varepsilon_1\dots\varepsilon_n\langle A_n(t-t_n)\dots A_1(t-t_1)\rangle_{\varepsilon x(t-\tau)}.$$

Taking into account the time-translational invariance of the unperturbed motion of the system, we can rewrite this equality in the form

$$a=\varepsilon_1\dots\varepsilon_n\langle A_n(-t_n)\dots A_1(-t_1)\rangle_{\varepsilon x(-\tau)}. \tag{22}$$

We now transform the initial average (17) in another way. We note that

$$S^+(t,\,0)\rho S(t,\,0)=q^{-1}\exp\{-H_0(t)/T\},\quad H_0(t)=S^+(t,\,0)H_0S(t,\,0). \tag{23}$$

We shall consider the derivative

$$\frac{d}{dt}H_0(t)=S^+(t,0)\frac{i}{\hbar}\{H(t)H_0-H_0H(t)\}S(t,0)$$
$$=x(t)S^+(t,0)\frac{i}{\hbar}\{H(t)Q-QH(t)\}S(t,0)=x(t)J(t),$$

where we have introduced the operator $J(t)\equiv dQ(t)/dt$. Hence follows

$$H_0(t)=H_0+E,\quad E=\int_0^t x(t')J(t')\,dt'.$$

Substituting this expression (which is analogous to the classical expression (2)) into (23) and using the well-known formula

$$e^{A+B}=\overrightarrow{\exp}\left\{\int_0^1 e^{A\alpha}Be^{-A\alpha}\,d\alpha\right\}e^A,$$

in which A and B are arbitrary operators, we obtain

$$S^+(t,0)\rho S(t,0)=\overrightarrow{\exp}\left\{-\frac{1}{T}\int_0^1 e^{-H_0\alpha/T}Ee^{H_0\alpha/T}\,d\alpha\right\}\rho.$$

Finally, from this and from (17) and (22) we obtain the following desired result:

$$\left\langle A_1(t_1)\dots A_n(t_n)\overrightarrow{\exp}\left\{-\frac{1}{T}\int_0^1 e^{-H_0\alpha/T}Ee^{H_0\alpha/T}\,d\alpha\right\}\right\rangle_{x(\tau)}$$
$$=\varepsilon_1\dots\varepsilon_n\langle A_n(-t_n)\dots A_1(-t_1)\rangle_{\varepsilon x(-\tau)}. \tag{24}$$

The start of the action of the external forces can now be taken at $-\infty$. The operator E in (24) is defined by the expression

$$E=\int_{-\infty}^{\infty}x(t)J(t)\,dt$$

and has the usual meaning of the operator of the energy absorbed by the system in the presence of the external perturbation.

The formula (24) relates the moment functions for the forward and time-reversed motions of the system. In the classical limit all the variables become commuting variables and the order of the factors under the averaging symbol is unimportant. The exponential in the left-hand side of (24) acquires the form $e^{-E/T}$ and the formula is considerably simplified:

$$\left\langle A_1(t_1)\dots A_n(t_n)\exp\left\{-\frac{1}{T}\int_{-\infty}^{\infty}x(t)J(t)\,dt\right\}\right\rangle_{x(\tau)}$$
$$=\varepsilon_1\dots\varepsilon_n\langle A_1(-t_1)\dots A_n(-t_n)\rangle_{\varepsilon x(-\tau)}.$$

Replacing A_k by Q_k here, we obtain a set of relations equivalent to the generating formula (4).

[1)]It is thereby assumed that the interaction with the thermostat is sufficiently weak, making it possible to introduce a system energy uniquely determined by the state of the system itself.

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Current fluctuations in semiconductors in the presence of a quantizing electric field

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The current fluctuations in a semiconductor are investigated under the conditions for "Stark quantization". It is shown that the fluctuations may be anomalously large. The obtained dependence of the fluctuations on the parameters of the scattering system and on the width of the energy band allow us to reach definite conclusions about the nature of the energy dissipation and band structure of the semiconductor.

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1. INTRODUCTION

A number of articles devoted to the investigation of semiconductors in strong electric fields have recently appeared. If the electric field is sufficiently strong (and the allowed band is relatively narrow), in such a field the electron is able to reach the top of the allowed band in energy space before being scattered. In such a situation the electron may undergo periodic motion in the Brillouin zone between collision events, which leads to qualitatively new quantum effects which are not observable in weak fields. The general theory of kinetic phenomena in semiconductors in a strong electric field is developed in the articles by Bryksin and Firsov.[1,2] In the single-band approximation they obtained[1] an expression for the current in an arbitrary electric field and an equation for the distribution function on the basis of a diagram technique. A quantum transport equation is presented and also a number of specific physical situations[2] are investigated. Similar questions are considered by Levinson and Yasevichyute in[3], where the quantum kinetic equation is solved and the current is calculated for a model of scattering. It should be noted that the solution of the problem by Levinson and Yasevichyute[3] is of a less general nature than the solution by Bryksin and Firsov[1,2] since the authors of[3] confined their attention to the case of weak electron-phonon coupling and to a specific choice for the form of the electron band.

It is known that the fluctuation-dissipation theorem is valid for a system in thermodynamic equilibrium; according to this theorem the problem of fluctuations reduces to a calculation of the linear response of the system to an external perturbation. There is no such generalized theorem for nonequilibrium systems, and in each specific case the calculation of the fluctuations requires special consideration. The theory of fluctuations in nonequilibrium electron-phonon systems is given in in[4–6]. In these articles current fluctuations were investigated under the quasi-classical condition $\bar{\varepsilon} \gg \hbar\omega$, where $\bar{\varepsilon}$ denotes the average energy of the electron and ω denotes the frequency of the fluctuations. High-frequency fluctuations in electron-phonon systems were investigated in[7].

The present article is devoted to a calculation of the current fluctuations in semiconductors in a strong electric field such that quantum effects due to the appearance of the "Stark levels"[8] begin to exert influence on the quantum effects. The existence of these levels has been experimentally established.[9,10] As far as the authors know, fluctuations under the conditions for quantization of the electron longitudinal motion have not been hitherto investigated.

Earlier[6,7] a method was proposed for a calculation of the fluctuations, based on the equations of motion for the quantum analog of the microscopic distribution function. In particular, this method enabled one to introduce outside sources of fluctuations into the equation for the fluctuating part of the distribution function without making any kind of assumption except those which are used in the derivation of the corresponding kinetic equations.

