ON THE FLUCTUATION-DISSIPATION THEOREM IN A STATIONARY STATE

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We consider the noise properties of systems which retain local equilibrium although a constant electrical current passes through them. We assume that heat exchange occurs fast so that the temperature in each point of the system is the same. We obtain from the quantum theory of irreversible processes for such systems a fluctuation-dissipation theorem, according to which the noise level of the system in a stationary state is determined not merely by the linear properties (active part of the impedance) but also by the non-linear properties of the system connected with quadratic detection. To illustrate the fluctuation-dissipation theorem it is applied to evaluate the noise of a p-n junction with a sufficiently large diffusion length of the minority carriers.

1. There are not many papers devoted to a consideration of fluctuations in a stationary state. Lax[1] used the theory of Markov processes but the region of applicability of the results obtained is small since he postulated for the connection between the correlation function and the macroscopic kinetic characteristics the validity of Onsager's assumption about the macroscopic character of the damping of the fluctuations. Bernard[3] used the quantum theory of irreversible processes to show that the fluctuation-dissipation theorem in its usual form does not occur in a stationary state. Bunkin[4] used the quantum theory of irreversible processes to give a definition of an effective noise temperature in a stationary state.

We must emphasize that in[3,4] as also in other papers on the quantum theory of non-linear irreversible processes (e.g., in[5]) systems are considered which are characterized by an interaction which is linear in the force which is acting. Only Stratonovich[6] mentions the desirability of studying systems with an interaction which is non-linear in the acting force.

In the present paper we consider systems which are characterized in general by an interaction which is non-linear in the applied force. The introduction of a non-linear interaction is dictated not only by a wish to have a general discussion but also by the necessity to elucidate the presence of rectifying properties in real systems. As was shown in[7], systems with an interaction which is linear in the force do not have rectifying properties.

2. We assume that the introduction of a thermodynamic force $F(t)$ (t—time) can be described by an additional term H' in the Hamiltonian. The term H' will be the interaction of the system studied with a perturbing system (i.e., with a signal generator). We have

$$H = H_0 + H', \tag{1}$$

where H_0 is the Hamiltonian of the unperturbed system. The interaction H' depends, because of the way it is introduced, not only on the dynamic variables (on the point in phase space) but also on the force F as a parameter. In particular, if the force F vanishes, the interaction H' also vanishes.

For small values of the force ($F = \Delta F$) the interaction H' can be written as a power series in the small quantity ΔF:

$$H' = -FQ = -\Delta F(Q_0 + \Delta F Q_1 + \Delta F^2 Q_2 + \ldots), \tag{2}$$

where $Q_0, Q_1, Q_2, \ldots$ depend only on the dynamic variables.

The correlation function $K_0(t)$ responding to a generalized current which is the thermodynamic conjugate of the force F can be expressed in equilibrium[8] in terms of the average of the anticommutator $[\dot{Q}_0(0), \dot{Q}_0(t)]_+$:

$$K_0(t) = \tfrac{1}{2}\langle[\dot{Q}_0(0), \dot{Q}_0(t)]_+\rangle_0 = \tfrac{1}{2}\mathrm{Sp}\{\rho_0[\dot{Q}_0(0), \dot{Q}_0(t)]_+\}. \tag{3}$$

We emphasize that the operator Q_0 is the non-trivial factor (coefficient) in the term linear in ΔF occurring in the interaction of the system with the signal generator. The time argument of the operator indicates that the operator is taken in the interaction representation. Thus

$$Q_0(t) = \exp(iH_0t/\hbar)Q_0\exp(-iH_0t/\hbar),$$

where i is the imaginary unit and $\hbar$ Dirac's constant. The pointed brackets (with index o) denote averages using the equilibrium density matrix ρ_0:

$$\rho_0 = \exp(-H_0/kT)/\mathrm{Sp}\{\exp(-H_0/kT)\},$$

where k is Boltzmann's constant and T the absolute temperature. The operator $\dot{Q}_0$ is defined by the usual relation $\dot{Q}_0 = (i\hbar)^{-1}[Q_0, H_0]$, where the square brackets indicate a commutator.

Let a force F^0, constant in time, act upon the system. After a relaxation process some state is established in the system which, strictly speaking, is not a stationary one. However, if the power dissipated in the system is small so that during time intervals of interest to us the change in the energy (and entropy) of the system is vanishingly small compared with the energy (entropy) itself we can introduce the concept of a quasi-stationary state. We denote the density matrix of such a quasi-stationary state by ρ^0.

Using the density matrix ρ^0, it is clearly impossible to evaluate the stationary current of the force J_0 but on the other hand one can use ρ^0 to evaluate the additional currents arising when we impose on the system an additional force ΔF. The density matrix ρ^0 must by virtue of the way it was introduced commute with the Hamiltonian of the stationary state H^0: $H^0 = H_0 - F^0Q^0$.

We expand the operator Q in powers of the additional force ΔF near the stationary state. We have $Q = Q^0 + \Delta F\, Q' + \frac{1}{2}\Delta F^2 Q'' + \ldots$ The operators Q^0, Q', and Q'' refer to the stationary state and depend on the force F^0 as parameter. We find for the Hamiltonian H, using the expansion for Q,

$$H = H^0 - \Delta FR - \Delta F^2 S - \ldots, \tag{4}$$

where R and S refer to the stationary state and we have for R and S: $R = Q^0 + F^0 Q'$, $S = Q' + \frac{1}{2}F^0 Q''$.

Among actually existing systems we can separate a rather wide class of systems which in a quasi-stationary state retain local equilibrium (or more precisely quasi-equilibrium). Just to this class of systems belong the systems considered in the thermodynamics of irreversible processes. We assume that heat exchange between different parts of the system takes place sufficiently rapidly. We can then characterize the whole system by a single temperature T (which, of course, increases with time, albeit slowly). The density matrix ρ^0 of a system with a fast internal heat exchange has an equilibrium structure when local equilibrium is present:

$$\rho^0 = \exp(-H^0/kT)/\mathrm{Sp}\,\{\exp(-H^0/kT)\}. \tag{5}$$

The validity of (5) indicates that the system under the action of the force F^0 goes over into a quasi-stationary state and that that state is already also a quasi-equilibrium state. A system reaching such a quasi-equilibrium state will fluctuate in about the same way as if it were in a new equilibrium state. The correlation function K(t) referring to the flux of the force ΔF must therefore be such that it can be written in the form

$$K(t) = \tfrac{1}{2}\langle[\dot R(0), \dot R(t)]_+\rangle = \tfrac{1}{2}\mathrm{Sp}\{\rho^0[\dot R(0), \dot R(t)]_+\}, \tag{6}$$

where the operator R is the non-trivial factor (coefficient) in the term which is linear in ΔF which occurs in the perturbation caused by the application of an additional force ΔF. The angle brackets (without the zero index) indicate averaging using the density matrix (5). The time argument here and henceforth shows that the operator is taken in the interaction representation using the stationary state Hamiltonian H^0. Thus

$$R(t) = \exp(iH^0t/\hbar) R \exp(-iH^0t/\hbar).$$

The operator $\dot R$ is defined by a commutator with the Hamiltonian already of the stationary state: $\dot R = (i\hbar)^{-1}[R, H^0]$.

We shall call the fluctuations occurring in the stationary state when (5) is satisfied thermal fluctuations. For the spectral density $\epsilon_T^2(\omega)$ of the thermal fluctuations we can according to the Wiener-Khinchin theorem [9] write

$$\overline{\varepsilon_T^2}(\omega) = 2\int_{-\infty}^{+\infty} e^{i\omega t}K(t)\,dt = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\tfrac{1}{2}\langle[\dot R(t), \dot R(0)]_+\rangle. \tag{7}$$

The density matrix ρ^0 satisfies the condition

$$\rho^0(H^0 + \hbar\omega) = \exp(-\hbar\omega/kT)\,\rho^0(H^0).$$

There exists therefore between the average values of the commutator and of the anticommutator of any two operators $\dot B(t)$ and $A(0)$ the general relation [10]

$$\int_{-\infty}^{+\infty} dt\, e^{i\omega t}\tfrac{1}{2}\langle[\dot B(t), A(0)]_+\rangle = E(T,\omega)\int_{-\infty}^{+\infty} dt\,(i\hbar)^{-1}e^{i\omega t}\langle[\dot B(t), A(0)]\rangle, \tag{8}$$

where $E(T, \omega)$ is the average energy of a quantum oscillator with eigenfrequency ω which is equal to

$$E(T,\omega) = \frac{\hbar\omega}{2}\,\frac{1+\exp(-\hbar\omega/kT)}{1-\exp(-\hbar\omega/kT)}. \tag{9}$$

Substituting into (8) $\dot B(t) = \dot R(t)$ and $A(0) = R(0)$ we find for the spectral density of the thermal noise

$$\overline{\varepsilon_T^2}(\omega) = 2E(T,\omega)\int_{-\infty}^{+\infty} dt\, e^{i\omega t}(i\hbar)^{-1}\langle[R(t), \dot R(0)]\rangle. \tag{10}$$

The function $i^{-1}\langle[R(t), \dot R(0)]\rangle$ is an even function of the time. Hence, we have instead of (10)

$$\overline{\varepsilon_T^2}(\omega) = 4E(T,\omega)\int_{-\infty}^{0} dt\,(i\hbar)^{-1}\cos\omega t\,\langle[R(t), \dot R(0)]\rangle. \tag{11}$$

We evaluate now the time average of the power $\overline{\Delta P}$ which is additionally dissipated in the system when an additional force ΔF is switched on:

$$\Delta F = V_0 e^{\varepsilon t}\cos\omega t, \quad \varepsilon > 0, \tag{12}$$

where ϵ is the parameter of the adiabatic switching on of the additional force, V_0 is a small quantity. We perform the calculation in the established regime in the first non-vanishing approximation in V_0 (i.e., in second order in the quantity V_0).

For the power ΔP we have

$$\Delta P = \langle (i\hbar)^{-1}[H^0, H]\rangle^{(2)} = \langle (i\hbar)^{-1}[H^0, H^0 - \Delta FR - \Delta F^2 S]\rangle^{(2)} = \Delta F\langle \dot R\rangle^{(1)} + \Delta F^2\langle \dot S\rangle.$$

The index on the angle brackets indicates what order in V_0 we must retain. Hence, $\Delta P = \Delta F\langle \dot R\rangle^{(1)}$.

We can rewrite the expression for $\langle \dot R\rangle^{(1)}$ using the general formula [8] for an arbitrary operator B:

$$\langle B\rangle^{(1)} = (i\hbar)^{-1}\int_{-\infty}^{t} dt_1\Delta F(t_1)\langle[R(t_1), B(t)]\rangle. \tag{13}$$

Putting B equal to $\dot R$ we find

$$\langle \dot R\rangle^{(1)} = \int_{-\infty}^{t} dt_1\,\Delta F(t_1)(i\hbar)^{-1}\langle[R(t_1), \dot R(t)]\rangle.$$

Bearing in mind that we can under the trace sign cyclically commute the operators and also that

$$\exp(iH^0t/\hbar)\exp(-iH^0t/\hbar) = 1; \quad [\rho^0, \exp(-iH^0t/\hbar)] = 0.$$

We get

$$\langle \dot R\rangle^{(1)} = \int_{-\infty}^{t} dt_1\,\Delta F(t_1)(i\hbar)^{-1}\langle[R(t_1 - t), \dot R(0)]\rangle.$$

We introduce a new integration variable $t_3 = t_1 - t$. We get

$$\langle \dot R\rangle^{(1)} = \int_{-\infty}^{0} dt_3\Delta F(t + t_3)(i\hbar)^{-1}\langle[R(t_3), \dot R(0)]\rangle. \tag{14}$$

The time average of the product $\cos\omega t\,\cos(\omega t + \omega t_3)$ is equal to $\frac{1}{2}\cos\omega t_3$. Hence we have for $\overline{\Delta P}$

$$\overline{\Delta P} = \tfrac{1}{2}V_0^2\int_{-\infty}^{0} dt_3\,(i\hbar)^{-1}\cos\omega t_3\,\langle[R(t_3), \dot R(0)]\rangle. \tag{15}$$

A comparison of (11) and (15) enables us to establish a fluctuation-dissipation theorem for systems in a quasi-stationary, quasi-equilibrium state:

$$\overline{\varepsilon_T^2}(\omega) = 4E(T, \omega)\Delta P/\overline{\Delta F^2}. \quad (16)$$

3. We shall be interested in electrical systems. It is clear from (16) that the level of the fluctuations is closely connected with such macroscopic characteristics of the electrical system as the coefficient (the non-trivial factor) in the additionally dissipating power. However, there arises some ambiguity in the choice of the power.

We are referring here to the fact that we can take for the force F either the electrical current or the gradient of the potential. In the first case, the current which is the thermodynamic conjugate of the force F will be the gradient of the potential; in the second case the current thermodynamically conjugate to the force will be the electrical current. In the first case Eq. (16) gives the magnitude of the level of the fluctuation emf when the leads of a two-terminal network are open for a variable current. In the second case Eq. (16) must give the magnitude of the level of the fluctuation current flowing through a two-terminal network in the regime where it has been briefly closed for a variable current. The levels of the fluctuating current and of the fluctuating emf must then be connected by the electrotechnical relation

$$\overline{I_T^2}(\omega) = \overline{\varepsilon_T^2}(\omega)/|Z(\omega)|^2, \quad (17)$$

where $Z(\omega)$ is the impedance of the two-terminal network in the stationary state with frequency ω. This is just the situation in the case of true equilibrium when there is no steady current flowing through the system.

When a steady current is present it is impossible to use Eq. (16) to calculate the level of the fluctuating emf and the level of the fluctuating current since then Eq. (17) is no longer valid. Hence, the choice of the force F to be either the electrical current or the gradient of the potential is no longer arbitrary but unambiguous. The force F must in all cases be either the electrical current or the gradient of the potential.

Let there be several independent two-terminal networks which subsequently are joined up in one large two-terminal network. If we assume that Eq. (16) with the same success must describe noise properties both of the separate two-terminal networks and the noise properties of the large two-terminal network it is necessary to reach the conclusion that we must take for the force F the electrical current. The level of the fluctuation current is determined from Eq. (17). From a comparison of (16) and (17) it is clear that the level of the fluctuation current $\overline{I_T^2}$ can also be calculated from Eq. (16) if we take for $\overline{\Delta P}$ the power which is additionally dissipated in the system when there is a permanent constant current and for $\overline{\Delta F^2}$ the average value of the square of the additional variable potential.

For an electrical two-terminal network we can express the value of $\overline{\Delta P}/\overline{\Delta F^2}$, in terms of $r(\omega)$, the active part of the impedance in a stationary state, of $I \equiv F^0$, the constant electrical current transferring the system into a stationary state, and of the quantity $\psi(\omega)$ characterizing the rectifying properties of the two-terminal network. As a result we get instead of (16)

$$\overline{\varepsilon_T^2}(\omega) = 4E(T, \omega)\{r(\omega) + I\Psi(\omega)\}. \quad (18)$$

It is well known[11] that when an additional current $\Delta I = \Delta F$ is switched on which varies with time according to (12) there arises in first approximation in the small quantity V_0 a variable component of the potential changing with the main frequency ω. In the second approximation in the amplitude V_0 there arises a component of the potential changing with twice that frequency and a shift in the constant potential $\overline{\Delta U}$ occurs with

$$\overline{\Delta U} = \Psi(\omega)\overline{\Delta I^2}. \quad (19)$$

Equation (19) is the definition of the quantiy $\psi(\omega)$.

When there is no constant current the second terms in the braces in (18) vanishes and the first one changes to the resistance corresponding to the equilibrium state. As a result (18) changes, as it should do, to the Nyquist formula.[12] We find from (18) that the effective noise temperature[13] is determined by the relation

$$E(T_{\text{eff}}, \omega) = E(T, \omega)\{r(\omega) + I\Psi(\omega)\}/r(\omega). \quad (18a)$$

Moreover, assuming that the distribution function has the form (5) we find according to Eq. (11a) of[13] that $T_{\text{eff}} = T$. This difference between Eq. (18a) and Eq. (11a) of[13] is a consequence of the non-linear character of the interaction of the system with the signal generator.

4. We consider a simple example. It is well known[9] that a diode made from a semiconductor such as germanium with a sufficiently large diffusion length of the minority carriers under well-known limitations has a current-voltage characteristic

$$I = I_0\{\exp(e_0U/kT) - 1\}, \quad (20)$$

where I_0 is a parameter, e_0 the electronic charge ($e_0 > 0$), U the potential, and I the current. When obtaining (20) we assumed that the electrons and holes in the region of the space charge (even though there is an electrical current passing through the sample) are distributed according to the Boltzmann law but taking into account the applied voltage. This means that when the current passes through the diode it changes into a quasi-equilibrium condition and we can thus use Eq. (18). Under the same conditions under which we obtained the characteristic (20) it turns out that

$$\Psi(\omega) = -\frac{e_0}{2kT}|Z(\omega)|^2, \quad (21)$$

where $Z(\omega)$ is the impedance of the p-n junction at frequency ω. For the level of the fluctuation current we can according to (18) write

$$\overline{I_T^2} = \overline{\varepsilon_T^2}/|Z(\omega)|^2 = 4E(T, \omega)\{g(\omega) + I\Psi(\omega)/|Z(\omega)|^2\}, \quad (22)$$

where $g(\omega)$ is the conductance at frequency ω. Using Eq. (21) for $\psi(\omega)$ we get instead of (22) (neglecting the fact that Planck's constant is finite)

$$\overline{I_T^2} = 4kTg(\omega) - 2e_0I. \quad (23)$$

If the frequency ω is much lower than the frequency of generation and recombination of the electrons and holes we can use the current-voltage characteristic (20) to calculate the conductivity $g(\omega)$. As a result we get an expression for the level of the thermal fluctuation currents

$$\overline{I_T^2} = 2e_0I_0\exp(e_0U/kT) + 2e_0I_0,$$

which has often been obtained before [9,14] by a formal application of the Schottky formula for shot noise for currents $I_0\exp(e_0U/kT)$ and I_0 the difference between which gives the resulting current passing through the diode.

We note that Eq. (23) is exactly the same as van der Ziel's Eq. (8.10a) from [9], obtained for p-n junctions by including the Schottky formula for shot noise.

If we assume that we can use Eq. (16) to calculate the level of the fluctuating current if we understand by $\overline{\Delta P}$ the average value of the power additionally dissipated in the system when the steady potential is constant, we get using the actual form (20) of the current-voltage characteristic

$$\overline{I_T^2} = 4e_0I_0\exp(e_0U/kT)\{1 + e_0U/2kT\}.$$

When $U = -2kT/e_0$ the average value of the square of the fluctuating current vanishes and when $U < -2kT/e_0$ this value becomes even negative. From this actual example of a semiconductor diode it is clear that the noise level is determined by the coefficient of the additional power corresponding to the regime of a constant steady current.

5. The quantities $r(\omega)$ and $\psi(\omega)$ can be evaluated directly from the responses in the first and second order of smallness. We can use (13) to write the change in the potential in first order in the small quantity V_0 in the form

$$\begin{aligned}\Delta U^{(1)} &= \langle (i\hbar)^{-1}[Q, H]\rangle^{(1)} = (i\hbar)^{-1}\langle [Q^0 + \Delta FQ',\ H^0 - \Delta FR]\rangle^{(1)} \\ &= \langle \dot{Q}^0\rangle^{(1)} - \Delta F(i\hbar)^{-1}\langle [Q^0, R]\rangle \\ &= (i\hbar)^{-1}\int_{-\infty}^{t} dt_1\Delta F(t_1)\langle [R(t_1),\ \dot{Q}^0(t)]\rangle + \Delta F(i\hbar)^{-1}\langle [R(0),\ Q^0(0)]\rangle.\end{aligned}$$

After standard transformations we get for the magnitude of the impedance from (24)

$$Z(\omega) = (i\hbar)^{-1}\mathrm{Sp}\left\{\rho^0\int_{-\infty}^{0} dt_3\, e^{\epsilon t_3}e^{i\omega t}[R(t_3), \dot{Q}^0(0)]\right\} + (i\hbar)^{-1}\mathrm{Sp}\{\rho^0[R(0), Q^0(0)]\}. \tag{25}$$

We have thus for the resistive component of the impedance

$$r(\omega) = (i\hbar)^{-1}\int_{-\infty}^{0} dt_3\, e^{\epsilon t_3}\cos\omega t_3\langle[R(t_3), \dot{Q}^0(0)]\rangle + (i\hbar)^{-1}\langle[R(0), Q^0(0)]\rangle. \tag{26}$$

For the second order response, taking the quadratic term in (4) into account we can write [8]

$$\langle B\rangle^{(2)} = (i\hbar)^{-2}\int_{-\infty}^{t} dt_1\int_{-\infty}^{t_1} dt_2\,\Delta F(t_1)\Delta F(t_2)\langle[R(t_2), [R(t_1), B(t)]]\rangle + (i\hbar)^{-1}\int_{-\infty}^{t} dt_1\,\Delta F(t_1)\Delta F(t_1)\langle[S(t_1), B(t)]\rangle, \tag{27}$$

where B is an arbitrary operator. For the second order change in the potential we have

$$\begin{aligned}\Delta U^{(2)} &= (i\hbar)^{-1}\langle[Q^0 + \Delta FQ' + {}^1/_2\Delta F^2Q',\ H^0 - \Delta FR - \Delta F^2S]\rangle^{(2)} \\ &= \langle\dot{Q}^0\rangle^{(2)} + \Delta F\langle\dot{Q}'\rangle^{(1)} - \Delta F(i\hbar)^{-1}\langle[Q^0, R]\rangle^{(1)} \\ &\quad - \Delta F^2(i\hbar)^{-1}\langle[Q', R]\rangle - \Delta F^2(i\hbar)^{-1}\langle[Q^0, S]\rangle.\end{aligned} \tag{28}$$

To evaluate $\langle\dot{Q}^0\rangle^{(2)}$ we must use Eq. (27) and to evaluate $\langle\dot{Q}'\rangle^{(1)}$ and $\langle[Q^0, R]\rangle^{(1)}$ we must use Eq. (13). After standard transformations and averaging over the time t we get

$$\Psi(\omega) = \overline{\Delta U^{(2)}}/\overline{\Delta F^2} = (i\hbar)^{-1}\langle[R(0), Q'(0)]\rangle + (i\hbar)^{-1}\int_{-\infty}^{0} dt_3\, e^{\epsilon t_3}\cos\omega t_3\langle[R(t_3), Q'(0)]\rangle. \tag{29}$$

From a macroscopic consideration it follows that the magnitude of the additionally dissipated power is determined by the expression

$$\overline{\Delta P} = {}^1/_2V_0^2\{r(\omega) + F^0\Psi(\omega)\}. \tag{30}$$

Substituting into (30) the expression for the resistivity (26) and the non-trivial part of the rectification $\psi(\omega)$ from (29) we are led to the magnitude of the power which is exactly the same as (15).

The magnitude of the rectification in the equilibrium state ψ_0 is obtained from (29) by the simple substitution $R \to Q_0$, $Q^0 \to Q_0$; $S \to Q_1$, $Q' \to Q_1$ where Q_0 and Q_1 are the coefficients in the expansion (2). As a result we get

$$\Psi_0(\omega) = (i\hbar)^{-1}\langle[Q_0, Q_1]\rangle_0 + (i\hbar)^{-1}\int_{-\infty}^{0} dt_3\cos\omega t_3\langle[Q_0(t_3), Q_1(0)]\rangle_0. \tag{31}$$

It is clear from (31) that systems with an interaction (with a signal generator) which is non-linear in the force exhibit, in contrast to systems with linear interactions [7], rectifying properties.

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