METHODOLOGICAL NOTES

Example of the description of dissipative processes in terms of reversible dynamic equations and some comments on the fluctuation-dissipation theorem

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The dynamics of a macroscopic oscillator which is interacting with a heat reservoir, which also consists of oscillators, is analyzed. This problem, which can be solved exactly in its general form in both the classical and quantum-mechanic cases, is used as an example for a study of the transition from a purely dynamic description to a statistical description. Since the system of linear oscillators is not ergodic, an averaging procedure must be regarded as taking an average over the time or over repeated measurements on a unique dynamic trajectory. Depending on the nature of the quadratic form of the potential energy, the oscillations of a macroscopic oscillator can decay in various ways, including exponentially, in the initial stage of the evolution. After a Poincaré cycle, the system returns to its initial state, and the damping of the oscillations gives way to a growth. The reversibility of the motion means that the Green's function of the system of oscillators is of odd parity in the time. Equilibrium fluctuations of a macroscopic oscillator are examined. In the classical case the Callen-Welton fluctuation-dissipation theorem can be formulated as follows: The derivative of the coordinate correlation function is proportional to the Green's function of the macroscopic oscillator. In a description in terms of frequencies, the odd parity of the Green's function gives rise to an imaginary part of the Fourier transform of this function in the fluctuation-dissipation theorem. This result is a consequence of the reversibility of the motion in time. The fluctuation-dissipation theorem is proved for Hamiltonian systems without dissipation, but it also applies to systems with dissipation. The exact microscopic Green's function is replaced in this case by the Green's function of a simplified phenomenological description, which explicitly contains dissipative parameters. In the quantum-mechanical case, the results are analogous. The classical and quantum-mechanical versions of the Nyquist relation which follow from the fluctuation-dissipation theorem when the Green's function is approximated by an exponentially damped sinusoidal oscillation are discussed.

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INTRODUCTION

In contrast with closed systems, which can be described by a Hamiltonian formalism, unclosed dissipative systems are described by phenomenological equations of one sort or another. If the description is carried out at the macroscopic level, this equation might be, for example, an equation of motion in which a friction force has been introduced. An example of phenomenological equations describing a system at a microscopic level might be kinetic equations. While a Hamiltonian description is based on "first principles" of physics, the use of phenomenological equations always involves some additional assumptions, whose validity is limited.[1] For example, certain theorems which are valid for Hamiltonian systems break down (e.g., the phase volume associated with those degrees of freedom in which a dissipation is introduced is no longer conserved). Dissipative parameters such as a friction force, an electrical resistance, and an effective collision rate are introduced in the equations as parameters describing the interaction of the system of interest with a heat reservoir and with other systems. Fundamental difficulties arise in a joint analysis of dissipative and quantum-mechanical phenomena, since a systematic quantum treatment is possible only for Hamiltonian systems.

It would be possible at least in principle to describe

jointly the system of interest and all the systems which are interacting with it (including the heat reservoir) within a common Hamiltonian formalism. In a description of this sort all the dissipative parameters should arise "automatically" in the course of the solution of the problem, and they should naturally be expressed in terms of the parameters of the complete Hamiltonian. This possibility is usually mentioned in the introductory sections of any course in statistical physics, but only as a potential possibility, which in reality is not implemented because of insurmountable technical difficulties.

The present methodological paper is devoted to an analysis of a simple but nontrivial problem in which that approach can be implemented. We consider the behavior of a macroscopic oscillator which is interacting with a heat reservoir, which also consists of oscillators, which are interacting both with each other and with the oscillator on which we are focusing.

Since the problem of a system of coupled oscillators can be solved *exactly* in both the classical and quantum-mechanical cases, in this example we can see the transition from a purely dynamic description based on reversible equations to a statistical description. A description of both the average motion of the oscillator and its fluctuations arises in a natural way. Our system executes a periodic (or nearly periodic) motion and has a time T_0 at which it returns precisely (or approximately) to its initial state (this is the length of the Poincaré cycle). The coefficients of the quadratic form of the potential energy can be chosen in such a way that in the initial ("dissipative") stage of the evolution of the system (at $T < T_0/2$) there is a damping of the oscillations of the macroscopic oscillator. As t approaches T_0, this damping gives way to a growth of the oscillations. The particular nature of the damping of the average motion is determined completely by the spectrum of normal oscillation modes of the overall system; it does not depend on the particular probability distribution of the coordinates and velocities of the oscillators of the reservoir. Those parameters which serve as "dissipative" parameters in the initial stage of the evolution are expressed in terms of quantities which are included in the *complete* Hamiltonian.

This model casts some light on the meaning of the Callen-Welton fluctuation-dissipation theorem. This theorem is proved for a *Hamiltonian* system, without dissipation; it couples the correlation function of fluctuations with the Green's function of this Hamiltonian system. In practice, however, the fluctuation-dissipation theorem is applied to *non-Hamiltonian* systems, which are described by phenomenological equations (microscopic or macroscopic) which explicitly contain dissipative parameters. This approach can be justified on the basis that these phenomenological equations describing the dissipative processes are actually capable of giving a good description of the behavior of the system, but only in the *initial* stage of its evolution, at $t < T_0/2$. These equations become definitely inapplicable at $t \sim T_0$. Fortunately, in the overwhelming majority of physics problems the time T_0 is so long that we are simply not interested in times comparable to it, and a phenomenological description using dissipative equations turns out in practice to be extremely accurate. If, however, we are attempting to reach an understanding of how dissipative characteristics appear in the fluctuation-dissipation theorem, despite the circum-

stance that this theorem is a consequence of a purely Hamiltonian description, we need to keep these points in mind.

Within the framework of the particular problem with which we are concerned here, we can also derive a Nyquist relation corresponding to an oscillatory electric circuit with a constant resistance. This relation can be found by making a corresponding assumption regarding the spectrum of normal oscillation modes of the system of oscillators under consideration.

Finally, in the model which we are considering here we can derive a quantum-mechanical Nyquist relation in a natural way from the reversible equations of quantum mechanics.

The problem of an oscillator which is interacting with a heat reservoir also consisting of oscillators has a characteristic feature which stems from the fact that this system is not ergodic. Specifically, if we think of our oscillatory system as consisting of a set of independent normal oscillations, we see that the energy of each of them is conserved separately. Consequently, as the system evolves it never goes into those parts of phase space which are incompatible with the initial distribution of the total energy among modes. Essentially the same difficulty is well known in the theory of equilibrium thermal radiation, where it is circumvented by incorporating in the system a negligibly small body which implements an exchange of energy among different modes. In the present paper we will take the following approach: In the stage of forming the initial conditions corresponding to a Gibbs distribution, i.e., at $t < 0$, we consider a more complex system, with additional interactions which make possible an exchange of energy among modes. An "expanded" system of this sort could in principle lead to the establishment of a Gibbs distribution through the realization of a regime of "dynamic chaos" in it.[2] After the initial conditions (at $t = 0$) are fixed, however, these additional interactions are turned off, and the system becomes purely oscillatory and linear.

A second distinctive feature which stems from the fact that the system is not ergodic is that we need to carry out a temporal rather than statistical averaging. A temporal averaging is more natural in our purely dynamic approach. A temporal averaging also corresponds to the procedure of measuring the average values in an experiment. An important point is that when measurements are repeated there is no need, as we will show below, to reformulate the initial conditions corresponding to a Gibbs distribution: All the repeated temporal averaging procedures for time-varying processes can be carried out on a unique dynamic trajectory which we examine in phase space.

A heat reservoir consisting of oscillators has been studied at a microscopic level from slightly different standpoints in many papers. For example, in an analysis of tunneling from a metastable state it turns out to be extremely important to incorporate dissipative effects. Since this phenomenon is definitely a quantum-mechanical phenomenon, a systematic analysis of it should be based on a Hamiltonian formalism. Here a heat reservoir of oscillators turns out to be an extremely convenient model (see the review by Caldeira and Leggett[3] and the bibliography there). An oscillator which is interacting with a heat reservoir which also consists of oscillators was studied in Refs. 4 and 5. We will examine these studies in more detail a bit further on.

1. SOLUTION OF THE PROBLEM OF THE MOTION OF A SYSTEM OF INTERACTING OSCILLATORS

We consider a system of n interacting oscillators with coordinates $q_1, ..., q_n$ and masses $m_1, ..., m_n$. In the case of electrical oscillations, q_i would be the charges on capacitors, and the masses m_i would be replaced by inductances L_i. The Lagrangian of the system is[2]

$$L = K - U = \frac{1}{2} \sum_{i=1}^{n} m_i \dot{q}_i^2 - \frac{1}{2} \sum_{i,j=1}^{n} \varkappa_{ij} q_i q_j. \tag{1.1}$$

The quadratic form of the potential energy U is positive definite; this situation corresponds to a stable position of the equilibrium at the point $q_1 = ... = q_n = 0$. We immediately assume that the quadratic form of the kinetic energy K is diagonal; this assumption does not restrict the generality of the results.[3]

We turn now to normal coordinates. We know (Ref. 6, for example) that a transformation of the type

$$q_i = m_i^{-1/2} \sum_{v=1}^{n} S_{iv} x_v, \tag{2.1}$$

where S_{iv} is a real orthogonal matrix, can put the Lagrangian (1.1) in diagonal form. The orthogonality of S_{iv} means that we have

$$\sum_{i=1}^{n} S_{iv} S_{i\mu} = \delta_{v\mu}, \tag{3a.1}$$

$$\sum_{v=1}^{n} S_{iv} S_{jv} = \delta_{ij}. \tag{3b.1}$$

The quadratic form of the kinetic energy remains diagonal for any choice of S_{iv} by virtue of (3a.1) and takes the form

$$K = \frac{1}{2} \sum_{i,v,\mu} S_{iv} S_{i\mu} \dot{x}_v \dot{x}_\mu = \frac{1}{2} \sum_{v=1}^{n} \dot{x}_v^2. \tag{4.1}$$

The quadratic form of the potential energy is diagonalized if we take S_{iv} to be a matrix which satisfies one of the equivalent conditions[4]

$$\sum_{i,j=1}^{n} \frac{\varkappa_{ij}}{(m_i m_j)^{1/2}} S_{iv} S_{j\mu} = \lambda_v \delta_{\mu v}, \tag{5a.1}$$

$$\sum_{i=1}^{n} \frac{\varkappa_{il}}{(m_i m_l)^{1/2}} S_{iv} = \lambda_v S_{lv}, \tag{5b.1}$$

$$\varkappa_{jl} = (m_j m_l)^{1/2} \sum_{v=1}^{n} \lambda_v S_{jv} S_{lv} \tag{5c.1}$$

It is easy to verify that these equalities are equivalent by virtue of the orthogonality conditions (3.1). It can be seen from (5b.1) that to find S_{iv} it is sufficient to find the eigenvectors and eigenvalues of the matrix $g_{il} = \varkappa_{il}/(m_i m_l)^{1/2}$, i.e., to find all the nontrivial solutions of the problem

$$\sum_{l=1}^{n} g_{il} \varphi_l = \lambda \varphi_i.$$

If we designate the various solutions of this problem by the index v, we see that after a corresponding normalization of the solutions $\varphi_i^{(v)}$ (and, possibly after they are rendered orthogonal if there is a degeneracy) we can set $S_{iv} = \varphi_i^{(v)}$. Equation (5c.1) gives a canonical expansion of the matrix g_{il} in its eigenvectors S_{iv}. From (5a.1) with $v = \mu$ we see

that we have $\lambda_v > 0$, by virtue of the positive definiteness of the matrix $\varkappa_{ij}$, i.e., by virtue of the stability of the equilibrium position $q_i = 0$.

Using (5a.1), we find that the Lagrangian (1.1) takes the form

$$L = \frac{1}{2} \sum_{v=1}^{n} (\dot{x}_v^2 - \lambda_v x_v^2). \tag{6.1}$$

We thus conclude that we have $\lambda_v = \omega_v^2$, where ω_v are the frequencies of the normal oscillations of the system of oscillators.

We can thus find ω_v^2, S_{iv} from the original quantities $m_i, \varkappa_{ij}$. According to (5c.1), the inverse is also true: Given ω_v^2, S_{iv}, and m_i, we can unambiguously reconstruct the original matrix $\varkappa_{ij}$:

$$\varkappa_{ij} = (m_i m_j)^{1/2} \sum_{v=1}^{n} \omega_v^2 S_{iv} S_{jv}. \tag{5d.1}$$

Consequently, if we are dealing with an oscillatory system of a general type, we can always assume that it is given by the set of quantities m_i, ω_v^2, S_{iv}. This is just what we will be assuming below.

Equations of motion corresponding to the Lagrangian (1.1) are

$$m_i \ddot{q}_i + \sum_{j=1}^{n} \varkappa_{ij} q_j = 0.$$

We have included external forces $F_i(t)$ on the right sides of these equations, so that the corresponding equations become

$$m_i \ddot{q}_i + \sum_{j=1}^{n} \varkappa_{ij} q_j = F_i(t). \tag{7.1}$$

Substituting in (2.1), and using (5b.1) and (3.1), we easily find the equations

$$\ddot{x}_v + \omega_v^2 x_v = f_v(t), \tag{8a.1}$$

$$f_v(t) = \sum_{j=1}^{n} S_{jv} F_j(t) (m_j)^{-1/2}. \tag{8b.1}$$

Their solution is

$$x_v(t) = x_v(0) \cos \omega_v t + \frac{\dot{x}_v(0)}{\omega_v} \sin \omega_v t$$
$$+ \frac{1}{\omega_v} \int_0^t \sin [\omega_v(t - t')] f_v(t') \, dt'. \tag{9.1}$$

We now return to the variables $q_i(t)$. Substituting (9.1) into (2.1), we find the formula

$$q_i(t) = \frac{1}{m_i^{1/2}} \sum_{v=1}^{n} S_{iv} \Big\{ x_v(0) \cos \omega_v t + \omega_v^{-1} \dot{x}_v(0) \sin \omega_v t$$
$$+ \omega_v^{-1} \int_0^t \sin [\omega_v(t - t')] f_v(t') \, dt' \Big\}. \tag{10.1}$$

We should eliminate the initial values $x_v(0)$ and $\dot{x}_v(0)$ from this formula, expressing them in terms of $q_i(0), \dot{q}_i(0)$. This can be done by noting that the transformation (2.1) can be generalized easily with the help of (3a.1):

$$x_v(t) = \sum_{j=1}^{n} m_j^{1/2} S_{jv} q_j(t).$$

We then find

$$x_v(0) = \sum_{j=1}^{n} m_j^{1/2} S_{jv} q_j(0), \quad \dot{x}_v(0) = \sum_{j=1}^{n} m_j^{1/2} S_{jv} \dot{q}_j(0).$$

Substituting these expressions into (10.1), and using (8b.1) and (2.1), we find the following expression for the solution of Eq. (7.1):

$$q_i(t) = \sum_{j=1}^{n} \left[\dot{G}_{ij}(t) \, m_j q_j(0) + G_{ij}(t) \, m_j \dot{q}_j(0) \right.$$

$$\left. + \int_0^t G_{ij}(t-t') \, F_j(t') \, dt' \right]; \qquad (11.1)$$

Here we have introduced

$$G_{ij}(t) = \frac{1}{(m_i m_j)^{1/2}} \sum_{v=1}^{n} \frac{S_{iv} S_{jv}}{\omega_v} \sin \omega_v t, \qquad (12.1)$$

$G_{ij}(t)$ is the Green's function of the problem (the response of oscillator i to an initial pulse acting on oscillator j).

Let us examine some general properties of the Green's function $G_{ij}(t)$. It can be seen from its definition, (12.1), that it is of *odd* parity in the time. This fundamental property follows from the *reversibility* of the motion in time. To find the reasons for this behavior, we write the quantity q_i given by (11.1) with $F_j = 0$ (i.e., this quantity describes the free motion of an oscillator) in the form $q_i(t; q^0, \dot{q}^0)$. Reversibility in time then means that if we change the signs of the initial velocities and the direction of time then quantities q_i will remain unchanged: $q_i(-t; q^0, -\dot{q}^\theta) = q_i(t; q^0, \dot{q}^0)$. Figure 1 illustrates this relation for the motion of a single oscillator. Substituting

$$q_i(t; q^0, \dot{q}^0) = \sum_{j=1}^{n} m_j \left[\dot{G}_{ij}(t) \, q_j^0 - G_{ij}(t) \, \dot{q}^0 \right],$$

into this equality, we find

$$\sum_{j=1}^{n} m_j \left[\dot{G}_{ij}(t) \, q_j^0 + G_{ij}(t) \, \dot{q}_j^0 \right]$$

$$= \sum_{j=1}^{n} m_j \left[\dot{G}_{ij}(-t) \, q_j - G_{ij}(-t) \, \dot{q}_j^0 \right].$$

This equation is satisfied only if the function $G_{ij}(t)$ is odd: $G_{ij}(-t) = -G_{ij}(t)$. The odd parity of the Green's function describing the response of a system to an external stimulus which drives it away from its equilibrium position is found not only in the particular problem with which we are concerned here but also in the more general case in which the potential energy of this system is examined in a small neighborhood of the equilibrium point and can therefore be as-
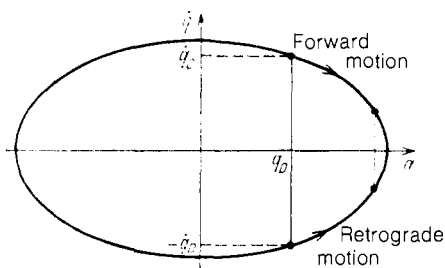

Forward motion

Retrograde motion

FIG. 1.

sumed to be a quadratic function of the coordinates. In this case, the external stimulus must be quite weak, or else it will drive the system out of this neighborhood.

It can also be seen from definition (12.1) that we have

$$G_{ij}(0) = 0, \quad \ddot{G}_{ij}(0) = 0, \quad \dot{G}_{ij}(0) = \delta_{ij} \, (m_i)^{-1} \qquad (13.1)$$

[the last inequality holds by virtue of (3b.1)].

Knowing the function $G_{ij}(t)$, we can also reconstruct the matrix $\varkappa_{ij}$. Specifically, we easily see that the following formula[51] follows from (12.1):

$$\varkappa_{ij} = -m_i m_j \dddot{G}_{ij}(0). \qquad (14.1)$$

2. AVERAGE MOTION OF A MACROSCOPIC OSCILLATOR AND COMPARISON OF IT WITH A PHENOMENOLOGICAL DESCRIPTION BASED ON OHM'S LAW

We start off with the assumption (which we will later discard) that at $-\infty < t < 0$ there is an ensemble of $K > 1$ systems of oscillators, each of which is identical to that discussed above, and each of which interacts with a "grand" reservoir at the temperature T. We assume that the nature of this interaction is such that the overall system is ergodic. At the time $t = 0$, the coordinates and momenta of the system of oscillators are then described by a Gibbs distribution. This statement means, in particular, that if we find the arithmetic mean of the coordinate or velocity of oscillator i at time $t = 0$ over all K identical copies of our system and then let $K \to \infty$ we will find values which are close to zero (of the order of $K^{-1/2}$).

For the time being we understand the averaging operation (in the first part of this section) to have precisely this meaning. At time $t = 0$ we "turn off" the interaction with the grand reservoir, and we find K systems of oscillators which are not interacting with each other and which have initial coordinates $q_i^{(\alpha)}(0)$ and initial velocities $\dot{q}_i^{(\alpha)}(0)$ such that in the limit $K \to \infty$ we find

$$\frac{1}{K} \sum_{\alpha=1}^{K} q_i^{(\alpha)}(0) \equiv \bar{q}_i(0) = O(K^{-1/2}) \to 0,$$

$$\frac{1}{K} \sum_{\alpha=1}^{K} \dot{q}_i^{(\alpha)}(0) = \overline{\dot{q}_i(0)} = O(K^{-1/2}) \to 0$$

(the index $\alpha = 1, ..., K$ specifies the particular copy of our system). For brevity, we say that $q_i(0)$ and $\dot{q}_i(0)$ are random quantities with zero mean values, and we refer to the averaging over the K copies of our system as an "averaging over thermal fluctuations." Let us assume that a macroscopic oscillator has an index $i = 1$, $m_1 = M$, $q_1(t) \equiv q(t)$. We also introduce the notation $G_{11}(t) = G(t)$, $F_1(t) = F(t)$. We write an expression for $q(t)$, setting $i = 1$ in (11.1), and singling out the term with $j = 1$:

$$q(t) = M q(0) \, \dot{G}(t) + M \dot{q}(0) \, G(t)$$

$$+ \int_0^t G(t-t') \, F(t') \, dt' + \tilde{q}(t). \qquad (1.2)$$

Here we have introduced

$$\widetilde{q}(t) = \sum_{j=2}^{n} \left[m_j q_j(0) \dot{G}_{1j}(t) + m_j \dot{q}_j(0) G_{1j}(t) \right.$$

$$\left. + \int_0^t G_{1j}(t-t') F_j(t') \, dt' \right] \qquad (2.2)$$

for the "noise" component of the motion of the macroscopic oscillator, which results from the initial conditions and the external forces associated with the oscillators of the reservoir.

We assume that an external force $F(t)$ begins to act on the macroscopic oscillator at the time $t = 0$, and we assume that this oscillator acquires an initial velocity $\dot{q}(0)$ which is large in comparison with the fluctuations. In (2.2), all the quantities $q_j(0)$, $\dot{q}_j(0)$ with $j = 2,3, ..., n$ are then random quantities (in the sense defined above) with zero mean values. The same is true of the quantity[6] $q(0)$. If we are interested in the mean value of the coordinate, $\bar{q}(t) \equiv Q(t)$ (the superior bar means an average over thermal fluctuations), then for $j = 2, ..., n$ we find $\bar{q}_j(0) = 0$, $\dot{q}_j(0) = 0$ after the averaging; with $F_j = 0$ (i.e., the external force is acting exclusively on the macroscopic oscillator) we find $\widetilde{q} = 0$. The average motion of the oscillator is thus described by the expression

$$Q(t) = M\dot{q}(0) G(t) + \int_0^t G(t-t') F(t') \, dt'. \qquad (3.2)$$

Introducing $A_\nu \equiv S^2_{1\nu}$ to streamline the equations, we have $\sum_{\nu=1}^{n} A_\nu = 1$ according to (3b.1), and according to (12.1) we have

$$G(t) = \frac{1}{M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu} \sin \omega_\nu t. \qquad (4.2)$$

Let us compare expression (3.2), which is written for the average motion of a macroscopic oscillator and which is derived from *microscopic* equations, with the motion described by a *phenomenological* equation of motion of an oscillator with a linear friction proportional to the velocity (in the case of electrical oscillations, this would be Ohm's law). Assigning an index R to the solution of the phenomenological equation, we have

$$M\ddot{Q}_R + R\dot{Q}_R + M\omega_0^2 Q_R = F(t). \qquad (5.2)$$

The solution of this equation with the same initial conditions, $Q_R(0) = 0$, $\dot{Q}_R(0) = \dot{Q}_0$, is

$$Q_R(t) = \dot{Q}_0 \bar{\omega}^{-1} \exp(-\gamma t) \sin \bar{\omega} t$$

$$+ \frac{1}{M\bar{\omega}} \int_0^t \exp[-\gamma(t-t')][\sin \bar{\omega}(t-t')] F(t') \, dt', \qquad (6.2)$$

where $\bar{\omega}^2 = \omega_0^2 - \gamma^2$, and $\gamma = R/2M$ (or $R/2L$, in the case of electrical oscillations). We can write solution (6.2) in the form in (3.2) with the Green's function $(M\bar{\omega})^{-1} \exp(-\gamma t) \sin \bar{\omega} t$.

It is clear that in considering an oscillatory system of a general type we can treat the set of frequencies ω_ν and the set of positive numbers A_ν as being arbitrary (the only restric-

tion on this set comes from the condition[7] $\sum_{\nu=1}^{n} A_\nu = 1$). Consequently, Eq. (5.2) generally does not reflect the properties of an average microscopic motion. In particular, we also conclude that Ohm's law with a frequency-independent resistance is not a universal consequence of (3.2).

At this point we pose the question in a different way: What assumptions should we make regarding A_ν and ω_ν if we wish to make Eq. (5.2) a *consequence* of the microscopic analysis?

We begin with the assumption (which we will later discard) that the frequencies ω_ν are equidistant: $\omega_\nu = \nu\Omega$. In this case, (4.2) is a finite Fourier sum:

$$G(t) = \frac{1}{M\Omega} \sum_{\nu=1}^{n} \frac{A_\nu}{\nu} \sin \nu\Omega t.$$

We obviously have $G(t + 2\pi/\Omega) = G(t)$; i.e., $G(t)$ is periodic with a repetition period $T_0 = 2\pi/\Omega$. In particular, we have $G(T_0) = G(0) = 0$. Furthermore, we have $G(T_0/2 + \tau) = -G(T_0/2 - \tau)$; i.e., the function $G(t)$ is odd with respect to the middle of the interval $(0, T_0)$. It follows from no more than these properties of $G(t)$ that the function $(M\omega)^{-1} + \exp(-\gamma t) \times \sin \omega t$ cannot be written in the form in (4.2). However, a Fourier sum of this form can be used to approximate (quite accurately if n is large) a function which on the interval $(0, T_0)$ has the form

$$G_R(t) = \frac{\exp(-\gamma t) \sin \bar{\omega} t - \exp[-\gamma(T_0-t)] \sin \bar{\omega}(T_0-1)}{M\bar{\omega}[1 + \exp(-\gamma T_0)]} \qquad (7.2)$$

and which is periodically continued in both directions outside this interval. Here $\bar{\omega} = N\Omega$, and N is an integer. If $\gamma T_0 \gg 1$, then in the initial interval (at $t < T_0/2$) function (7.2) is essentially indistinguishable from $(M\bar{\omega})^{-1} \exp(-\gamma t) \sin \bar{\omega} t$, but it satisfies the necessary conditions of periodicity and oddness. Function (7.2) on the interval $(0, T_0)$ can also be written in the form

$$G_R(t) = \mathrm{ch}\left[\gamma\left(\frac{T_0}{2} - t\right)\right] \sin \bar{\omega} t \cdot \left(M\bar{\omega} \, \mathrm{ch} \, \gamma \frac{T_0}{2}\right)^{-1}. \qquad (8.2)$$

The normalization factor has been chosen in such a way that the condition $\dot{G}_R(0) = M^{-1}$ holds; this condition must be satisfied by $G(t)$. It can be seen from (7.2) and (8.2) that we have $G_R(0) = G_R(T_0) = 0$ (i.e., the periodicity condition holds) and that $G(T_0/2 + \tau)$ is an odd function (Fig. 2).

The reason for the periodicity of $G(t)$ [or $G_R(t)$] is that in the absence of external forces our system is conserva-
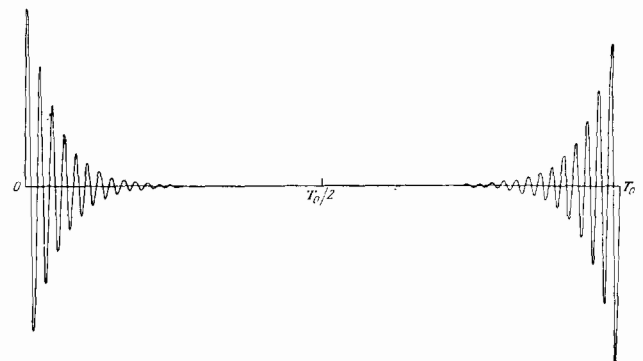

FIG. 2.

tive and executes a finite motion. In general, it would then follow that the Poincaré theorem[7-9] regarding the returns of a system to its original state will hold arbitrarily accurately. In the case of an equidistant spectrum, these returns occur at intervals of the period T_0, and the system returns *exactly* to its original state.

If, however, the time T_0 is extremely large, and the condition $\gamma T_0 \gg 1$ holds (T_0 is estimated for some simple situations[8] in Refs. 2 and 7), then we will actually be interested in only the *initial* stage of the process which (if the number of oscillators, n, is sufficiently large) will be essentially indistinguishable from the process described by the solution of Eq. (5.2).

What should the coefficients A_v be in order to satisfy the "equality" $G(t) \approx G_R(t)$? With $n = \infty$ we can satisfy the *exact* equality $G(t) = G_R(t)$ by finding the coefficients A_v from the expansion of function (7.2) in a Fourier series in $\sin v\Omega t$. If, on the other hand, n is finite but quite large, we find a rather good approximation of the function $G_R(t)$ by a finite Fourier sum (this is the best approximation in the sense of the mean square deviation).

We thus write an expansion of function (7.2), expressed in terms of the variable $\tau = t - (T_0/2)$ in the region $|\tau| < T_0/2$, as a Fourier series of the type in (4.2), but with infinite n:

$$\frac{(-1)^N}{M\overline{\omega}\,\mathrm{ch}\,(\gamma T_0/2)}\,\mathrm{ch}\,\gamma\tau\cdot\sin N\Omega\tau = \sum_{v=1}^{\infty}\frac{(-1)^v A_v}{v\Omega M}\sin v\Omega\tau.$$

Multiplying this expansion by $\sin\mu\Omega\tau$ and integrating over τ from $(-T_0/2)$ to $(T_0/2)$, we easily find the coefficients A_v. Using the equalities $\overline{\omega} = N\Omega$, $\omega_v = v\Omega$ and introducing the eigenfrequency (ω_0) of the macroscopic oscillator by means of the standard equation $\overline{\omega}^2 = \omega_0^2 - \gamma^2$, we find, after some simple manipulations,

$$A_v = \frac{4}{\pi}\frac{\gamma\omega_v^2\Omega\,\mathrm{th}\,(\gamma T_0/2)}{(\omega_v^2 - \omega_0^2)^2 + 4\gamma^2\omega_v^2}. \tag{9.2}$$

If the solution of the problem of the motion of an oscillator in a reservoir consisting of a set of other oscillators is to correspond in its initial stage (at $t < T_0/2$) to the solution of phenomenological equation (5.2), we thus need to choose the matrix S_{iv} in a special way. Alternatively, in accordance with (5d.1), we need to choose a special form for the matrix $\varkappa_{ij}$. Specifically, according to (9.2) the quantities S_{1v}^2, which determine the coupling of the macroscopic oscillator with the oscillators of the reservoir must lie on a Lorentzian resonant curve[9] as a function of the frequencies ω_v.

It follows that phenomenological equation (5.2), in which the action of the thermostat on the macroscopic oscillator is described by the term $R\dot{Q}_R$ (in particular, by Ohm's law), is not a universal equation. Other laws describing the damping of the oscillation amplitude $C(t)$ of the macroscopic oscillator would also be consistent with the microscopic description.[10] As an example we might cite the paper by Razavy,[10] in which functions $C(t)$ other than $\exp(-\gamma t)$ were given for a one-dimensional chain of oscillators directly in terms of the quantities m_i and $\varkappa_{ij}$.

Clearly, if some *arbitrary* amplitude damping law compatible with the symmetry conditions which we have mentioned is given, and if n is sufficiently large, then we can indicate a reservoir of oscillators which is of such a nature

that in it the microscopic Green's function can have a given form:

$$\frac{1}{M}\sum_{v=1}^{\infty}\frac{A_v}{\omega_v}\sin\omega_v t = C(t)\sin\overline{\omega}t.$$

For this purpose it is sufficient to solve the last equation for the numbers A_v as was done in the derivation of (9.2) and then construct some orthogonal matrix S_{iv} for which the relation $S_{1v}^2 = A_v$ holds. We can then find the corresponding matrix $\varkappa_{ij}$ from (5d.1).

An exponential damping law for the oscillation amplitude was found approximately in Refs. 4 and 5 by an approach which was equivalent to adopting less-restrictive assumptions regarding the form of the matrix $\varkappa_{ij}$. Specifically, these less-restrictive assumptions reduced to the following assumptions:

a) The oscillators of the reservoir interact only with the macroscopic oscillator—not with each other.

b) The so-called "rotating-wave approximation" (Ref. 11, for example), which is equivalent to an averaging method, is applicable. In the case at hand, this approximation reduces to the following approximation of the Hamiltonian:

$$H = \sum_{i=1}^{n}\left(\frac{p_i^2}{2m_i} + \frac{\varkappa_{ii}q_i^2}{2}\right) + \frac{1}{2}\sum_{i\neq j}\varkappa_{ij}q_i q_j$$

$$\rightarrow \sum_{i=1}^{n}\left(\frac{p_i^2}{2m_i} + \frac{\varkappa_{ii}q_i^2}{2}\right)$$

$$+ \frac{1}{4}\sum_{i\neq j}\left[\varkappa_{ij}q_i q_j + \frac{\varkappa_{ij}}{(\varkappa_{ii}\varkappa_{jj})^{1/2}}\frac{p_i p_j}{(m_i m_j)^{1/2}}\right].$$

c) The Wigner-Weisskopf approximation holds (Ref. 11, for example). In this approximation, the solution is sought immediately in the form of an exponentially damped sinusoidal oscillation.

From the standpoint of the set of solutions derived in Refs. 4 and 5, an exponential law is clearly an approximation which includes in addition to the exact solution of this type, certain solutions which are close to the exact solution.

If the damping law of the oscillation amplitude is not exponential, phenomenological equation (5.2) evidently will no longer hold. Generally speaking, it should be less accurate than a linear equation of higher order. It is clear that if we eliminate the variables of the reservoir oscillators from the system of equations of motion we can generally find an equation of order $2n$ for $q(t)$. However, if we *require* that the phenomenological equation correspond to a linear oscillator with *one* degree of freedom, then we necessarily find (5.2). Nevertheless, that requirement can by no means always be justified physically.

Even if Eq. (5.2), which describes an irreversible motion, holds in the initial region ($t \ll T_0/2$), the exact equation which function (7.2) must obey is the following equation, as is easily verified:

$$\frac{d^4Q_R}{dt^4} + 2(\omega_0^2 - 2\gamma^2)\frac{d^2Q_R}{dt^2} + \omega_0^4 Q_R = 0. \tag{10.2}$$

This equation contains derivatives of exclusively even order, so that it is invariant under the substitution $t \rightarrow -t$ and describes a *reversible* periodic motion if the coefficients in the expression for its general solution are chosen appropriately:

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$$Q_R(t) = a e^{(i\overline{\omega}-\gamma)t} + b e^{(-i\overline{\omega}-\gamma)t}$$

$$+ c e^{(i\overline{\omega}+\gamma)t} + d e^{(-i\omega+\gamma)t}.$$

Although Eq. (10.2) describes a reversible motion, it explicitly contains a dissipative parameter: the resistance[11] $R = 2\gamma L$.

There is yet another important circumstance to be noted here. If we work from the microscopic equations of motion, the "dissipative" (in a phenomenological description) parameter γ or the corresponding resistance $R = 2\gamma L$ appears as a quantity characterizing the potential-energy matrix $\varkappa_{ij}$. Specifically, since the parameter γ appears explicitly in the expression for A_ν, it therefore also appears in $S_{1\nu} = (A_\nu)^{1/2}$ and thus $\varkappa_{ij}$, since this matrix is related to $S_{1\nu}$ by Eq. (5d.1). In other words, the dissipative parameter γ *is contained* in the complete Hamiltonian as a parameter of the interaction of the macroscopic oscillator with the reservoir oscillators (it unavoidably appears in the expressions for $\varkappa_{ij}$).

In this model, of a reservoir consisting of oscillators, we can of course find Eq. (5.2) only under some extremely contrived assumptions, which reduce to the validity of (9.2) The only important point is that Eq. (5.2) for $t < T_0/2$ *does not contradict* the exact microscopic equations.

When this problem is approached in other ways, which are based immediately on irreversible kinetic equations, an exponential oscillation damping law (and also Ohm's law) can be derived under other, more natural assumptions (e.g., through an appropriate approximation of the collision integral). Such approaches are of course far more convenient in practice for dealing with various specific problems, but we are deliberately avoiding kinetic equations here since our purpose is to study dissipation on the basis of reversible microscopic equations.

Finally, we note that we derived (3.2) and (4.2) for the average motion on the sole basis of the vanishing of the mean values of the initial coordinates and velocities of the oscillators of the reservoir; the specific type of probability distribution of these quantities was of no importance.

In deriving (9.2) we used the assumption that the spectrum of normal oscillations is equidistant. We will now analyze the consequences of giving up that assumption. We assume that the frequencies $\omega_1, \omega_2, ..., \omega_n$ are not equidistant but that their ratios are rational numbers. Each of the frequencies can then be written in the form $\omega_\nu = N_\nu \Omega$, where the numbers N_ν are integers, and Ω is the largest frequency scale at which such a representation is possible. Going back to (4.2), we see that again in this case we have $G(t + T_0) = G(t)$, where $T_0 = 2\pi/\Omega$; i.e., $G(t)$ is a periodic function of period T_0. As in the case of the equidistant spectrum, $G(t)$ is odd with respect to the point $t = T_0/2$. The set of functions $\sin(N_n \Omega t)$ is orthogonal on $(0, T_0)$, but these functions do not form a complete system. Incidentally, the functions $\sin(\nu \Omega t)$ also did not form a complete system, since their number is finite. The distinction is that in the case of the equidistant spectrum all the high-frequency harmonics were removed from the complete set of functions, while in the case of a nonequidistant spectrum some of the low-frequency harmonics are also removed. It is nevertheless clear that if within the Lorentzian line (9.2) there is a fairly large number of frequencies $\omega_\nu = N_\nu \Omega$, and they are distributed

over the interval $(\overline{\omega} - \gamma, \overline{\omega} + \gamma)$ at least approximately uniformly, then a function of the type in (7.2) can be represented extremely accurately by expansion (4.2). To clarify this point we note that the function $(M\overline{\omega})^{-1} e^{-\gamma|t|} \sin \overline{\omega} t$ can be represented by the Fourier integral

$$\frac{e^{-\gamma|t|}}{M\overline{\omega}} \sin \overline{\omega} t = \int_{-\infty}^{\infty} e^{i\omega t} \cdot \frac{2i\gamma\omega}{\pi M} \frac{d\omega}{(\omega^2 - \omega_0^2)^2 + 4\gamma^2\omega^2}$$

$$= \int_{-\infty}^{\infty} e^{i\omega t} \varphi(\omega) \, d\omega.$$

The integral on the right side of this equation can be approximated by an integral sum, so that the expansion becomes

$$\int_{-\infty}^{\infty} e^{i\omega t} \varphi(\omega) \, d\omega \approx \sum_{\nu} e^{i\omega_\nu t} \varphi(\omega_\nu) \Delta\omega_\nu.$$

Here it is not at all necessary that the frequencies ω_ν be chosen equidistant. The only requirements are that in the region $\omega \sim \widetilde{\omega}$, which is important for the integration, the condition max $\Delta\omega_\nu \ll \gamma$ hold and that a sufficiently large number of points ω_ν fall in this region. For a nonequidistant arrangement of the frequencies ω_ν in the case in which the ratios of the frequencies are rational, we thus see that again there exist a time T_0 after which the system will return *exactly* to its initial state.

Finally, if the ratios of the normal frequencies are arbitrary, even irrational, they can nevertheless be approximated arbitrarily accurately by rational numbers. We then return to the preceding case with this accuracy.

For arbitrary ω_ν we thus find a near-period $T_0(\varepsilon)$ instead of the period of an exact return; this near-period is of such a nature that the inequality

$$| G(t + T_0(\varepsilon)) - G(t) | < \varepsilon$$

holds for arbitrary t, and after a time T_0 the system returns to its original state within an error of the order of ε. Functions of this sort (Fourier series with arbitrary frequencies) are called "nearly periodic." The Poincaré return theorem[7-9] specifically asserts that a finite motion of a conservative system is nearly periodic. In the particular case with which we are concerned in this paper, this assertion reduces to the assertion that the function $G(t)$ is nearly periodic for arbitrary ω_ν.

We now return to the averaging question, which we discussed at the beginning of this section of the paper. We discard the assumption that there are K copies of the system. We assume that at $t < 0$ our single system of n oscillators interacts vanishingly weakly with a "grand" reservoir having a temperature T. We assume that the nature of this interaction is such that the overall system is ergodic (in particular, because of the interaction with the reservoir, the energies of the individual normal oscillations are not conserved). In this case, we know[7-9,12-15] that a Gibbs distribution is established in the system. We "switch off" the interaction of the system of oscillators with the grand reservoir at the time $t = 0$. At this time, all the coordinates $q_i(0)$ and velocities $\dot{q}_i(0)$ have certain values which constitute a specific sample of the set of random quantities which obey the Gibbs distribution. These quantities are initial values which determine the subsequent evolution of the system of oscillators. At $t > 0$, this evolution proceeds (we would like to stress this

point) in accordance with Eqs. (11.1). At $t > 0$, we treat the system of oscillators with indices $j > 2$ as a reservoir with respect to the oscillator with index 1. In the course of the evolution, the initial values $q_i(0)$ and $\dot{q}_i(0)$ are fixed, and it is not possible to take an average over them. At $t > 0$, an average can be taken only over the time. The initial values $q_i(0)$ and $\dot{q}_i(0)$, however, retain a "memory" of the contact with the reservoir which occurred at $t < 0$. In particular, this statement means that the characteristic values of $q_i(0)$ and $\dot{q}_i(0)$ agree with the Gibbs distribution

$$W(q, \dot{q}) = \mathcal{N} \exp\left[-H\left(q(0), \dot{q}(0)\right)(kT)^{-1} \right], \quad (11.2)$$

where $\mathcal{N}$ is a normalization factor, and

$$H = \frac{1}{2} \sum_{i=1}^{n} m_i \dot{q}_i^2(0) + \frac{1}{2} \sum_{i,j=1}^{n} \varkappa_{ij} q_i(0) q_j(0)$$

is the Hamiltonian expressed in terms of variables referring to the time $t = 0$.

For the analysis below it is convenient to express the Hamiltonian in terms of the normal coordinates x_ν. We obviously have

$$H = \frac{1}{2} \sum_{\nu=1}^{n} \left[\dot{x}_\nu^2(0) + \omega_\nu^2 x_\nu^2(0) \right]. \quad (12.2)$$

In the limit $n \to \infty$, the spectrum of normal frequencies becomes far more dense. Let us examine a group of $K > 1$ normal oscillations with approximately equal frequencies $\omega_{\nu_1} \leqslant \omega_{\nu_2} \leqslant \ldots \leqslant \omega_{\nu_K}$, which are such that the relation $\omega_{\nu_K} - \omega_{\nu_1} \ll \gamma_0$ holds, where γ_0 is some given resolving power.[12] Frequencies which differ from each other by less than γ_0 will not be distinguishable experimentally. The circumstance that the quantities $x_{\nu_1}(0), \ldots, x_{\nu_K}(0), \dot{x}_{\nu_1}(0), \ldots, \dot{x}_{\nu_K}(0)$ constitute a sample of a normally distributed set obeying the distribution

$$W(x(0), \dot{x}(0)) = \mathcal{N} \exp\left\{ -\frac{1}{2kT} \sum_{\nu=1}^{n} \left[\dot{x}_\nu^2(0) + \omega_\nu^2 x_\nu^2(0) \right] \right\} \quad (13.2)$$

means that when K is sufficiently large the arithmetic mean values $\left(\text{here } \nu = K^{-1} \sum_{\alpha=1}^{K} \nu_\alpha \right)$

$$\bar{x}_\nu(0) \equiv \frac{1}{K} \sum_{\alpha=1}^{K} x_{\nu_\alpha}(0) \approx 0, \quad \bar{\dot{x}}_\nu(0) \equiv \frac{1}{K} \sum_{\alpha=1}^{K} \dot{x}_{\nu_\alpha}(0) \approx 0 \quad (14a.2)$$

are small. In other words, in absolute value they are much smaller than the characteristic values of each of the terms $(kT)^{1/2}/\omega_\nu$ and $(kT)^{1/2}$, respectively. The mean square values of the initial coordinates and velocities over the same sample are approximately equal to the mean square values determined by distribution (13.2); i.e.,

$$\overline{x_\nu^2}(0) \equiv \frac{1}{K} \sum_{\alpha=1}^{K} x_{\nu_\alpha}^2(0) \approx \frac{kT}{\omega_\nu^2},$$

$$\overline{\dot{x}_\nu^2}(0) \equiv \frac{1}{K} \sum_{\alpha=1}^{K} \dot{x}_{\nu_\alpha}^2(0) \approx kT. \quad (14b.2)$$

Relations (14.2) are consequences of the law of large numbers in probability theory (in the limit $K \to \infty$, these re-

lations hold within an error of the order of $K^{-1/2}$). At $t > 0$, an averaging over time leads, by virtue of relations (14.2), to mean values and variances of the dynamic variables which correspond to Gibbs distribution.

We turn now to the process of measuring the mean value $\bar{q}(t) = Q$. In a real experiment, we impart an additional initial momentum $M\dot{Q}_0$ to the macroscopic oscillator at $t = 0$, so that the initial conditions on the motion of the system of oscillators are, according to (10.1),

$$q_i(0) = \frac{1}{m_i^{1/2}} \sum_{\nu=1}^{n} S_{i\nu} x_\nu(0), \quad i = 1, 2, \ldots, n,$$

and

$$\dot{q}_i(0) = \frac{1}{m_i^{1/2}} \sum_{\nu=1}^{n} S_{i\nu} \dot{x}_\nu(0), \quad i = 2, \ldots, n, \quad (15.2)$$

for $i \neq 1$, or

$$\dot{q}_0 = \frac{1}{M^{1/2}} \sum_{\nu=1}^{n} S_{1\nu} \dot{x}_\nu(0) + \dot{Q}_0 = \dot{Q}_0 + \dot{q}_1(0)$$

for $i = 1$. Here $\dot{q}_0$ is the initial velocity of the macroscopic oscillator, where the additional initial momentum $M\dot{Q}_0$ has been taken into account.

The subsequent motion of the macroscopic oscillator occurs in accordance with (11.1), in which the contribution from the initial momentum $M\dot{Q}_0$ has been singled out:

$$q(t) = M\dot{Q}_0 G(t) + \sum_{j=1}^{n} m_j \left[q_j(0) \dot{G}_{1j}(t) + \dot{q}_j(0) G_{1j}(t) \right]. \quad (16.2)$$

The second term is the noise component of the motion, which is unrelated to the initial momentum $M\dot{Q}_0$. Let us assume, for example, that the spectrum of the system of oscillators is Lorentzian, so that under the condition $t \ll T_0/2$ the function $G(t)$ represents an exponentially damped oscillation. (As will be seen below, this assumption is not mandatory. All that is required is that in the initial stage of the evolution there exists a characteristic relaxation time; the damping law for the oscillation amplitude need not be exponential.) Under the condition $t \gg \gamma^{-1}$ (but still under the condition $t < T_0/2$) the first term in (16.2) is damped, in contrast with the second term. In other words, the regular response to the initial momentum "drowns" in the noise. After this stage, we return (from the macroscopic standpoint) to the original position, as it was just before the time $t = 0$, before the initial momentum $M\dot{Q}_0$ had been imparted to the system. We can thus "repeat the experiment," being in the same initial state (the same from the macroscopic standpoint). In other words, we can again impart to the macroscopic oscillator at a time $t_1 \gg \gamma^{-1}$ (but $t_1 \ll T_0/2$) the same momentum, $M\dot{Q}_0$. Equivalently, at the time t_1 the macroscopic oscillator is subjected to a force $F_1(t) = M\dot{Q}_0 \delta(t - t_1)$. According to (11.1), at $t > t_1$ we then have

$$q(t) = M\dot{Q}_0 G(t) + M\dot{Q}_0 G(t - t_1)$$
$$+ \sum_{j=1}^{n} m_j \left[q_j(0) \dot{G}_{1j}(t) + \dot{q}_j(0) G_{1j}(t) \right].$$

Since we are now interested in values $t \gg \gamma^{-1}$, however, the

first term here is exponentially small and can be ignored; we thus write

$$q(t) = M\dot{Q}_0 G(t - t_1) + \sum_{j=1}^{n} m_j [q_j(0) \dot{G}_{1j}(t) + \dot{q}_j(0) G_{1j}(t)]. \tag{17.2}$$

At $t - t_1 \gg \gamma^{-1}$ the first term here is also damped, and we again cannot distinguish the state of the macroscopic oscillator from the initial state. At a time $t_2 \gg t_1 + \gamma^{-1}$ (but $t_2 \ll T_0/2$) we can then repeat the experiment "under the same initial conditions," imparting a momentum $M\dot{Q}_0$ to the macroscopic oscillator [i.e., we can apply a force $F_1(t) = M\dot{Q}_0 \delta(t - t_2)$]. As a result, at $t > t_2$ we have

$$q(t) = M\dot{Q}_0 G(t - t_2) + \sum_{j=1}^{n} m_j [q_j(0) \dot{G}_{1j}(t) + \dot{q}_j(0) G_{1j}(t)]. \tag{18.2}$$

This procedure can be repeated $K > 1$ times (under the condition $K\gamma^{-1} \ll T_0/2$). The second terms in (16.2), (17.2), (18.2), etc., are identical; they differ only in the values of their argument t. In this sense they *are not a random noise*, since in principle they could be predicted on the basis of a necessary *finite* number of measurements. What we are interested in, however, is the average response, over all the experiments, of the macroscopic oscillator to the momentum imparted to it, $M\dot{Q}_0$. We will accordingly compare and average the coordinate values which are equidistant from the time at which the corresponding experiment begins. In other words, we are interested in a mean value of the type

$$Q(t) = \frac{1}{K+1} [q(t) + q(t_1 + t) + q(t_2 + t) + \ldots + q(t_K + t)]$$

$$= M\dot{Q}_0 G(t) + \sum_{j=1}^{n} m_j \left[q_j(0) (K+1)^{-1} \sum_{\alpha=0}^{K} \dot{G}_{1j}(t_\alpha + t) \right.$$

$$\left. + \dot{q}_j(0) (K+1)^{-1} \sum_{\alpha=0}^{K} G_{1j}(t_\alpha + t) \right] \tag{19.2}$$

(here $t_\alpha = 0$ for $\alpha = 0$). The functions $G_{ij}(t_\alpha + t)$ and $\dot{G}_{ij}(t_\alpha + t)$ consist of terms of the type $\sin(\omega_\nu t + \omega_\nu t_\alpha)$ and $\cos(\omega_\nu t + \omega_\nu t_\alpha)$. Since the times at which the repeated measurements are begun t_α are totally unmatched with the periods $2\pi/\omega_\nu$, however, the phase shifts $\omega_\nu t_\alpha$ can be regarded as random. In this case, however, as we know quite well (Ref. 16, for example), the mean value of a sum of harmonic oscillations with random phases of the type

$$(K+1)^{-1} \sum_{\alpha=0}^{K} \sin \omega_\nu t_\alpha, \quad (K+1)^{-1} \sum_{\alpha=0}^{K} \cos \omega_\nu t_\alpha,$$

tends toward zero as $K^{-1/2}$ as K increases. Consequently, during the averaging procedure the second term in (19.2) is of order $K^{-1/2}$, and at large values of K it becomes negligibly small in comparison with $M\dot{Q}_0 G(t)$.

Accordingly, despite the fact that the "interference" [the second term in (16.2)] is not random, its role in the averaging procedure is reduced, as in the "buildup" of a useful signal against a noisy background. As we have seen, this interference is cancelled by the introduction of an element of randomness in the choice of the point at which the next experiment is begun.

We have examined a procedure for averaging time-varying processes in a situation in which repeated measurements should be carried out under identical (from the macroscopic standpoint) initial conditions. In the following section of this paper we examine equilibrium fluctuations in a case in which there is no ordered motion of any sort of the macroscopic oscillator, and its motion is caused exclusively by the interaction with the oscillators of the reservoir. In this case, no particular time is distinguished from other times from the macroscopic standpoint, and an averaging can be carried out over the time. For example, the mean value of the coordinate or of any other quantity $f(t)$ which depends on only one time can be found from the formula[13]

$$\bar{f}(t) = \bar{f} = \frac{1}{T_0} \int_0^{T_0} f(t) \, dt. \tag{20a.2}$$

If we are instead interested in the mean values of quantities which depend on two times, e.g., correlations of the type $f(t_1)\varphi(t_2)$, we take a sliding average over the time with a fixed value of the temporal shift of the arguments:

$$\overline{f(t) \varphi(t+\tau)} = \frac{1}{T_0} \int_0^{T_0} f(t) \varphi(t+\tau) \, dt = B_{f\varphi}(\tau). \tag{20b.2}$$

3. EQUILIBRIUM FLUCTUATIONS; DISCUSSION OF THE FLUCTUATION-DISSIPATION THEOREM AND THE NYQUIST RELATION

Now that we have examined the average motion of the oscillators, we turn to the fluctuations in this motion. We restrict the discussion here to *equilibrium* fluctuations, for which the mean values of the coordinate and momentum of the macroscopic oscillator are zero. To calculate the equilibrium fluctuations in the coordinate $q(t) = q_1(t)$ of the macroscopic oscillator, it is most convenient to use (10.1) with $f_\nu = 0$:

$$q(t) = \frac{1}{(M)^{1/2}} \sum_{\nu=1}^{n} S_{1\nu} \left[x_\nu(0) \cos \omega_\nu t + \frac{\dot{x}_\nu(0)}{\omega_\nu} \sin \omega_\nu t \right]. \tag{1.3}$$

We recall that $x_\nu(0)$ and $\dot{x}_\nu(0)$ are fixed numbers here—a specific sample of a set of random numbers which obey a Gibbs distribution and therefore satisfy conditions (14a.2) and (14b.2). The time average is evidently $q = 0$ [in the sense of (20a.2)]. We now consider the correlation function

$$B_q(\tau) = q\overline{(t) q(t+\tau)} = \frac{1}{T_0} \int_0^{T_0} q(t) q(t+\tau) \, dt. \tag{2.3}$$

Substituting (1.3) into this expression, we find some mean values which can be calculated easily:

$$\overline{\cos \omega_\nu t \cos \omega_\mu (t+\tau)} = \overline{\sin \omega_\nu t \sin \omega_\mu (t+\tau)}$$

$$= \frac{1}{2} \delta_{\nu\mu} \cos \omega_\nu \tau,$$

$$\overline{\cos \omega_\nu t \sin \omega_\mu (t+\tau)} = -\overline{\sin \omega_\nu t \cos \omega_\mu (t+\tau)}$$

$$= \frac{1}{2} \delta_{\nu\mu} \sin \omega_\nu \tau \tag{3.3}$$

(note the minus sign in one of the expressions on the second line). As a result we find

$$B_q(\tau) = \frac{1}{2M} \sum_{\nu=1}^{n} S_{1\nu}^2 \left[x_\nu^2(0) + \frac{\dot{x}_\nu^2(0)}{\omega_\nu^2} \right] \cos \omega_\nu \tau. \tag{4.3}$$

We now need to relate the quantities $x_\nu^2(0)$ and $\dot{x}_\nu^2(0)$ to the

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temperature. For this purpose we call on Eq. (14b.2). We assume that when the spectrum of normal oscillations is sufficiently dense the quantities $S_{1\nu}^2 = A_\nu$ and $\cos \omega_\nu \tau$ are smooth functions of the index ν. The quantities $x_\nu(0)$ and $\dot{x}_\nu(0)$, on the other hand, may be greatly different from each other, even at adjacent indices ν, by virtue of their "origin."

Let us consider a group of terms in (4.3) with approximately equal indices ν, chosen in such a way that we have $|\omega_{\nu+K} - \omega_\nu| \ll \gamma_0$, where γ_0 is the given resolution (which may correspond to the actual resolution of a spectrum analyzer in an experiment). In this case, taking the smoothly varying quantities through the summation sign, we find

$$J \equiv \sum_{|\nu-\nu_0|<K/2} S_{1\nu}^2 \cos \omega_\nu \tau \cdot \left(x_\nu^2(0) + \frac{\dot{x}_\nu^2(0)}{\omega_\nu^2} \right)$$
$$\approx S_{1\nu_0}^2 \cos \omega_{\nu_0} \tau \sum_{|\nu-\nu_0|<K/2} \left(x_\nu^2(0) + \frac{\dot{x}_\nu^2(0)}{\omega_{\nu_0}^2} \right).$$

Using expressions (14b.2), which are based on the law of large numbers and which express the sum which appears here in terms of the temperature, we find

$$J \approx S_{1\nu_0}^2 \cos \omega_{\nu_0}\tau \cdot K \frac{2kT}{\omega_{\nu_0}^2} \approx 2kT \sum_{|\nu-\nu_0|<K/2} S_{1\nu}^2 \cos \omega_\nu\tau \cdot \omega_\nu^{-2}$$

(in writing the last expression, we have again written $KS_{1\nu_0}^2 \cos \omega_{\nu_0}\tau/\omega_{\nu_0}^2$ as a sum). Substituting the value found for the partial sum J into (4.3), we find

$$B_q(\tau) = \frac{kT}{M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu^2} \cos \omega_\nu \tau \qquad (A_\nu = S_{1\nu}^2). \tag{5.3}$$

This expression could have been derived from (1.3) in a far simpler way, by assuming that $x_\nu(0)$ and $\dot{x}_\nu(0)$ are random quantities obeying a Gibbs distribution. That approach, however, would require preparing initial conditions for the system of oscillators *many times* and taking an average over a set of initial conditions. The more complicated derivation which we have gone through here had the goal of showing that the time scale for the establishment of a Gibbs distribution is unimportant in the derivation of expression (5.3) for the correlation function. In view of the demonstrated equivalence of these two logically different methods of deriving (5.3), in the analysis of a quantum-mechanical fluctuation-dissipation theorem below we will use the second method, which is the shorter one. We will not carry out a preliminary summation over the group of frequencies of normal oscillations, although that approach would also be possible in the quantum-mechanical case.

We turn now to an analysis of (5.3). Each normal oscillation contributes to $B_q(\tau)$ and vice versa: The fluctuation spectrum consists exclusively of the frequencies of normal oscillations. Let us compare (5.3) with expression (4.2) for the Green's function of this system. Differentiating (5.3) with respect to τ, we find

$$\dot{B}_q(\tau) = -\frac{kT}{M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu} \sin \omega_\nu\tau,$$

which in turn, along with (4.2), leads to an important relation between $B_q(\tau)$ and $G(\tau)$:

$$\dot{B}_q(\tau) = -kTG(\tau). \tag{6.3}$$

Equation (6.3) is a particular case of the classical (not quantum-mechanical) fluctuation-dissipation theorem (FDT),[12,13,16,17] which relates fluctuations (more precisely, the correlation function of the coordinate) to the Green's function of this system, i.e., to the function $G(t)$, which determines the response of a macroscopic oscillator *which is interacting with a reservoir* to an external stimulus. Significantly, none of the quantities ω_ν, A_ν is explicitly present in (6.3). Accordingly, we can find $B_q(\tau)$ without knowing them; it is sufficient to determine $G(t)$, e.g., by imparting to the oscillator an initial momentum $M\dot{Q}_0$ and using the formula

$$G(t) = \frac{Q(t)}{M\dot{Q}_0}.$$

The quantity $\bar{q}^2 = B_q(0)$ can also be expressed in terms of the Green's function $G(t)$. Since $G(t)$ is odd with respect to the point $t = T_0/2$, we can find the following expression, which holds for finite T_0:

$$\bar{q}^2 = kT \int_0^{T_0/2} \left(1 - \frac{2t}{T_0} \right) G(t)\, dt. \tag{7.3}$$

This expression simplifies in the limiting case $T_0 \to \infty$, in which the process becomes irreversible. In that case we have

$$\bar{q}^2 = kT \int_0^{\infty} G(t)\, dt. \tag{7a.3}$$

It is not difficult to see that this expression follows from (6.3) under the condition $B_q(\infty) = 0$. In general, on the other hand, when expression (7.3) holds, the correlation function $B_q(\tau)$ does not fall off to zero; furthermore, we have $B_q(T_0) = B_q(0)$.

As we know, the FDT is proved under extremely general assumptions for Hamiltonian systems of an arbitrary type. It essentially reflects the fact that the quantum-mechanical dynamics of a system is determined by the evolution operator $\hat{U}(t) = \exp(-it\hat{H}/\hbar)$, while the Gibbs distribution is specified by the statistical operator $\hat{\rho}(T) = \exp(-\hat{H}/kT)$. We thus have $\hat{\rho}(-i\hbar/kt) = \hat{U}(t)$. This operator equation generates a series of fluctuation-dissipation relations,[18] one of which, in the classical limit, is (6.3).

It should be noted, however, that while the left side of (6.3) does indeed describe equilibrium fluctuations the right side of this relation describes not a dissipation but a *purely dynamic* response of a *Hamiltonian* system to an external stimulus.[14]

The FDT, however, is usually applied to dissipative, rather than Hamiltonian, systems. The Green's function of a *Hamiltonian* system, which appears in the FDT on its right side, is accordingly replaced by a *phenomenological* Green's function, which does not meet the restrictions which follow from the reversibility of the initial equations. A replacement of this sort can be justified if the phenomenological, non-Hamiltonian description of the macroscopic process reflects the nature of the average motion well, so that a satisfactory *approximation* of the microscopic Green's function of the Hamiltonian system is found in the initial (dissipative) stage of the evolution. It can thus be assumed that at $t < T_0/2$ the phenomenological equations make it possible to find accurately a *microscopic* function $G(t)$ for which the FDT holds.

Such a construction makes it possible to extend an FDT, which holds for Hamiltonian systems to non-Hamiltonian (dissipative) systems, and it justifies the second part of the name of this theorem. It is in this stage that the parameters which, in the complete Hamiltonian of this system and in its exact Green's function, describe the interaction of a macroscopic object with a reservoir are expressed in terms of parameters describing dissipation. To avoid a logical contradiction with the initial reversible equations from which the FDT was derived it is sufficient simply to note that such a replacement is legitimate only in the initial stage of the evolution of the system.

It should be kept in mind that since the correlation function $B_q(\tau)$ is an even function by definition, the function $\dot{B}_q(\tau)$ is odd. Also present on the right side of (6.3) is the Green's function $G(t)$, which is odd (by virtue of the reversibility of the equations of motion). Let us examine how we would formulate an FDT in terms of frequencies, rather than times, and, in particular, the consequence of the condition that both sides of (6.3) are odd. We introduce the spectral decompositions

$$B_q(\tau) = \int_{-\infty}^{\infty} \Phi(\omega) e^{i\omega\tau} d\omega, \tag{8.3}$$

$$G(t) = \frac{1}{\pi} \int_{-\infty}^{\infty} \tilde{G}(\omega) e^{i\omega t} d\omega, \tag{9a.3}$$

$$\tilde{G}(\omega) = \frac{1}{2} \int_{-\infty}^{\infty} e^{-i\omega t} G(t) dt. \tag{9b.3}$$

Although the functions $B(\tau)$ and $G(t)$ are periodic and are decomposed in Fourier series we will use more general and more convenient representations in the form of Fourier integrals, bearing in mind that the functions $\Phi(\omega)$ and $\tilde{G}(\omega)$ may be of the form of a sum of δ-functions.

Let us examine some general properties of the functions $\Phi(\omega)$ and $\tilde{G}(\omega)$. Since $B^* = B$ and $G^* = G$, the following conditions hold on the real ω axis, i.e., for $\omega^* = \omega$:

$$\Phi^*(\omega) = \Phi(-\omega), \quad \tilde{G}^*(\omega) = \tilde{G}(-\omega).$$

It follows from the parity and positive definiteness (Ref. 16, for example) of the correlation function $B_q(\tau)$ that we have

$$\Phi(-\omega) = \Phi(\omega) = \Phi^*(\omega) \geqslant 0.$$

The odd parity of $G(t)$ implies that $\tilde{G}(\omega)$ is odd, so that we have $-\tilde{G}(\omega) = \tilde{G}(-\omega) = \tilde{G}^*(\omega)$. We thus have $\mathrm{Re}\,\tilde{G}(\omega) = 0$ and

$$\tilde{G}(\omega) = i\,\mathrm{Im}\,\tilde{G}(\omega) \quad \text{for} \quad \omega^* = \omega. \tag{10.3}$$

Substituting in decompositions (8.3) and (6.3), we find a spectral form of the classical FDT:

$$\Phi(\omega) = i\frac{kT}{\pi\omega}\tilde{G}(\omega) = -\frac{kT}{\pi\omega}\,\mathrm{Im}\,\tilde{G}(\omega). \tag{11.3}$$

The appearance of an *imaginary* part of $\tilde{G}(\omega)$ in (11.3) follows from (10.3), i.e., from the odd parity of $G(t)$ and thus from the *reversibility* of the equations of motion. The FDT, however, can be written in the form of either the first or the second equation in (11.3); the first of these equations does not contain the symbol "Im." However, this observation applies only to the *exact* formulation of the FDT, in which the Green's function which is the solution of the reversible equa-

tions of motions appears on its right side. If we instead replace the exact Green's function $G(t)$ by some approximation $G_R(t)$, which is not necessarily an odd function, then the FDT should be used only in the form of the second equation in (11.3). This conclusion follows from the circumstance that the imaginary part of a Fourier transform of an arbitrary real function is always an odd function.

The Green's function $G(t)$ is frequently replaced by a so-called *retarded* Green's function

$$G^{\mathrm{ret}}(t) = \theta(t) G(t), \quad \theta(t) = \begin{cases} 1 & \text{at} & t > 0, \\ 0 & \text{at} & t < 0. \end{cases} \tag{12.3}$$

We define its spectral density $\tilde{G}^{\mathrm{ret}}(\omega)$ by the relations

$$G^{\mathrm{ret}}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}\tilde{G}^{\mathrm{ret}}(\omega)\,d\omega, \quad \tilde{G}^{\mathrm{ret}}(\omega) = \int_{0}^{\infty} e^{-i\omega t}G(t)\,dt \tag{13.3}$$

[note the difference in numerical factors in (9.3) and (13.3)]. In contrast with $\tilde{G}(\omega)$, the function $\tilde{G}^{\mathrm{ret}}(\omega)$ has both real and imaginary parts. Making use of the odd parity of $G(t)$, we find from (13.3)

$$\mathrm{Im}\,\tilde{G}^{\mathrm{ret}}(\omega) = -\int_{0}^{\infty}\sin\omega t\,G(t)\,dt$$

$$= -\frac{1}{2}\int_{-\infty}^{\infty}\sin\omega t\,G(t)\,dt = \mathrm{Im}\,\tilde{G}(\omega), \tag{14.3}$$

i.e., the imaginary parts of the functions $\tilde{G}(\omega)$ and $\tilde{G}^{\mathrm{ret}}(\omega)$ are the same in the case $\omega^* = \omega$. At the same time, the real part of the function $\tilde{G}^{\mathrm{ret}}(\omega)$,

$$\mathrm{Re}\,\tilde{G}^{\mathrm{ret}}(\omega) = \int_{0}^{\infty}\cos\omega t\,G(t)\,dt \tag{15.3}$$

is nonzero. Using the familiar equality

$$\cos\omega t = \frac{1}{\pi}\,\barint_{-\infty}^{\infty}\frac{\sin\omega' t}{\omega' - \omega}\,d\omega'$$

(the bar through the integral sign means the Cauchy principal value), we can rewrite (15.3) as a Hilbert transformation (or dispersion relation):

$$\mathrm{Re}\,\tilde{G}^{\mathrm{ret}}(\omega) = -\frac{1}{\pi}\,\barint_{-\infty}^{\infty}\frac{\mathrm{Im}\,\tilde{G}^{\mathrm{ret}}(\omega')}{\omega' - \omega}\,d\omega'. \tag{16.3}$$

Returning to the spectral formulation of the FDT and using (14.3), we can write (11.3) in the more common form

$$\Phi(\omega) = -\frac{kT}{\pi\omega}\,\mathrm{Im}\,\tilde{G}^{\mathrm{ret}}(\omega). \tag{17.3}$$

In the quantum-mechanical case, the general formulation of the FDT for one degree of freedom is (Refs. 12, 16, and 17, for example)

$$\Phi(\omega) = -\frac{\theta(\omega, T)}{\pi\omega}\,\mathrm{Im}\,\tilde{G}^{\mathrm{ret}}(\omega), \tag{18.3}$$

where

$$\theta(\omega, t) = \frac{\hbar\omega}{2}\,\mathrm{cth}\,\frac{\hbar\omega}{2kT} \tag{19.3}$$

is the mean energy of an oscillator with a resonant frequency ω, including the contribution from zero-point oscillations, $\hbar\omega/2$. Since we have $\theta(\omega, T) \approx kT$ at $kT \gg \hbar\omega$, we see that (17.3) is the classical limit of (18.3). The transition from

the classical FDT to its quantum-mechanical formulation can be carried out formally by making the replacement

$$kT \rightarrow \frac{\hbar\omega}{2} \operatorname{cth} \frac{\hbar\omega}{2kT}. \tag{20.3}$$

We turn now to the Nyquist relation, which we can use to find the spectral densities of fluctuations in the current or the emf in quasisteady electric circuits. This relation can be found as a particular case of the FDT under certain additional specific assumptions which are not necessary in the general case.

The Nyquist relation asserts that the spectral density of the fluctuating emf which arises across a resistance R at temperature T is

$$g_{\mathscr{E}}(\omega) = \frac{2}{\pi} kTR, \tag{21.3}$$

regardless of the type of electric circuit of which this resistance is a part.[15]

We can find the Nyquist relation without going beyond the model which we have been examining here, if we assume that the generalized coordinates q_i are the charges on corresponding capacitors, while the velocities $\dot{q}_i$ are currents. We seek the spectral density of the equilibrium fluctuations of the charge $q(t)$ of a macroscopic oscillator (an oscillating circuit). It is clear that since the Nyquist relation contains the resistance R we can derive it only if we assume that the spectrum of normal oscillations has a Lorentzian shape. As we will show below, such a spectrum leads in the initial, dissipative stage of the evolution to phenomenological equation (5.2), which corresponds to Ohm's law with a frequency-independent resistance.

We write (5.3) for the charge correlation function as

$$B_q(\tau) = \sum_{\nu=1}^{n} \Phi_\nu \cos\omega_\nu\tau, \quad \Phi_\nu = \frac{kTA_\nu}{L\omega_\nu^2}$$

(below we will use notation corresponding to an electric circuit). Substituting expression (9.2) for the coefficients A_ν in here, we find the following expression, in whose numerator we have substituted $2\gamma = R/L$:

$$\frac{\Phi_\nu}{\Omega} = \frac{2kTR}{\pi L^2} \frac{\operatorname{th}(\gamma T_0/2)}{(\omega_\nu^2 - \omega_0^2)^2 + 4\gamma^2\omega_\nu^2} = g_q(\omega_\nu).$$

The quantity Φ_ν/Ω is the spectral *density* of the charge fluctuations. Since the current is $I = \dot{q}$, the spectral density of its fluctuations, $g_I(\omega_\nu)$, is $\omega_\nu^2 g_q(\omega_\nu)$; i.e.,

$$g_I(\omega_\nu) = \frac{2kTR}{\pi L^2} \operatorname{th}\left(\frac{\gamma T_0}{2}\right) \frac{\omega_\nu^2}{(\omega_\nu^2 - \omega_0^2)^2 + 4\gamma^2\omega_\nu^2}.$$

Phenomenological equation (5.2), which corresponds (in the limit $\gamma T_0 \rightarrow \infty$) to this expression, can be associated with an electric circuit consisting of a series connection of an inductance L, a capacitance C, and a resistance R in a "ring." The electrical impedance Z of such a circuit is $Z = R + i\omega L - (i/\omega C)$. The current I and the emf $\mathscr{E}$ are related by $\mathscr{E} = ZI$; we then find $g_\mathscr{E}(\omega_\nu) = |Z(\omega_\nu)|^2 g_I(\omega_\nu)$ for the spectral densities. Since we have $|Z(\omega_\nu)|^2 = (L/\omega_\nu)^2[(\omega_\nu^2 - \omega_0^2)^2 + 4\gamma^2\omega_\nu^2]$, we find for $g_\mathscr{E}(\omega_\nu)$ [assuming $\tanh(\gamma T_0/2) = 1$]

$$g_\mathscr{E}(\omega_\nu) = \frac{2}{\pi} kTR.$$

This expression differs from Nyquist relation (21.3), given above, only in the index ν, which specifies that normal fre-

quency which determines the spectral density of the noise in the given frequency interval. It is clear, however, that if the measurement instrument cannot resolve the individual normal frequencies, so that many normal oscillations always fall in its bandwidth $\Delta\omega$, such an instrument cannot distinguish a signal with a continuous spectrum from one with a discrete spectrum. Formally, this argument reduces to the assertion that the following approximation of an integral by an integral sum holds very well:

$$\sum_{\Delta\omega} \varphi_\nu \equiv \sum_{\Delta\omega} \frac{\varphi_\nu}{\Omega}\Omega \approx \int_{\Delta\omega} g_\varphi(\omega)\,d\omega.$$

Under these conditions, the index ν in the expression derived here can be discarded, and the expression becomes identical to the Nyquist relation.

We now wish to compare Nyquist relation (21.3) with FDT (17.3). We see that the former is a particular case of the latter under certain additional assumptions regarding the spectrum of normal oscillations. These additional assumptions essentially justify the introduction of a frequency-independent electrical resistance R, and the Nyquist relation applies specifically to this case. Yet another distinction between the FDT and the Nyquist relation stems from the circumstance that a necessary condition for the applicability of the latter is that the phenomenological equation correspond to the model of a linear system with *one* degree of freedom (an oscillator with a friction $R\dot{Q}_R$), while the FDT also applies to far more general phenomenological models which incorporate the possible appearance of new degrees of freedom at high frequencies. Long before quantum-mechanical effects come into play (see the following section of this paper), the Nyquist relation may thus become inapplicable because of such effects as a breakdown of the quasisteady approximation, a skin effect, or the appearance of parasitic capacitances and inductances. In none of these cases can the Nyquist relation be used to calculate the noise, while the FDT can always be used for this purpose.

It might appear that the following argument could be cited to justify the universality of the Nyquist relation: That relation is derived from extremely general considerations regarding detailed balance (Refs. 16 and 17, for example), so that the particular model on the basis of which it is derived would be unimportant. However, the fact is that even before we call upon the considerations of detailed balance we make the implicit assumption that Ohm's law with a frequency-independent resistance holds. If this law does hold, then we can derive the Nyquist relation. If, however, Ohm's law in this form is not called upon in this derivation in the Nyquist relation, then it is not possible to justify the latter relation. In this case the Nyquist relation yields to a more general relation: the FDT.

4. QUANTUM-MECHANICAL FLUCTUATION-DISSIPATION THEOREM AND THE NYQUIST RELATION

In this section we examine the question of incorporating quantum-mechanical fluctuations in our problem. One result of the analysis below is the derivation of a quantum-mechanical Nyquist relation, which some time ago was the subject of some debate,[19-22] which has flared up again.[23,24,32]

For the quantum-mechanical study of this problem, we could use one of the many equivalent formulations of quan-

tum mechanics. We will use here a formalism which is close to the classical formalism and which is based on the representation of quantum mechanics in the phase space of coordinates and momenta (the Wigner-function formalism). In this formalism, one introduces, in place of the coordinate operation $\hat{x}$ and the momentum operator $\hat{\pi}$, the c-number variables x and π, which have the properties of random quantities; the state vector $|\psi\rangle$ is replaced by the quasiprobabilistic Wigner function $W(x,\pi)$, which plays the role of a joint probability density of random values of the coordinates and momenta. The quantum-mechanical expectation values of any functions of the operators $\langle\psi|f(\hat{x},\hat{\pi})|\psi\rangle$ is made exactly equal to the expectation values calculated with the help of the quasiprobabilistic Wigner function by introducing the functions $f_W(x,\pi)$, the "Weyl symbols" of the operator $f(\hat{x},\hat{\pi})$, which are selected in a special way for each operator $f(\hat{x},\hat{\pi})$, in such a way that the following equality holds:

$$\langle\psi|f(\hat{x},\hat{\pi})|\psi\rangle = \int\int_{-\infty}^{\infty} f_W(x,\pi)\, W(x,\pi)\, dx\, d\pi. \quad (1.4)$$

We refer the reader who is interested in the subtleties of this formalism to the specialized reviews[25-27] and the monograph by de Groot and Suttorp,[28] in which this formalism is used systematically. In the present review we offer only an elementary derivation of the basic expression, (1.4), and of the quantities which appear in it. We will not go into a detailed discussion of the physical content of this representation.

We denote by $|x\rangle$ the eigenfunctions of the operator $\hat{x}$ (i.e., $\hat{x}|x_1\rangle = x_1|x_1\rangle$), which form an orthonormal ($\langle x_1|x_2\rangle = \delta(x_1 - x_2)$) and complete ($\int|x\rangle dx\langle x| = 1$) basis. We denote by $f(\hat{x},\hat{\pi})$ the operator representing some physical quantity and we denote by $|\psi\rangle$ the state vector of the quantum-mechanical system ($\langle\psi|\psi\rangle = 1$), so that $\langle x|\psi\rangle = \psi(x)$ and $\langle\psi|x\rangle = \psi^*(x)$ are wave functions in the coordinate representation. The expectation value of $f(\hat{x},\hat{\pi})$ in the state $|\psi\rangle$ is defined by

$$\langle f\rangle \equiv \langle\psi|f(\hat{x},\hat{\pi})|\psi\rangle.$$

We will now go through a chain of simple identity transformations which lead to representation (1.4). We have

$$\langle f\rangle = \langle\psi|f(\hat{x},\hat{\pi})|\psi\rangle = \langle\psi|\hat{1}f(\hat{x},\hat{\pi})\hat{1}|\psi\rangle$$

$$= \int\int_{-\infty}^{\infty} \langle\psi|x_1\rangle\, dx_1\, \langle x_1|f(\hat{x},\hat{\pi})|x_2\rangle dx_2\langle x_2|\psi\rangle.$$

Setting $x_1 = x + (\xi/2)$ and $x_2 = x - (\xi/2)$ ($dx_1 dx_2 = dx\, d\xi$), we write

$$\langle f\rangle = \int\int_{-\infty}^{\infty} \psi^*\left(x + \frac{\xi}{2}\right)\psi\left(x - \frac{\xi}{2}\right)$$

$$\times \left\langle x + \frac{\xi}{2}\middle|f(\hat{x},\hat{\pi})\middle|x - \frac{\xi}{2}\right\rangle dx\, d\xi$$

$$= \int\int\int_{-\infty}^{\infty} \psi^*\left(x + \frac{\xi_1}{2}\right)\psi\left(x - \frac{\xi_1}{2}\right)\delta(\xi_1 - \xi_2)$$

$$\times \left\langle x + \frac{\xi_2}{2}\middle|f(\hat{x},\hat{\pi})\middle|x - \frac{\xi_2}{2}\right\rangle dx\, d\xi_1\, d\xi_2.$$

Finally, substituting in

$$\delta(\xi_1 - \xi_2) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\frac{i\pi(\xi_1 - \xi_2)}{\hbar}\, d\pi,$$

we find

$$\langle f\rangle = \frac{1}{2\pi\hbar}\int\int\int_{-\infty}^{\infty}\int \psi^*\left(x + \frac{\xi_1}{2}\right)\psi\left(x - \frac{\xi_1}{2}\right)$$

$$\times e^{i\pi\xi_1/\hbar}\left\langle x + \frac{\xi_2}{2}\middle|f(\hat{x},\hat{\pi})\middle|x - \frac{\xi_2}{2}\right\rangle$$

$$\times e^{-i\pi\xi_2/\hbar}\, dx\, d\pi\, d\xi_1\, d\xi_2.$$

We now introduce two functions: the quasiprobability density or Wigner function

$$W(x,\pi) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \psi^*\left(x + \frac{\xi}{2}\right)\psi\left(x - \frac{\xi}{2}\right)e^{i\pi\xi/\hbar}\, d\xi \quad (2.4)$$

and the Weyl $f_W(x,\pi)$ of the operator $f(\hat{x},\hat{\pi})$,

$$f_W(x,\pi) \equiv \int_{-\infty}^{\infty}\left\langle x + \frac{\xi}{2}\middle|f(\hat{x},\hat{\pi})\middle|x - \frac{\xi}{2}\right\rangle e^{-i\pi\xi/\hbar}\, d\xi. \quad (3.4)$$

[The correspondence between $f(\hat{x},\hat{\pi})$ and $f_W(x,\pi)$ is sometimes denoted by $f(\hat{x},\hat{\pi}) \to f_W(x,\pi)$.] The last equality for $\langle f\rangle$ then takes the form indicated above, in (1.4).

The function $W(x,\pi)$ which depends quadratically on ψ, i.e., on the state of the system, is an analog of the joint probability density for random c-number values of the coordinate and the momentum. The function $f_W(x,\pi)$ is called the "Weyl symbol" of the operator $f(\hat{x},\hat{\pi})$ and represents this operator in the phase space (x,π). Equation (1.4) can be discussed in terms of probability theory as an averaging of the function $f_W(x,\pi)$ of random c-number coordinates and momenta over the probability density $W(x,\pi)$. The Wigner function actually has many properties characteristic of a probability density and allows [with the help of (1.4)] an *exact* calculation of quantum-mechanical expectation values. In particular,

$$\int_{-\infty}^{\infty} W(x,\pi)\, d\pi = |\langle x|\psi\rangle|^2 = W(x),$$

$$\int_{-\infty}^{\infty} W(x,\pi)\, dx = |\langle\pi|\psi\rangle|^2 = W(\pi)$$

are the actual probability densities of the coordinate and the momentum.

On the other hand, the probabilistic interpretation of the function W is not perfect. The primary reasons are the two following properties of this function:

1. In certain parts of the (x,π) plane, W can take on negative values.

2. If $\langle f\rangle = \langle\psi|\hat{f}|\psi\rangle = \int\int f_W^{(1)}(x,\pi)W(x,\pi)\, dx\, d\pi$ is the mean value of the quantity f, then its mean square value $\langle f^2\rangle = \langle\psi|\hat{f}^2|\psi\rangle$ is given by an expression of the same type:

$$\langle f^2\rangle = \int\int f_W^2(x,\pi)\, W(x,\pi)\, dx\, d\pi.$$

However, if $f^2(\hat{x},\hat{\pi})$ depends on *both* of the variables $\hat{x},\hat{\pi}$ then we have $f_W^{(2)} \neq (f_W^{(1)})^2$.

For a harmonic oscillator with a resonant frequency ω_v, the function $W(x,\pi)$ is known for any excited state $|n\rangle$ ($\hat{H}(\hat{x}_v,\hat{\pi}_v)|\hat{n}\rangle = \hbar\omega_v(n + \frac{1}{2})|n\rangle$) (Ref. 25, for example):

$$W_n (x_\nu, \pi_\nu) = \frac{(-1)^n}{\pi \hbar} \exp \left[-\frac{2}{\hbar \omega_\nu} H (x_\nu, \pi_\nu) \right]$$
$$\times L_n \left(\frac{4}{\hbar \omega_\nu} H (x_\nu, \pi_\nu) \right); \qquad (4.4)$$

Here ν specifies both the resonant frequency and the phase variables of the νth normal oscillation, and

$$H (x_\nu, \pi_\nu) = \frac{1}{2} (\pi_\nu^2 + \omega_\nu^2 x_\nu^2). \qquad (5.4)$$

The Laguerre polynomials $L_n (x)$ in (4.4) are determined by the generating function

$$(1-z)^{-1} \exp [-zx (1-z)^{-1}] = \sum_{n=0}^{\infty} z^n L_n (x); \qquad (6.4)$$

specifically, $L_0(x) = 1$, $L_1(x) = 1 - x$, $L_2(x) = 1 - 2x + (x/2^2)$, ...). As can be seen from (4.4), at $n > 1$ the functions $W_n (x_\nu, \pi_\nu)$ can take on negative values.

If the oscillator is in one of the pure states $|n\rangle$, then any mean values of its parameters can be found with the help of (1.4), provided that we first use (3.4) to find the Weyl symbol of the corresponding operator.

What we are interested in, however, is another problem. After contact with a ("grand") reservoir which existed at $t < 0$ (this point was discussed in more detail earlier) each of the normal oscillators is in a *mixed* state, of such a nature that its probability to be in the nth excited state $|n\rangle$ is determined by the Gibbs distribution

$$p_n = (1 - e^{-\hbar \omega_\nu / kT}) e^{-n \hbar \omega_\nu / kT}. \qquad (7.4)$$

The mixed state of the νth oscillator is described by the equilibrium Wigner function

$$\overline{W}_\nu (x_\nu, \pi_\nu) = \sum_{n=0}^{\infty} p_n W_n (x_\nu, \pi_\nu). \qquad (8.4)$$

This function can be found by substituting (4.4) and (7.4) into (8.4), and (6.4) can be used for the summation. After some simple calculations we find the equilibrium Wigner function of the νth normal oscillation:

$$\overline{W}_\nu (x_\nu, \pi_\nu) = \left(\pi \hbar \, \mathrm{cth} \, \frac{\hbar \omega_\nu}{2kT} \right)^{-1}$$
$$\times \exp \left[-\frac{\pi_\nu^2}{2\theta (\omega_\nu, T)} - \frac{x_\nu^2}{2\theta (\omega_\nu, T)/\omega_\nu^2} \right], \quad (9.4)$$

where

$$\theta (\omega_\nu, T) = \frac{\hbar \omega_\nu}{2} \, \mathrm{cth} \, \frac{\hbar \omega_\nu}{2kT} \qquad (10.4)$$

is the mean energy of an oscillator with resonant frequency ω_ν at the temperature T (the energy of the zero-point oscillations is included).

Distribution (9.4) is Gaussian and is determined completely by the mean values and second moments of the quantities x_ν, π_ν:

$$\overline{\langle x_\nu \rangle} = 0, \quad \overline{\langle \pi_\nu \rangle} = 0,$$
$$\overline{\langle x_\nu^2 \rangle} = \frac{\theta (\omega_\nu, T)}{\omega_\nu^2}, \quad \overline{\langle \pi_\nu^2 \rangle} = \theta (\omega_\nu, T), \quad \overline{\langle x_\nu \pi_\nu \rangle} = 0. \qquad (11.4)$$

Here the angle brackets refer to an averaging over quantum-mechanical fluctuations, while the superior bar refers to an averaging over thermal fluctuations. Equilibrium Wigner function (9.4) thus offers a simultaneous and common de-

scription of both the quantum-mechanical and thermal fluctuations of the coordinate and momentum of the oscillator.

It can be shown that distribution (9.4) is a steady-state distribution, i.e., does not vary over time (proving this assertion would require use of the quantum-mechanical Liouville equation, which we will not reproduce here).

We turn now to the correlation functions of the fluctuations. To calculate them we need information on the state of the system at two different but otherwise arbitrary times. It is thus not sufficient to know simply the Wigner function corresponding to one time. We will accordingly use Heisenberg equations of motion for the operators $\hat{x}_\nu$ and $\hat{\pi}_\nu$:

$$\frac{d\hat{\pi}_\nu (t)}{dt} = \frac{i}{\hbar} [H (\hat{x}_\nu, \hat{\pi}_\nu), \hat{\pi}_\nu] = -\omega_\nu^2 \hat{x}_\nu (t),$$
$$\frac{d\hat{x}_\nu (t)}{dt} = \frac{i}{\hbar} [H (\hat{x}_\nu, \hat{\pi}_\nu), \hat{x}_\nu] = \hat{\pi}_\nu (t). \qquad (12.4)$$

It is easy to verify that a solution of these equations is

$$\hat{x}_\nu (t) = \hat{x}_\nu (0) \cos \omega_\nu t + \frac{\hat{\pi}_\nu (0)}{\omega_\nu} \sin \omega_\nu t,$$
$$\hat{\pi}_\nu (t) = \hat{\pi}_\nu (0) \cos \omega_\nu t - \omega_\nu \hat{x}_\nu (0) \sin \omega_\nu t. \qquad (13.4)$$

We are interested in the coordinate correlation function. Using (13.4), we can easily calculate the operator corresponding to this function:

$$B_\nu (t_1, t_2) \equiv \frac{1}{2} [\hat{x}_\nu (t_1) \hat{x}_\nu (t_2) + \hat{x}_\nu (t_2) \hat{x}_\nu (t_1)]$$
$$= \frac{1}{2} \left[\hat{x}_\nu^2 (0) + \frac{\hat{\pi}_\nu^2 (0)}{\omega_\nu^2} \right] \cos \omega_\nu (t_1 - t_2)$$
$$+ \frac{1}{2} \left[\hat{x}_\nu^2 (0) - \frac{\hat{\pi}_\nu^2 (0)}{\omega_\nu^2} \right] \cos \omega_\nu (t_1 + t_2)$$
$$+ \omega_\nu^{-1} [\hat{x}_\nu (0) \hat{\pi}_\nu (0) + \hat{\pi}_\nu (0) \hat{x}_\nu (0)]$$
$$\sin \omega_\nu (t_1 + t_2). \qquad (14.4)$$

We should now take an average of this expression. In the formalism which we are using, one associates with the initial values of the operators, $\hat{\pi}_\nu (0)$, $\hat{x}_\nu (0)$, and combinations thereof, some random numbers which are their Weyl symbols. Their probability distribution is described by Wigner function (9.4). Accordingly, we should first find the Weyl symbols of the operators in (14.4), so that we can substitute them, along with (9.4), into (1.4).

The Weyl symbol of the operator $F(\hat{x}_\nu)$ is equal to $F(x_\nu)$, as is easily verified: Using definition (3.4), we can write (omitting the index ν)

$$\int \left\langle x + \frac{\xi}{2} \middle| F (\hat{x}) \middle| x - \frac{\xi}{2} \right\rangle e^{-i\pi \xi / \hbar} d\xi$$
$$= \int F \left(x - \frac{\xi}{2} \right) \delta (\xi) e^{-i\pi \xi / \hbar} d\xi = F (x).$$

In precisely the same way it can be proved that we have $F(\hat{\pi}) \to F(\pi)$ (the proof involves transforming to a basis of the eigenvectors of the momentum operator). We are left with the problem of finding the Weyl symbol of the operator $\hat{x}\hat{\pi} + \hat{\pi}\hat{x}$ (for brevity, we will omit the index ν and the argument $t = 0$ from the intermediate calculations). By definition we have

$$\int \left\langle x + \frac{\xi}{2} \middle| \hat{x}\hat{\pi} + \hat{\pi}\hat{x} \middle| x - \frac{\xi}{2} \right\rangle e^{-i\pi \xi / \hbar} d\xi$$

$$= \int \left[\left(x + \tfrac{\xi}{2} \right) \left\langle x + \tfrac{\xi}{2} \left| \hat{\pi} \right| x - \tfrac{\xi}{2} \right\rangle \right.$$
$$\left. + \left\langle x + \tfrac{\xi}{2} \left| \hat{\pi} \right| x - \tfrac{\xi}{2} \right\rangle \left(x - \tfrac{\xi}{2} \right) \right] e^{-i\pi\xi/\hbar} \, d\xi$$

$$= 2x \int \left\langle x + \tfrac{\xi}{2} \left| \hat{\pi} \right| x - \tfrac{\xi}{2} \right\rangle e^{-i\pi\xi/\hbar} \, d\xi.$$

Using

$$\langle x_1 | F(\hat{\pi}) | x_2 \rangle = F\left(-i\hbar \frac{\partial}{\partial \eta} \right) \delta(\eta)|_{\eta = x_1 - x_2},$$

we find[6]

$$\hat{x}_\nu(0) \, \hat{\pi}_\nu(0) + \hat{\pi}_\nu(0) \, \hat{x}_\nu(0) \to -2i\hbar x \int \delta'(\xi) \, e^{-i\pi\xi/\hbar} \, d\xi$$

$$= 2x_\nu(0) \, \pi_\nu(0).$$

To find now the correlation function of the fluctuations of the coordinate of oscillator ν, it is sufficient to replace the operators $\hat{x}_\nu^2(0)$, $\hat{x}_\nu^2(0)$ and $\hat{x}_\nu(0)\hat{\pi}_\nu(0) + \hat{\pi}_\nu(0)\hat{x}_\nu(0)$ in (14.4) by their Weyl symbols $x_\nu^2(0)$, $\pi_\varphi^2(0)$ and $2x_\nu(0)\pi_\nu(0)$, which are, according to (9.4), Gaussian random numbers, and to take an average over this Gaussian distribution. The result is of course given by (11.4); for the correlation function of the coordinate, $B_\nu(t_1, t_2)$, we find

$$B_\nu(t_1, t_2) = \frac{\theta(\omega_\nu, T)}{\omega_\nu^2} \cos \omega_\nu \tau, \quad \tau = t_1 - t_2 \qquad (15.4)$$

If we had first taken an average over the time $t = (t_1 + t_2)/2$ at a fixed τ in (14.4), we would have found the functional dependence $B_\nu \sim \cos \omega_\nu \tau$. A time dependence of the type $\cos \omega_\nu \tau$ is thus determined exclusively by the dynamics of this system, while the numerical coefficient in (15.4) depends on the relation between the quantum-mechanical and thermal fluctuations.

Correlation function (15.4) has been derived for a normal oscillation, i.e., for an *isolated* oscillator, which is not coupled with anything else. As can be seen from (15.4), the mean square value of the fluctuations of the coordinate of such an oscillator is determined by the quantity $\theta(\omega_\nu, T)$, i.e., by the energy of the oscillator at its *own resonant* frequency.

We turn now to the fluctuations of the coordinate of a macroscopic oscillator which *is interacting* with the system of the $(n-1)$ other oscillators. The operator representing the coordinate of the macroscopic oscillator, $\hat{q}_1(t)$, is related to the operators $\hat{x}_\nu(t)$ by

$$\hat{q}_1(t) = \frac{1}{M^{1/2}} \sum_{\nu=1}^{n} S_{1\nu} \hat{x}_\nu(t). \qquad (16.4)$$

We first note that all the results referring to the average motion of a classical macroscopic oscillator can be transferred without any changes to the average motion of the quantum-mechanical oscillator. This conclusion follows from the circumstance that after we take an average over any quantum state the Heisenberg equations of motion of a linear oscillator become the corresponding classical equations. This is a consequence of the general Ehrenfest theorem for motion in a quadratic potential. Consequently, all the results derived for the average motion of a classical macroscopic oscillator remain valid in the quantum-mechanical case.

We turn now to a calculation of the correlation function for fluctuations in the coordinate of the macroscopic oscillator. From (16.4) we have

$$\hat{B}_q(t_1, t_2) = \frac{1}{2} [\hat{q}_1(t_1) \, \hat{q}_1(t_2) + \hat{q}_1(t_2) \, \hat{q}_1(t_1)]$$

$$= \frac{1}{2M} \sum_{\nu, \mu=1}^{n} S_{1\nu} S_{1\mu} [\hat{x}_\nu(t_1) \, \hat{x}_\mu(t_2) + \hat{x}_\nu(t_2) \, \hat{x}_\mu(t_1)]. \qquad (17.4)$$

Before we average this expression, we note that in the case $\nu \neq \mu$ the operators $\hat{x}_\nu(t_i)$, $\hat{x}_\mu(t_j)$ act in different state spaces and are thus averaged independently:

$$\langle \psi_\nu, \psi_\mu | \hat{x}_\nu \hat{x}_\mu | \psi_\nu, \psi_\mu \rangle = \langle \psi_\nu | \hat{x}_\nu | \psi_\nu \rangle \langle \psi_\mu | \hat{x}_\mu | \psi_\mu \rangle.$$

As was shown above [see (11.4)], the equilibrium expectation values are $\overline{\langle x_\nu \rangle} = 0$. Consequently, when we average (17.4) we should retain only the term with $\nu = \mu$; using (14.4) and (15.4), we then find

$$B_q(t_1, t_2) = \frac{1}{M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu^2} \theta(\omega_\nu, T) \cos \omega_\nu \tau. \qquad (18.4)$$

As in the classical case, the function $B_q(\tau)$ is periodic (or nearly periodic). This property reflects the reversibility of the initial equations. In the limiting case $\hbar \omega_\nu \ll kT$ we find the classical expression (5.3) from (18.4).

From (18.4) we can construct a quantum-mechanical formulation of the fluctuation-dissipation theorem (FDT). As above, we introduce decompositions of $B_q(\tau)$ and $G^{\text{ret}}(t)$ in Fourier integrals:

$$\Phi(\omega) = \frac{1}{2\pi} \int e^{-i\omega\tau} B_q(\tau) \, d\tau$$

$$= \frac{\hbar}{4M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu} \operatorname{cth} \left(\frac{\hbar \omega_\nu}{2kT} \right) [\delta(\omega + \omega_\nu) + \delta(\omega - \omega_\nu)].$$

Using the identity $F(\omega_\nu) \delta(\omega_\nu \pm \omega) = F(\mp \omega) \delta(\omega_\nu \pm \omega)$ and also making use of the circumstance that the function $F(\omega_\nu) = \omega_\nu^{-1} \operatorname{cth}(\hbar \omega_\nu / 2kT)$ is of even parity with respect to ω_ν, we find

$$\Phi(\omega) = \frac{\hbar}{4M\omega} \operatorname{cth} \left(\frac{\hbar \omega}{2kT} \right) \sum_{\nu=1}^{n} A_\nu [\delta(\omega + \omega_\nu) + \delta(\omega - \omega_\nu)]. \qquad (19.4)$$

As was mentioned above, the Green's function of the system of oscillators refers to the average motion, so that in quantum theory it is the same as that given by the classical expression found above, (4.2): $G(t) = \frac{1}{M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu} \sin \omega_\nu t$. We use the imaginary part of the decomposition in a Fourier integral of the retarded function $G^{\text{ret}}(t) = \theta(t) G(t)$:

$$\operatorname{Im} \widetilde{G}^{\text{ret}}(\omega) = -\int_0^\infty \sin \omega t \cdot \frac{1}{M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu} \sin \omega_\nu t \, dt$$

$$= \frac{\pi}{2M} \sum_{\nu=1}^{n} \frac{A_\nu}{\omega_\nu} [\delta(\omega - \omega_\nu) - \delta(\omega - \omega_\nu)].$$

Since $\omega_\nu^{-1} \delta(\omega + \omega_\nu) = -\omega^{-1} \delta(\omega + \omega_\nu)$ and $\omega_\nu^{-1} \delta(\omega - \omega_\nu) = \omega^{-1} \delta(\omega - \omega_\nu)$, we have

$$\operatorname{Im} \widetilde{G}^{\mathrm{ret}}(\omega) = -\frac{\pi}{2M\omega} \sum_{\nu=1}^{n} A_\nu \left[\delta(\omega + \omega_\nu) + \delta(\omega - \omega_\nu) \right]. \tag{20.4}$$

Comparing (19.4) and (20.4) we find a quantum-mechanical FDT:

$$\Phi(\omega) = -\frac{\hbar}{2\pi} \operatorname{cth}\left(\frac{\hbar\omega}{2kT}\right) \operatorname{Im} \widetilde{G}^{\mathrm{ret}}(\omega)$$

$$= -\frac{\theta(\omega, T)}{\pi\omega} \operatorname{Im} \widetilde{G}^{\mathrm{ret}}(\omega). \tag{21.4}$$

Equality (21.4) holds for arbitrary ω. If $\omega \neq \pm \omega_\nu$, then both sides of this equality are zero, while if $\omega = \pm \omega_\nu$ we have an equality of nonzero quantities: generalized functions. As usual, such an equality should be understood as the equality of integrals of the two sides, after they have first been multiplied by some smooth function. In physical measurements, the role of this function is played by the frequency characteristic of a filter, which always has a finite bandwidth $\Delta\omega$. In a real experiment, therefore, with a given $\Delta\omega$ which satisfies the condition $\Delta\omega \gg T_0^{-1}$, it is not possible to answer the question of whether this spectrum is continuous or discrete, since many discrete frequencies ω_ν fall simultaneously in the filter bandwidth $\Delta\omega$. There is accordingly no need to make a special point of taking the limit of a continuous spectrum (correspondingly, taking the limit $T_0 \to \infty$), since these situations are indistinguishable from the experimental standpoint. Consequently, expression (21.4) is identically applicable in the two situations: before and after the limit $T_0 \to \infty$ is taken.

We might also note that the total measurement time τ_0 and the bandwidth $\Delta\omega$ are related by $\tau_0 \Delta\omega \sim 1$, so that the condition $T_0 \Delta\omega \gg 1$ leads to the condition $\tau_0 \ll T_0$; i.e., a measurement can always be carried out in the initial ("dissipative") stage of the evolution of the system.

We turn now to the quantum-mechanical Nyquist relation. Clearly, we can find such a relation by transforming from the general formulation of the FDT if we assume that the spectrum of normal oscillations is determined by (9.2), which corresponds to an exponential decay of the oscillations of a macroscopic oscillator. In this case, (18.4) takes the form (we are substituting $2\gamma = R/L$)

$$B_q(\tau) = \sum_{\nu=1}^{n} \Phi_\nu \cos \omega_\nu \tau, \quad \Phi_\nu$$

$$= \frac{\Omega}{\pi} \frac{\hbar R}{L^2} \operatorname{th}\left(\frac{\gamma T_0}{2}\right) \frac{\omega_\nu \operatorname{cth}(\hbar\omega_\nu/2kT)}{(\omega_\nu^2 - \omega_0^2)^2 + 4\gamma^2 \omega_\nu^2}. \tag{22.4}$$

If $\gamma T_0 \gg 1$ we can assume $\operatorname{th}\left(\frac{\gamma T_0}{2}\right) = 1$. Furthermore, in this case we have $\Omega \ll \gamma$, and a very large number of discrete frequencies, separated by distances Ω, fit in the resonant linewidth γ. In this case, even near the maximum of the resonance curve, i.e., at $\omega_\nu \sim \omega_0$, we can approximate the sum $\Sigma \Phi_\nu \cos \omega_\nu \tau$ very accurately by an integral; this approximation becomes especially accurate far from the resonance. Accordingly, using the notation $\Delta\omega = \Omega$, we can write

$$B_q(\tau) = \sum_{\nu=1}^{n} \Phi_\nu \cos \omega_\nu \tau$$

$$= \sum_{\nu=1}^{n} \frac{\Phi_\nu}{\Omega} \cos \omega_\nu \tau \Delta\omega \approx \int_{\omega_{\min}}^{\omega_{\max}} g_q(\omega) \cos \omega\tau \, d\omega;$$

Here $g_q(\omega) = \frac{\Phi_\nu}{\Omega}$ is the spectral *density* of the charge fluctuations, i.e., the contribution of a unit frequency interval to the mean square value of the fluctuations. Expression (22.4) thus gives us the following expression for the spectral density of charge fluctuations:

$$g_q(\omega) = \frac{\hbar R}{\pi L^2} \frac{\omega \operatorname{cth}(\hbar\omega/2kT)}{(\omega^2 - \omega_0^2)^2 + 4\gamma^2 \omega^2}. \tag{23.4}$$

In this expression we are no longer writing the index ν, which distinguishes the various normal frequencies, since it has been shown that the summation over all ω_ν in (22.4) and the integration over the variable ω in (23.4) lead to identical values of $B_q(\tau)$ or $\overline{q^2}$.

The spectral density of the current $I = \dot{q}$ can be found by multiplying the right side of (23.4) by ω^2: $g_I(\omega) = \omega^2 g_q(\omega)$. Proceeding as we did above in the derivation of the classical Nyquist relation, we transform to the spectral density of the emf: $g_{\mathscr{E}}(\omega) = |Z(\omega)|^2 g_I(\omega)$, where $|Z|^2 = (L/\omega)^2 \left[(\omega^2 - \omega_0^2)^2 + 4\gamma^2 \omega^2 \right]$. As a result we find the quantum-mechanical Nyquist relation

$$g_{\mathscr{E}}(\omega) = \frac{2}{\pi} \theta(\omega, T) R = \frac{2}{\pi} \frac{\hbar\omega}{2} \operatorname{cth}\left(\frac{\hbar\omega}{2kT}\right) R. \tag{24.4}$$

As was already mentioned, a quantum-mechanical formulation of the FDT can be found from the classical formulation through replacement (20.3), i.e., through the replacement

$$kT \to \theta(\omega, T) = \frac{\hbar\omega}{2} \operatorname{cth} \frac{\hbar\omega}{2kT}. \tag{25.4}$$

Precisely the same replacement converts the classical Nyquist relation into the quantum-mechanical relation (22.4); this is the approach taken in the original study by Nyquist.[17]

In the debate[23,24] over the quantum-mechanical Nyquist relation, which we mentioned earlier, the possibility of the alternative replacement

$$kT \to \theta(\omega_0, T) = \frac{\hbar\omega_0}{2} \operatorname{cth} \frac{\hbar\omega_0}{2kT} \tag{26.4}$$

was discussed, where ω_0 is the resonant frequency of the macroscopic oscillator. This expression differs substantially from (25.4), since in it the equivalent temperature is independent of the frequency, in contradiction of (25.4). The result is a very different asymptotic behavior of the noise at high frequencies. Replacement (26.4) is actually valid for an isolated oscillator with an *infinitely large* quality factor, as can be seen from expression (15.4). The oscillations of such an oscillator, however, are not damped (its correlation function is proportional to $\cos \omega_\nu \tau$). If we instead consider an oscillator which *is interacting* with other oscillators and is therefore capable of transferring energy to them, i.e., if we are dealing with a *damped* oscillator with a finite quality factor, then—as can be seen from (18.4) and (22.4)—its noise is caused specifically by the contributions from the normal oscillations at other frequencies, $\omega_\nu \neq \omega_0$, each of which has an "equivalent temperature" corresponding to its own normal frequency, according to (26.4). As a result we find (25.4), where the "equivalent temperature" turns out to depend on the frequency.

That replacement (26.4) holds only in the single case of an oscillator of infinite quality factor and cannot be correct in general is clear from the following simple observation: The same replacement $kT \to \Theta(\omega, T)$ sends the classical FDT into the quantum-mechanical FDT, regardless of the

particular system to which the FDT is applied. In particular, the system might be, instead of an oscillating circuit, a system in which there is no special frequency ω_0 at all or a system in which there are several such special frequencies. In all these cases, the meaning of ω_0 in expression (26.4) would be completely unclear.[18]

Let us go back to the question of the mean kinetic (or magnetic) energy of a macroscopic oscillator. The momentum operator $\hat{p}_1$ which is the canonical conjugate of $\hat{q}_1$ is expressed in terms of $\hat{\pi}_\nu$ by the following formula, as is easily verified:

$$\hat{p}_1 = M^{1/2} \sum_{\nu=1}^{n} S_{1\nu} \hat{\pi}_\nu. \tag{27.4}$$

Making use of the independence of $\hat{\pi}_\nu$ and $\hat{\pi}_\mu$ with $\nu \neq \mu$ along with (11.4), we then find the mean square value of this operator to be

$$\overline{\langle p_1^2 \rangle} = M \sum_{\nu=1}^{n} S_{1\nu}^2 \overline{\langle \pi_\nu^2 \rangle} = M \sum_{\nu=1}^{n} A_\nu \theta(\omega_\nu, T).$$

The mean kinetic energy is therefore

$$\langle \overline{K} \rangle = \frac{\overline{\langle p_1^2 \rangle}}{2M} = \frac{1}{2} \sum_{\nu=1}^{n} A_\nu \theta(\omega_\nu, T). \tag{28.4}$$

In the classical limit, with $\hbar\omega_\nu \ll kT$, we have $\theta(\omega_\nu, T) \approx kT$, and from (28.4) we find, using the equality $\sum_{\nu=1}^{n} A_\nu = 1$,

$$\langle \overline{K} \rangle = \frac{1}{2} kT \sum_{\nu=1}^{n} A_\nu = \frac{1}{2} kT. \tag{29.4}$$

This result agrees with the theorem of uniform distribution of energy among the degrees of freedom. Expression (28.4) could also be derived from the classical expression (29.4) by again using replacement (25.4), if we first introduce a factor $1 = \sum_{\nu=1}^{n} A_\nu$ in the expression $\langle \overline{K} \rangle = kT/2$.

In the quantum-mechanical case, as we see from (28.4), the expectation value of the kinetic energy *does depend* on the relation among the various A_ν. In the case of Lorentzian spectrum, for example, it would also depend on the resistance R. The same conclusion is reached by a direct calculation on the interaction of a charged oscillator with a thermal electromagnetic field, which was carried out in Ref. 30.

The last topic which we will take up in connection with the debate regarding the quantum-mechanical Nyquist relation deals with the analysis of those arguments which have been advanced regarding the question of whether the dissipative parameter R can or cannot appear in the expression for the mean square value of the fluctuations of the charge and the current. It might appear that since R does not enter the Hamiltonian of the oscillator, $H_0 = (LI^2/2) + (q^2/2C)$, the resistance would not be contained in the Gibbs distribution for the oscillator, $W \sim \exp(-H_0/kT)$, so that it therefore could not appear in the expressions for $\overline{I}^2, \overline{q}^2$. However, we can use the Gibbs distribution $\exp(-H_0/kT)$ for an isolated oscillator only if its interaction with the reservoir is *so weak* that it affects only the distribution of the values of its energy, without broadening its infinitely narrow resonant curve (Ref. 14, for example). If we instead wish to incorporate a finite width of the resonance curve then we should examine not an isolated oscillator, which in this case is not itself described by a Hamiltonian, but an oscillator which is interacting with a reservoir. In other words, we should use a Gibbs distribution for the overall system.

As has been mentioned repeatedly, however, the quantity R *is contained* in the total Hamiltonian. In the classical case, if the spectrum of normal oscillations is Lorentzian, so that a resistance R can be introduced, it nevertheless drops out of the final expressions for q^2 and I^2. This result, however, is not a consequence of any fundamental factor but somewhat "fortuitous." It is a simple matter to construct a phenomenological model with another spectrum of normal oscillations, for which the dissipative parameters no longer drop out of the classical formulas for $\overline{q}^2$ and $\overline{I}^2$. The Lorentzian model of the spectrum has the disadvantage that the envelope of the corresponding Green's function is not differentiable at the origin; i.e., it allows an arbitrarily fast response to an external stimulus. Even a slight alteration of this model, e.g., the replacement of the phenomenological Green's function (in the limit $\gamma T_0 \to \infty$)

$$G_R^{\text{ret}}(t) = \frac{\theta(t)}{M\tilde{\omega}} \exp(-\gamma t) \sin \tilde{\omega} t \tag{30.4}$$

by another phenomenological model (also in the limit $\gamma T_0 \to \infty$)

$$G_R^{\text{ret}}(t) = \frac{\theta(t)}{M\tilde{\omega}} \frac{\gamma' \exp(-\gamma t) - \gamma \exp(-\gamma' t)}{\gamma' - \gamma} \sin \tilde{\omega} t, \tag{31.4}$$

where $\gamma' > \gamma$, both erases the discrepancy when the quantum-mechanical Nyquist relation is used[19] and gives rise to dissipative parameters γ and γ' not only in the quantum-mechanical expressions [as has also been shown for model (30.4)] but also in the classical expressions for[20] $\overline{q}^2$ and $\overline{I}^2$. On the other hand, functions (30.4) and (31.4) are essentially indistinguishable outside the region $t < (\gamma\gamma')^{-1.2}$. Consequently, the disappearance of R from the expressions for $\overline{q}^2$ and $\overline{I}^2$ in the case in which the classical Nyquist relation is applicable is not a "crude feature"; it ceases as soon as the conditions for the applicability of this expression cease to hold. In particular, even upon a very slight deviation from Ohm's law, or when we go from the classical Nyquist relation to the quantum relation, R appears in the expressions for $\overline{q}^2$ and $\overline{I}^2$. It is quite possible that there will be deviations from the Nyquist relation (as a result of the appearance of frequency dispersion, for example); such deviations will not contradict the FDT. However, the corrections to the Nyquist relation which were discussed in Ref. 31 are of a different nature and are based on an incorrect interpretation of the FDT. This theorem is an *exact* relation between the noise spectrum and the response of this system, which in general must be calculated in the first order of a time-dependent quantum-mechanical perturbation theory (Ref. 12, for example). If one instead uses some other approximation for the response, the equality of the quantities appearing in the FDT will be disrupted. This is precisely how the FDT and the Nyquist relation which follows from it were "refined" in Ref. 31 (the Wigner-Weisskopf approximation was used instead of perturbation theory).

SUMMARY

It of course cannot be claimed that the very simple model which we have discussed here offers a general description of various physical phenomena. The purpose in analyzing

this model has been a different one: Since this model is exactly solvable at the level of reversible microscopic equations, it can be used as an example to cast light on the logical relationship among different methods for describing dissipative processes and to refine those prerequisites which are required here.

In summarizing this paper we would like to point out the following. From the standpoint of the microscopic reversible equations, a dissipative process may be thought of as just the initial stage of a periodic (or nearly periodic) motion of the overall system, although this initial stage is "infinitely long." The transition to irreversible motion is made by letting the return time T_0 go to infinity; to do this, we also need to increase the total number of oscillators in the reservoir.

The nature of the average motion of a macroscopic object does not depend on the particular probability distribution of the coordinates and velocities of the reservoir particles; it is determined exclusively by the nature of the spectrum of the normal oscillations of the system. In the initial (dissipative) stage there may be a damping of the oscillations of the macroscopic oscillator, which then gives way to a growth of these oscillations. Even in the dissipative stage, however, the average motion does not necessarily obey the usual equation for damped oscillations with a friction force proportional to the velocity (or with a voltage drop proportional to the current). The parameters which describe the dissipation of the energy in the initial stage of the motion of the system, in particular, the resistance, are expressed in terms of the parameters of the total Hamiltonian of the system.

Turning now to equilibrium fluctuations of a macroscopic oscillator, we note that the most general description of these fluctuations within the framework of the second statistical moments is given by the Callen-Welton fluctuation-dissipation theorem. At high temperatures, where quantum-mechanical effects are unimportant, this theorem can be formulated as the assertion that the derivative of the correlation function of the fluctuations of the coordinate is proportional to the microscopic Green's function, which, by virtue of the time reversibility of the equations of motion, is an odd function of the time.

We should point out that the FDT is proved for Hamiltonian systems, which have no dissipation at all. In applications of the FDT, however, the Green's function of the microscopic equations of motion (which usually cannot be found, because of the complexity of the problem) is replaced by a Green's function determined for the initial stage of the evolution of this system through a solution of phenomenological equations (macroscopic or microscopic) which give an approximate description of the average motion and which do contain dissipative parameters *which have been introduced* in them. It is in this stage of the replacement of the Green's function in the FDT that dissipative parameters appear.

The Nyquist relation follows from the FDT in the case in which it is possible to ignore frequency dispersion and in which the average motion in the dissipative stage of the evolution can be described by means of a friction proportional to the velocity (or to the current). At the level of a microscopic description, in the model which we have discussed here, this situation corresponds to a special (Lorentzian) shape of the spectrum of normal oscillations.[2][1]

Corresponding results can be found in the quantum-mechanical case. Here the exact solution of the model problem which we have been discussing leads to a result which was in fact pointed out by Nyquist: A quantum-mechanical fluctuation-dissipation theorem and a quantum-mechanical Nyquist relation can be found (in spectral form) from the corresponding classical relations by replacing the temperature by the average energy of a quantum-mechanical oscillator whose resonant frequency is equal to the frequency in which we are interested in the fluctuation spectrum (the instantaneous frequency).

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[1] Prigogine's recent book[1] expresses exactly the opposite point of view: that physics must be based on equations which explicitly incorporate the fundamental irreversibility of processes. It is doubtful that such a radical change in the fundamental principles of physics is necessary.

[2] In the number labeling an equation, the digit following the decimal point is the section number.

[3] In general (with nonorthogonal curvilinear coordinates or in the presence of mutual inductance coefficients), the quadratic form of K may not be diagonal. In such a case, it can be put in the form in (1.1); as a result, U will also be altered. Since U is taken in the form of a quadratic form of a general type, however, this transformation of it is not important.

[4] Throughout this paper, the summation sign is always written out explicitly, since the summation index appears more than two times in many places [e.g., in (5c.1)]. Consequently, the repetition of an index in an equation [as on the right side of (5a.1)] does not imply a summation.

[5] It should be kept in mind that the quantity $\varkappa_{ii}/m_i$ is the square of the so-called partial frequency of oscillator i, i.e., the square of its frequency when the other oscillators of the system are fixed at their equilibrium positions. The square of the *eigenfrequency* of oscillator i is given by the expression $\Omega_i^2 = \sum_{j=1}^{n} (\varkappa_{ij}/m_i)$. Consequently, in order to find Ω_1^2 with the help of (14.1), for example, we need to know all the functions $G_{1j}(t)$.

[6] We might also deal with the more general case $q(0) \neq 0$. In that case, however, the mean values of the coordinates of all the oscillators of the reservoir would also be nonzero, since the coupling of the oscillators means that a deflection of a macroscopic oscillator causes displacements of the other oscillators also. To avoid complicating the calculations, we will restrict the discussion to the case $q(0) = 0$.

[7] The orthogonal matrix S_{iv} can be specified by the following procedure: Its first row, $\mathbf{S}_1 = (S_{11}, S_{12}, ..., S_{1n})$, is an arbitrary unit vector. Its second row is an arbitrary unit vector $\mathbf{S}_2$ which is orthogonal to $\mathbf{S}_1$, etc. Its last row is determined unambiguously by all the preceeding rows, as the unit vector which is orthogonal with respect to $\mathbf{S}_1, ..., \mathbf{S}_{n-1}$. Consequently, the first row and thus the numbers A_v can be specified *arbitrarily*.

[8] According to the estimate in Ref. 7, the duration of the Poincaré cycle for one mode of neon at room temperature and atmospheric pressure is of the order of $\exp(10^{25})$ s, while the lifetime of the universe is "only" of the order of $\exp(40)$ s.

[9] This type of interaction between an oscillator which we have singled out

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and oscillators of a reservoir (in the limit $n \to \infty$) occurs in the following mechanical model: A semi-infinite stretched string is attached to oscillator No. 1 in the direction perpendicular to its displacements.[33] The quantum-mechanical problem corresponding to this model was solved in Ref. 34.

[10]In this case, of course, Eq. (5.2) will no longer hold.

[11]Equation (10.2) is formally equivalent to the system of equations of motion for two interacting oscillators, one having a negative mass and a negative potential energy.

[12]Here, in contrast with the discussion above, K is the number of normal oscillations of approximately the same frequency which have been combined into a single group.

[13]To simplify the arguments here, it is convenient to choose the averaging time T_0 equal to the length of the Poincaré cycle, although this choice is not mandatory.

[14]The Green's function $G(t)$ which enters the FDT doubles as the response of a system to an instantaneous initial momentum (a shock) and the response function for a continuously acting external force. Accordingly, in the formulation of an FDT it is not at all necessary, although this is usually done, to add an additional term $-F\hat{q}$ to the initial Hamiltonian $\hat{H}$. All that is required in order to introduce this term is to excite oscillations in a system which has previously been in its equilibrium position. However, the same could be done with the help of appropriately chosen initial conditions. The FDT therefore applies not only to a system with a Hamiltonian $\hat{H} - F\hat{q}$ but also to a system with a Hamiltonian $\hat{H}$.

[15]The spectral density g_γ (ω) is defined here in such a way that the mean square value of the fluctuating emf is equal to an integral over positive frequencies:

$$\overline{\mathscr{E}^2} = \int_0^\infty g_{\mathscr{E}} (\omega) \, d\omega.$$

The same comment applies to the spectral charge density g_q (ω) and the spectral current density g_I (ω).

[16]In the three examples considered here, it turns out that the Weyl symbol of the operator is found from the operator itself through the substitutions $\hat{\pi}_\gamma \to \pi_\gamma$, $\hat{x}_\gamma \to x_\gamma$. In general, on the other hand, this is not the case. For example we have

$$\hat{x} \, \hat{\pi}^2 \hat{x} \to x^2 \pi^2 + \frac{\hbar^2}{2}.$$

[17]Nyquist's paper[29] dealt for the most part with a justification of classical formula (21.3). Nyquist concluded his paper by pointing out that he had made use of an equipartition law, which stated that the total energy per degree of freedom is kT. He wrote that if we instead take the energy per degree of freedom to be

$$h\nu \, (e^{h\nu/kT} - 1)^{-1},$$

where h is Planck's constant (Nyquist did not include the energy of zero-point oscillations here), the expression for the emf in the frequency interval $d\nu$ would become

$$E_\nu^2 \, d\nu = 4R_\nu h\nu \, d\nu \, (e^{h\nu/kT} - 1)^{-1}.$$

Nyquist wrote that in an interval of frequencies and temperatures in which the experimental data are valid (he was thinking of the paper by Johnson, which was printed just before Nyquist's own paper), this expression is indistinguishable from that derived on the basis of energy equipartition.

[18]When (26.4) is used, the quantity g_γ (ω) in the corresponding Nyquist relation would depend not only on R but also on the values of the reactive parameters L and C, which determine ω_0. In other words, the noise emf would depend not only on the properties of the noisy element of the circuit but also on precisely to what it was connected.

[19]The divergences which stem from the use of the quantum-mechanical Nyquist relation are consequences of the zero-point oscillations, which are not detected in measurements. For this reason, the divergences are eliminated after the quantity $\hbar\omega/2$ is subtracted from $\theta(\omega,T)$.

[20]As can be seen easily by substituting (31.4) into (7a.3).

[21]As we know, under actual conditions both Ohm's law and the Nyquist relation hold very well. This circumstance means that exponential damping is not only an exact solution in some extremely particular model (as in the present paper) but also a good approximation in a far more general formulation of the problem. Since we have not considered approximate solutions here, the question of the reason for such a broad applicability of the Nyquist relation remains outside the scope of this paper.

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