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AN EXACTLY SOLVABLE MODEL FOR BROWNIAN MOTION

IV. SUSCEPTIBILITY AND NYQUIST'S THEOREM

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Synopsis

By means of an exactly solvable model, treated in a previous paper[1]), the relation between the microscopic and macroscopic susceptibility is discussed. Furthermore, the limits of the validity of Nyquist's theorem are given.

1. *Introduction.* In this paper we extend the system of linearly coupled oscillators, considered in previous papers[1]) (quoted hereafter as I, II and III) with an external force which acts on the central oscillator or the heavy mass. In sect. 2 the susceptibility of the central oscillator is calculated. It turns out that this can be expressed in terms of the secular function $G(z)$. Furthermore, the condition is found for which the macroscopic and microscopic susceptibilities are equal. In sect. 3 a short discussion is given of the susceptibilities of the elastically bound electron in the electromagnetic radiation field (cf. sect. I.6) and the heavy mass in the linear chain (cf. III). In sect. 4 the Nyquist theorem is derived without applying perturbation theory. The same assumptions must be made as with the derivation of the Langevin equation and Fokker-Planck equation in I and II. Furthermore, the results are compared with the criticism of MacDonald[2]) on the extension of the theorem to the quantummechanical case.

2. *Susceptibility.* The case will be considered where the central oscillator moves in an external field $\mathfrak{F}(t)$. Then the Hamiltonian (I.1) is completed with a term $-Q\mathfrak{F}(t)$ to

$$H = \tfrac{1}{2}(P^2 + \Omega_0^2 Q^2) + \sum_n \tfrac{1}{2}(p_n^2 + \omega_n^2 q_n^2) + \sum \varepsilon_n q_n Q - Q\mathfrak{F}(t). \tag{1}$$

Again the quadratic part is transformed to the diagonal form by means of the transformation (I.6). One obtains

$$H = \sum_\nu \tfrac{1}{2}(p_\nu^2 + s_\nu^2 q_\nu^2 - X_{0\nu} q_\nu \mathfrak{F}(t)). \tag{2}$$

This leads to the inhomogeneous equations of motion

$$\ddot{q}_\nu + s_\nu^2 q_\nu = X_{0\nu}\mathfrak{F}(t). \tag{3}$$

$\mathfrak{F}(t)$ is written as a Fourier transform,

$$\mathfrak{F}(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(\omega)\, e^{i\omega t}\, d\omega. \tag{4}$$

Solving the equations of motion (3) and transforming back to the original variables P, Q, p_n and q_n one obtains

$$Q(t) = \dot{A}Q(0) + AP(0) + \sum_n \{\dot{A}_n q_n(0) + A_n p_n(0)\} +$$
$$+ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega f(\omega) \left\{ \sum_\nu \frac{X_{0\nu}^2}{\omega^2 - s_\nu^2} \cos s_\nu t + i\omega \sum_\nu \frac{X_{0\nu}^2}{\omega^2 - s_\nu^2} \frac{\sin s_\nu t}{s_\nu} \right\} -$$
$$- \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega\, e^{i\omega t} f(\omega) \sum_\nu \frac{X_{0\nu}^2}{\omega^2 - s_\nu^2}. \tag{5}$$

In order to find how to deal with the poles in the integrals we impose on the system the causality condition, i.e. the contribution of $\mathfrak{F}(t)$ to $Q(t)$ vanishes for $t < 0$ if $\mathfrak{F}(t)$ is zero for $t < 0$. Therefore we suppose $\mathfrak{F}(t) = 0$ for $t < 0$. This implies that $f(\omega)$ has a holomorphic continuation in the lower half plane. From the causality condition follows that the path of integration in eq. (5) passes below the points s_ν. Hence, we transform the path of integration to a line parallel to the real axis in the lower half plane at a distance ε. This is allowed due to the analytic properties of $f(\omega)$.

Waiting for a time $t = \Gamma^{-1}$ and averaging at $t = 0$ over the canonical ensemble of the small oscillators the first line of eq. (5) vanishes. There remains the effect of the external force $\mathfrak{F}(t)$. The coefficient of $f(\omega)$ in the first integral can be written by means of the theorem of Cauchy (cf. eq. (I.21)),

$$\sum_\nu \frac{X_{0\nu}^2}{\omega^2 - s_\nu^2} \cos s_\nu t + i\omega \sum_\nu \frac{X_{0\nu}^2}{\omega^2 - s_\nu^2} \frac{\sin s_\nu t}{s_\nu} =$$
$$= - \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left(\frac{1}{G_-(s^2)} - \frac{1}{G_+(s^2)} \right) \frac{e^{ist}}{s - \omega}\, ds, \tag{6}$$

where ω lies in the lower half plane. The integral can be calculated for $t > 0$ by contour integration in the upper half plane. Consequently the pole $s = \omega$ does not contribute. As is demonstrated in app. I.A the result consists of terms proportional to $\exp(-\Gamma t)$. Hence, for $t \gg \Gamma^{-1}$ these terms can be neglected and $Q(t)$ can be written as

$$Q(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty - i\varepsilon}^{+\infty - i\varepsilon} \mathrm{d}\omega \, \mathrm{e}^{i\omega t} f(\omega) \, \alpha(\omega), \tag{7}$$

where

$$\alpha(\omega) = -\sum_{\nu} \frac{X_{0\nu}^2}{\omega^2 - s_\nu^2} \tag{8}$$

is interpreted as the susceptibility. By means of Cauchy's theorem

$$\alpha(\omega) = -\frac{1}{2\pi i} \oint_C \frac{1}{\omega^2 - z} \frac{1}{G(z)} \mathrm{d}z, \tag{9}$$

where C encloses R_+, but not ω^2 in the z-plane. As the integrand tends rapidly to zero for $|z|$ going to infinity, the contour C can be extended to a contour C' as drawn in fig. 1,

$$\alpha(\omega) = \frac{1}{2\pi i} \oint_{C'} \frac{1}{z - \omega^2} \frac{1}{G(z)} \mathrm{d}z. \tag{10}$$

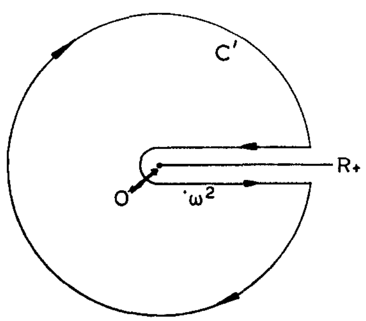

Fig. 1. Path of integration, C', for the calculation of $\alpha(\omega)$.

This yields

$$\alpha(\omega) = -G^{-1}(\omega^2). \tag{11}$$

Remembering that ω lies in the lower half plane of s one finds in the limit ε to zero the microscopic susceptibility (cf. eq. (I.28)),

$$\alpha_{\mathrm{mic}}(\omega) = \lim_{\varepsilon \to 0} \alpha(\omega) = -G_-^{-1}(\omega^2). \tag{12}$$

If again $\gamma(\omega)$ satisfies the Hölder condition one obtains

$$\alpha_{\text{mic}}(\omega) = \left(\Omega_0^2 - \omega^2 - P \int_0^\infty \frac{\gamma(s)}{s^2 - \omega^2}\, \mathrm{d}s + i\pi\, \frac{\gamma(\omega)}{2\omega}\right)^{-1}. \tag{13}$$

Knowing $\gamma(\omega)$ one can calculate $Q(t)$ exactly by means of the eqs. (7) and (13). However, in most cases one does not know $\gamma(\omega)$ but only the macroscopic equation,

$$\ddot{Q} + 2\Gamma\dot{Q} + \Omega_1^2 Q = F(t), \tag{14}$$

by which the motion of $Q(t)$ is governed. Therefore we will investigate under which conditions the macroscopic susceptibility, $\alpha_{\text{mac}}(\omega)$, corresponding to eq. (14) and defined by

$$Q(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \alpha_{\text{mac}}(\omega)\, f(\omega)\, \mathrm{e}^{i\omega t}\, \mathrm{d}\omega, \tag{15}$$

equals the microscopic susceptibility, $\alpha_{\text{mic}}(\omega)$.

Clearly,

$$\alpha_{\text{mac}}(\omega) = (\Omega_1^2 - \omega^2 + 2i\omega\Gamma)^{-1}. \tag{16}$$

Hence it follows that $\alpha_{\text{mac}}(\omega)$ equals $\alpha_{\text{mic}}(\omega)$ if

$$\Omega_1^2 = \Omega_0^2 - P \int_0^\infty \gamma(s)(s^2 - \omega^2)^{-1}\, \mathrm{d}s, \tag{17}$$

$$\Gamma = (\pi/4)\, \omega^{-2}\gamma(\omega). \tag{18}$$

In app. I.A it is shown that the terms on the right hand side are almost independent of ω if $\omega^{-2}\gamma(\omega)$ varies slowly in the region $\omega = \Omega_0$. Moreover, $\omega^{-2}\gamma(\omega)$ must tend rapidly enough to zero for $\omega > \omega_1 = \tau_t^{-1}$; hence, only forces may be considered which contain Fourier components with low frequencies, $\omega \ll \omega_1$.

3. *Examples.* Let us check these results for the system of an electron in an electromagnetic field. The strength function is given by eq. (I.49). For the susceptibility we find

$$\alpha_{\text{mic}}(\omega) = \left(\Omega_0^2 - \frac{\Omega_0^2\alpha^3}{\kappa_0(\alpha^2 + \omega^2)} - \omega^2 + i\, \frac{\Omega_0^2\alpha^2\omega}{\kappa_0(\alpha^2 + \omega^2)}\right)^{-1}. \tag{19}$$

If we assume $\Omega_0 \ll \alpha$, $\alpha \ll \kappa_0$, $\omega \ll \alpha$ then

$$\alpha_{\text{mic}}(\omega) = (\Omega_1^2 - \omega^2 + 2i\omega\Gamma)^{-1} = \alpha_{\text{mac}}(\omega), \tag{20}$$

with the known expressions for Ω_1 and Γ (cf. eq. (I.31)). Summarizing we conclude that in addition to the assumptions and conditions, needed for the derivation of the Langevin equation and Fokker-Planck equation, we must require that the external force contains only Fourier components with frequencies, low compared to the cutoff frequency ω_1.

In III we studied the motion of a heavy mass in a linear chain. For that system the Langevin equation reads

$$\ddot{q} + \mu\omega_0\dot{q} = M^{-1}F(t), \tag{21}$$

so that the macroscopic susceptibility is given by

$$\alpha_{\mathrm{mac}}(\omega) = -M^{-1}(\omega^2 - i\mu\omega\omega_0)^{-1}. \tag{22}$$

For the microscopic susceptibility one obtains

$$\alpha_{\mathrm{mic}}(\omega) = -M^{-1}G_{-}^{-1}(\omega) = -M^{-1}(\omega^2 - i\mu\omega\sqrt{\omega_0^2 - \omega^2})^{-1}, \tag{23}$$

from which immediately follows that $\alpha_{\mathrm{mac}}(\omega)$ equals $\alpha_{\mathrm{mic}}(\omega)$ if

$$\omega \ll \omega_0, \tag{24}$$

which condition is similar to $\omega \ll \omega_1$. In practice we have in actual substances $\omega_0 \simeq 10^{13}\,\mathrm{sec}^{-1}$. The highest ultrasonic frequency is about $10^9\,\mathrm{sec}^{-1}$, so that the condition (24) is reasonable.

4. *Nyquist's theorem*. The spontaneous voltage fluctuations between the terminals of a resistor are related to the resistance R by Nyquist's theorem[3]),

$$\langle\delta V_\omega^2\rangle = \frac{2}{\pi} RkT\,\mathrm{d}\omega. \tag{25}$$

Here $\langle\delta V_\omega^2\rangle$ is the mean square fluctuation of the voltage in the range $(\omega, \omega + \mathrm{d}\omega)$, T the temperature of the resistor. Furthermore, Nyquist proposed to replace kT by $\hbar\omega(\mathrm{e}^{\hbar\omega/kT} - 1)^{-1}$ if quantum effects are significant for the fluctuations ($\hbar\omega \gg kT$). Callen and Welton[4]) gave a quantummechanical derivation of the theorem using first order perturbation theory. It turned out that the zero-point energy had to be taken also into account, so that in eq. (25) kT must be replaced by $E(\omega, T) = (\hbar\omega/2)\coth(\hbar\omega/2kT)$.

In the present model the theorem can be discussed without relying on perturbation theory. In I the Langevin equation

$$\ddot{Q} + 2\Gamma\dot{Q} + \Omega_1^2 Q = F(t) \tag{26}$$

was derived. This equation is similar to the equation of motion of a charge q in an electric circuit with a resistance R, a selfinductance L and a capacity C,

$$L\ddot{q} + R\dot{q} + C^{-1}q = V(t). \tag{27}$$

Clearly, we can restrict ourselves to the discussion of $F(t)$, which is due to the interaction between the central oscillator and the thermal bath of small oscillators.

The impedance function $Z(\omega)$ of a system is defined by

$$Z(\omega)\,\dot{Q}(\omega) = f(\omega), \tag{28}$$

when $\dot{Q}_\omega$ and $f(\omega)$ are respectively the Fourier components of $\dot{Q}(t)$ and $F(t)$. Subsequently, $Z(\omega)$ can be expressed in terms of the susceptibility

$$Z(\omega) = -i\omega^{-1}\alpha^{-1}(\omega). \tag{29}$$

The resistance $R(\omega)$ is given by

$$R(\omega) = \operatorname{Re} Z(\omega) = \operatorname{Im}(\omega^{-1}\alpha^{-1}(\omega)). \tag{30}$$

In our model $R(\omega)$ becomes

$$R(\omega) = \frac{\pi}{2}\,\frac{\gamma(\omega)}{\omega^2}. \tag{31}$$

Due to the properties of $\gamma(\omega)$ this reduces for $\omega \ll \omega_1$ to

$$R(\omega) = 2\Gamma, \tag{32}$$

which just represents the macroscopic resistance.

The fluctuation spectrum F_ω^2 of $F(t)$ is related to the autocorrelation function by (cf. eq. (I.83))

$$\Phi_F(\tau) = \int_0^\infty F_\omega^2 \cos\omega\tau \,\mathrm{d}\omega, \qquad t \gg \omega^{-1}, \tag{33}$$

$$F_\omega^2 = \frac{2}{\pi}\,R(\omega)\,\frac{(\Omega_1^2-\omega^2)^2+4\Gamma^2\omega^2}{G_+(\omega)\,G_-(\omega)}\,E(\omega, T). \tag{34}$$

Under the same conditions as needed for the derivation of the Langevin equation in sect. I.11 and the Fokker-Planck equation in sect. II.4 eq. (34) reduces to

$$F_\omega^2 = \frac{2}{\pi}\,2\Gamma E(\omega, T) = \frac{2}{\pi}\,RE(\omega, T). \tag{35}$$

This represents Nyquist's theorem by which the microscopic quantity F_ω^2 is related to the macroscopic quantity, $R = 2\Gamma$. In the classical case $E(\omega, T)$ is replaced by kT.

Summarizing we conclude that in addition to the known conditions about $\gamma(\omega)$ we must require for the validity of Nyquist's theorem that only frequencies are considered which satisfy

$$\omega \ll \omega_1. \tag{36}$$

MacDonald[2]) raised objections against the quantummechanical version of Nyquist's theorem. His idea was that there exists a quantumstatistical time $\tau_q = \hbar/kT$, within which irreversible description in terms of a resistance or a friction, and a temperature T is inadequate. Following this reasoning he doubted the significance of Nyquist's theorem for frequencies $\omega \gtrsim kT/\hbar$ where the factor $E(\omega, T)$ begins to differ from kT.

Our result is (cf. sect. II.11) that calculation of the fluctuation of the displacement Q by means of the equation of motion, (26), and the fluctuation spectrum of $F(t)$, (35), indeed yields only correct results if times are considered for which $t \gg \hbar/kT$. However, we also showed that the quantum-statistical factor $E(\Omega_0, T)$ is meaningful if the condition $\hbar\Gamma \ll kT \ll \hbar\Omega_0$ is fulfilled. This condition shows that Nyquist's theorem is still valid for frequencies for which $E(\omega, T)$ differs from kT.

Furthermore, we want to remark that a white fluctuation spectrum of $F(t)$ is not possible. The first reason is that $\omega^{-2}\gamma(\omega)$ cannot be constant because of the condition (I.25), which is required to prevent self-accelerating solutions. Clearly, the second reason is that $E(\omega, T)$ varies with ω.

5. *Conclusion.* The macroscopic susceptibility equals the microscopic susceptibility if one makes the same assumptions and approximations needed for the derivation of the Langevin and Fokker-Planck equations. Moreover, the external force may only contain Fourier components with frequencies which are small compared to the inverse of the transient time, $\omega \ll \omega_1 = \tau_t^{-1}$.

Under the conditions mentioned above the Nyquist theorem holds. Without use of perturbation theory it is shown that extension to the quantum-mechanical case is valid, provided the quantumstatistical transient time is small compared to the relaxation time, $\hbar/kT \ll \Gamma^{-1}$.

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