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Fluctuation-dissipation theorems from the generalised Langevin equation

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Abstract. The generalised Langevin equation (GLE), originally developed in the context of Brownian motion, yields a convenient representation for the mobility (generalised susceptibility) in terms of a frequency-dependent friction (memory function). Kubo has shown how two deep consistency conditions, or fluctuation-dissipation theorems, follow from the GLE. The first relates the mobility to the velocity auto-correlation in equilibrium, as is also derivable from linear response theory. The second is a generalised Nyquist theorem, relating the memory function to the auto-correlation of the random force driving the velocity fluctuations. Certain subtle points in the proofs of these theorems have not been dealt with sufficiently carefully hitherto. We discuss the input information required to make the GLE description a complete one, and present concise, systematic proofs starting from the GLE. Care is taken to settle the points of ambiguity in the original version of these proofs. The causality condition imposed is clarified, and Felderhof's recent criticism of Kubo's derivation is commented upon. Finally, we demonstrate how the 'persistence' of equilibrium can be used to evaluate easily the equilibrium auto-correlation of the 'driven' variable (e.g., the velocity) from the transient solution of the corresponding stochastic equation.

Keywords. Generalised Langevin equation; fluctuation-dissipation theorem; Brownian motion; correlations; mobility.

1. Introduction and discussion

The generalised Langevin equation (GLE), originally developed in the context of Brownian motion, is an archetypal stochastic equation for the study of fluctuations and the approach to equilibrium in a variety of physical problems, ranging from superionic conductors to mechanical relaxation. Besides being consistent with linear response theory (LRT) for classical variables (see, e.g., Kubo 1966), the GLE yields a convenient representation for the generalised susceptibility concerned (e.g., the mobility in the case of Brownian motion). The effect of the environment or 'bath' on the system of interest is summarised in a memory function or kernel. This quantity may be estimated or modelled on the basis of physical considerations in a given situation. Considerable progress has been made in this direction, particularly in connection with the study of liquids, and a vast literature exists on the subject.

In a certain sense, the GLE is the most general linear stochastic equation possible (Mori 1965; Tokuyama and Mori 1976). Such an equation must satisfy a certain fundamental consistency condition which goes under the general name, 'fluctuation-dissipation (FD) theorem'. Kubo (1966) has shown explicitly how the FD theorem is obtained in the case of the GLE for the velocity of a classical Brownian particle. In what he terms the *first* FD theorem, the mobility is related to the velocity auto-correlation function *in equilibrium*, i.e., in the absence of an applied force. This is, of course, at the heart of LRT.* A corollary to the above relation, called the *second* FD theorem, is also obtained by Kubo. This is a generalisation of the familiar Nyquist theorem. It relates the memory function to the auto-correlation of the random force that is responsible for the fluctuations in the velocity of the Brownian particle.

Kubo's treatment is a exhaustive one, covering a number of other topics (e.g., LRT) as well, and the final forms obtained for the FD theorems are certainly correct. There are, however, a few points in the course of the derivations which need an improved treatment so as to exhibit the chain of reasoning clearly and to make the proofs logically consistent. The first such point is an explanation (based on physical grounds) of the need for, and mode of, constructing an effective non-stationary force $R(t;\, t_0)$ over and above the true stationary random force $L(t)$ originally introduced in the GLE. A closely related matter is the causality condition in terms of R; we shall comment further on this shortly. The second point occurs in the proof of the second FD theorem using the relation between the power spectra of the driving force L and the driven variable v, the velocity. We show how the proof may be carried to completion without lack of rigour by a simple argument based on the analyticity of certain quantities that occur. Finally, we consider the alternative derivation of the theorem directly from the GLE. In this route it is necessary at the last stage to establish, *independently*, the equality of the auto-correlation functions of L and R. By doing so, we take care of the lacuna in the original derivation. These are the modest objectives of the present paper, in which the final results arrived at (the FD theorems) are already known. Our aim is to present straightforward and logically consistent derivations of these directly from the GLE. In § 3 we make a brief but pertinent digression into the LRT version of the FD theorem for the mobility. Sections 4, 5 and 6 concerned with the actual derivation of the FD theorems from the GLE. Finally, in § 7, we draw attention (with examples) to a very simple method of obtaining the auto-correlation in equilibrium of the driven variable from the solution of a stochastic equation such as the GLE.

We are concerned here only with the FD theorems associated with the GLE. The conditional and joint probability distribution functions characterising the statistics of the velocity variable are not considered. Recently, in a very interesting paper, Fox (1977) has solved the latter problem for the case of a stationary Gaussian driving force $L(t)$: the velocity inherits the Gaussian property, and its auto-correlation function determines all its distribution functions. The FD theorem (in the form expressed by equation (28) below) is of course built into the GLE right from the start, in equation (2) of Fox.

Before turning to the derivations proper, it is instructive (for the sake of clarity) to identify the further input information needed to supplement the GLE and thereby to make such a stochastic model a complete one.

(i) The GLE is a *stochastic* equation. The statistical properties of the random or Langevin force $L(t)$ driving the velocity fluctuations must be specified. The basic assumption is that L is a stationary process with zero mean.

*A lucid account of the connection between response, relaxation and fluctuations may be found in Kubo (1973).

(ii) The solution $v(t)$ of the GLE, averaged over the statistics of L, still refers to an average over a sub-ensemble corresponding to a *given* initial condition $v(t_0)=v_0$. Complete averages must be found by a further integration over the single-variable or first probability distribution $P_1(v_0, t_0)$, as pointed out long ago by Uhlenbeck and Ornstein (1930). This distribution must be specified separately. We are generally concerned with an equilibrium situation. In particular, this means that $P_1(v_0, t_0)$ is a stationary, stable distribution $P_1(v_0)$. Equilibrium, or the damping out of spontaneous fluctuations (which is the principle underlying the FD concept), means that the conditional probability $P_2(v, t \mid v_0, t_0)$ approaches precisely the original stable distribution $P_1(v)$ as $(t-t_0)\to\infty$ (Doob 1942). As Fox (1977) puts it succinctly, 'the Maxwellian persists.'* It is this crucial property that relates the strength of the random force to the friction coefficient in the Langevin equation (a special case of (28)), or, equivalently, relates the coefficient of the gradient term $\partial(vP_2)/\partial v$ to that of the diffusion term $\partial^2P_2/\partial v^2$ in the standard Fokker-Planck equation for P_2. The powerful nature of this inner consistency criterion is illustrated in § 7, where we obtain the equilibrium auto-correlation almost effortlessly.

(iii) The velocity response we are interested in is the retarded response. In the language of LRT, the mobility $\mu(\omega)$ is the retarded generalised susceptibility $\chi_{vx}^{\mathrm{ret}}(\omega)$. The evaluation of this quantity naturally requires that the appropriate boundary condition be put in. In LRT (Kubo 1966), one may do so by choosing the appropriate solution of the Liouville equation for the density matrix. In the stochastic GLE model, one must explicitly put in a causality condition that mathematically expresses the physical statement: 'The velocity at time t_0 is uncorrelated with the driving force (to be properly chosen) at a later time (t_0+t)'. This is precisely what has been done by Kubo (1966). We have, in § 4, explained the reasoning behind the choice of the force $R(t_0+t; t_0)$ that is uncorrelated to $v(t_0)$. Recently, Felderhof (1978) has criticised Kubo's derivation of the FD theorem. According to him, the causality condition $\langle v(t_0)R(t_0+t; t_0)\rangle=0$ is really a *corollary* of the FD theorem, whereas in Kubo's method of derivation it is part of the *input* information. Felderhof establishes the FD theorem by appealing to the Nyquist theorem (actually, a generalised Onsager relation): to be specific, by *putting in* a certain analyticity property of the response of a 'passive linear system'. The vanishing of $\langle v(t_0)R(t_0+t; t_0)\rangle$ is then shown to follow as an incidental corollary. We do not feel that Felderhof's criticism is justified. After all, where does the crucial analyticity property referred to above come from, if not from (macro-) causality? As used in Felderhof, this property is a general one that obtains in LRT. If we use this information in the GLE, we are directly assuming that the GLE and LRT are compatible (which of course they are). But the whole point of using the GLE is to have an explicit, stochastic model for the study of fluctuations and related dynamics on a footing that is more or less *independent* of LRT. We should like to answer questions regarding correlations, the approach to stable

*The GLE (or even the LE) *can* be consistent with stable equilibrium distributions *other* than the Maxwellian (i.e., a Gaussian); see Doob (1942). We do not go into this technicality here. Nor are we concerned with the possibility that the asymptotic solution of a Fokker-Planck type equation for a Markov process may in some cases be different from a Gaussian. This issue has been beautifully clarified by Van Kampen (1977).

equilibrium distributions, the response to external stimuli, etc. without borrowing from the results of LRT as and when needed. True, the FD theorem (a generalised Onsager relation) is basic (as Felderhof states). Before using the GLE for *other* purposes, it is therefore necessary to check that it is compatible with the FD theorem. Deriving the FD theorem from the GLE is just a convenient, direct method of establishing this compatibility. And the causality condition is a piece of supplementary information needed for this purpose.* The last four sentences summarise, in our opinion, the motivation behind Kubo's derivation. Such a derivation should not be misconstrued as a claim that the causality condition is more basic than the FD theorem, as Felderhof has interpreted it, so that one proceeds to assume the latter to 'derive' the former as a corollary!

2. Generalised Langevin equation and the mobility

We consider a Brownian particle subjected to the action of an external force $F(t)$ that is switched on at $t=-\infty$. The GLE for the velocity of the particle is, in standard notation,

$$m\dot{v}(t)+m\int_{-\infty}^{t} dt'\,\gamma(t-t')\,v(t')=L(t)+F(t), \tag{1}$$

where $L(t)$ is the random force and $\gamma(t-t')$ is the memory function or kernel representing the friction due to the medium. The statistical properties of $L(t)$ are supposed to be independent of the applied force $F(t)$. In particular, it is assumed that $L(t)$ is a stationary random process, and $\langle L(t)\rangle=0$.

The (velocity) response of the particle is described by its frequency-dependent mobility $\mu(\omega)$, defined as follows. A 'monochromatic' force

$$F(t) = \mathrm{Re}\,[F_0 \exp(-i\omega t)] \tag{2}$$

is turned on at $t=-\infty$. At any finite value of t, the transient effects would have disappeared. The average velocity response is then given by

$$\langle v(t)\rangle = \mathrm{Re}\,[\mu(\omega)\, F_0 \exp(-i\omega t)]. \tag{3}$$

As already stated, the GLE provides a convenient representation for $\mu(\omega)$ in terms of the memory function: it follows from (1) that

$$m\,\mu(\omega) = [\bar{\gamma}(\omega) - i\omega]^{-1}, \tag{4}$$

where
$$\bar{\gamma}(\omega) = \int_{0}^{\infty} dt\, \gamma(t) \exp(i\omega t), \tag{5}$$

is the Fourier-Laplace transform** of the kernel $\gamma(t)$.

*The 'necessary and sufficient' nature of this condition in the case of the ordinary Langevin equation has already been discussed *with full mathematical rigour* by Doob (1942).

**If the integral in (5) does not exist, we mean by $\bar{\gamma}(\omega)$ the analytic continuation to $p=-i\omega$ of the Laplace transform of $\gamma(t)$. This goes for all Fourier-Laplace transforms in this paper.

3. The (first) fluctuation-dissipation theorem from response theory

The mobility $\mu(\omega)$ is of course just the generalised susceptibility $\chi_{vx}(\omega)$ in the sense of Kubo (1966), for the applied force $F(t)$ corresponds to a perturbation $-xF(t)$ added to the unperturbed Hamiltonian H_0 of the system. LRT for classical variables yields the expression

$$\mu(\omega) \equiv \chi_{vx}(\omega) = \beta \int_0^\infty dt \, \langle v(o)v(t)\rangle_{\text{eq}} \exp(i\omega t), \tag{6}$$

where $\beta = 1/k_B T$. $\langle v(o)\, v(t)\rangle_{\text{eq}}$ is the velocity auto-correlation in equilibrium, in the absence of $F(t)$. The velocity is a stationary random process in this situation. Equation (6) is the first FD theorem. (Strictly speaking, the term 'FD theorem' should be reserved for (10) below, relating the Fourier transforms of the 'symmetrised' and 'antisymmetrised' correlations.)

We may recapitulate briefly some further properties that are obtainable from LRT (Kubo 1966). It follows from the definition of the velocity that

$$\beta \langle v(t)\, v(t)\rangle_{\text{eq}} = \langle \{x(t), v(t)\}\rangle_{\text{eq}}, \tag{7}$$

where $\{,\}$ stands for the Poisson bracket. We thus have the equipartition theorem

$$\langle v^2\rangle_{\text{eq}} = k_B T/m. \tag{8}$$

Further, the stationarity of $v(t)$ in equilibrium implies the symmetry property for the response function

$$\langle v(0)\, v(t)\rangle_{\text{eq}} \equiv \phi_{vx}(t) = \phi_{vx}(-t). \tag{9}$$

This in turn means that the weight function in the spectral representation of the generalised susceptibility $\chi_{vx}(\omega)$ is equal to $(1/\pi)$ times the *real* part of $\chi_{vx}(\omega)$. The relation between the symmetrised correlation and the response function then reads (again in the classical limit)

$$\langle [x(t'), v(t)]_+\rangle_{\text{eq}} = (2/i\pi\beta) \int_{-\infty}^{\infty} d\omega\, \omega^{-1}\, \chi'_{vx}(\omega) \exp[-i\omega(t-t')], \tag{10}$$

where $[\,,]_+$ is the anti-commutator and χ' is the real part of χ. Differentiating both sides with respect to t' then setting $t'=t$, and using (4) and (8), we finally find that

$$\text{Re} \int_{-\infty}^{\infty} d\omega\, [\tilde{\gamma}(\omega) - i\omega]^{-1} = \pi. \tag{11}$$

This might appear to be a constraint on the memory function. However, it is merely a direct consequence of the analyticity of the generalised susceptibility. Equation

(11) is trivially verified in the case of the ordinary Langevin equation, which corresponds to a white noise assumption for $L(t)$—and hence also to the form

$$\gamma(t) = \gamma\delta(t), \quad \tilde{\gamma}(\omega) = \gamma \; (= \text{const.}), \tag{12}$$

for the kernel. It is not difficult to establish that (11) is true in general. Macro-causality says that the retarded susceptibility $\mu(\omega)$ is analytic in the upper half-plane. Therefore

$$\int_{-\infty}^{\infty} d\omega \; \mu(\omega) + \int_{\Gamma} d\omega \; \mu(\omega) = 0, \tag{13}$$

where Γ is a semicircle in the upper half plane with radius $\to \infty$. Now the memory function $\gamma(t)$ can at best be instantaneous, as in (12), so that $\tilde{\gamma}(\omega)$ must either tend to a constant as $\omega \to \infty$, or else vanish. Using this fact in the representation (4) for $\mu(\omega)$, the contribution from the integral over Γ is equal to $-\pi$. Equation (11) follows at once. We remark once again that the crucial ingredient in the above is causality in the macroscopic sense.

4. Direct proof of the FD theorem from the GLE

We wish to emphasise that, once the GLE is written down as a stochastic equation based on physical considerations (mentioned earlier), it is a self-contained microscopic model in a certain sense. There should be no further need to borrow results from LRT. We have already discussed the auxiliary input information required to supplement the GLE model, and argued that causality is a boundary condition that is no more *intrinsic* to one formalism than to another. We shall now show clearly how the FD theorem follows from the GLE.

Our aim is to compute the equilibrium auto-correlation function

$$\langle v(t_0) \, v(t_0 + t) \rangle_{\text{eq}},$$

where $t > 0$ and t_0 is some fiducial instant of time. In the absence of an applied force, the GLE at time $(t_0 + t)$ is

$$m\dot{v}(t_0 + t) + m \int_{t_0}^{t_0+t} dt' \, \gamma(t_0 + t - t') \, v(t') = L(t_0 + t) - m \int_{-\infty}^{t_0} dt' \cdot \gamma(t_0 + t - t') \, v(t') \equiv R(t_0 + t; t_0). \tag{14}$$

The purpose of splitting up the frictional force in the above manner (Kubo 1966) is as follows. The friction is merely the 'systematic' part of the *total* random, internal (medium-originated) force, and is in fact responsible for the correlation or memory effects. When causality is expressed by the statement that the velocity at time t_0 is uncorrelated to the force at subsequent instants of time, we must take care to ensure that this force *includes** the correct systematic component. We are concerned with the values of the relevant variable (here, velocity) from time t_0 onwards. The systematic part of the internal force on the Brownian particle at time t_0 is equal to

$$-m \int_{-\infty}^{t_0} dt' \, \gamma\,(t_0 - t')\, v\,(t'). \tag{15}$$

At time $(t_0 + t)$, the systematic part of the internal force that depends on the (velocity) history of the particle *upto* time t_0 is precisely the second term on the right in (14). For the purpose of evaluating the velocity auto-correlation (in which the earlier time label is t_0), we must thus define the effective force at time $(t_0 + t)$ as

$$R\,(t_0 + t;\, t_0) \equiv L\,(t_0 + t) - m \int_{-\infty}^{t_0} dt' \, \gamma\,(t_0 + t - t')\, v\,(t') \tag{16}$$

It is *this* force with which $v\,(t_0)$ is uncorrelated for $t > 0$. We have already said that there is nothing artificial or extraneous about this expression of causality: the physical requirement of causality has to be imposed just as axiomatically in any other formalism, no more or less.

Macrocausality in the GLE approach is thus expressed by the condition

$$\langle v(t_0)\, R\,(t_0 + t;\, t_0)\rangle_{\text{eq}} = 0 \;(t > 0). \tag{17}$$

This immediately shows that the truly random part $L(t)$ of the internal force *is* correlated with the velocity; after some manipulations using the stationarity property in equilibrium, this correlation may be written in the compact form

$$\langle v(t_0)\, L\,(t_0 + t)\rangle_{\text{eq}} = m \int_0^{\infty} d\tau \; \gamma(t + \tau) \langle v(0) v(\tau)\rangle_{\text{eq}},\; (t > 0). \tag{18}$$

Returning to (14), we multiply both sides by $v\,(t_0)$ and take the equilibrium ensemble average. The right hand side vanishes because of (17). Multiply by $\exp\,(i\omega t)$ and integrate over t from 0 to ∞. Using the stationarity property of the velocity in equilibrium, we obtain after some algebra

$$\int_0^{\infty} dt\, \langle v(t_0)\, v\,(t_0 + t)\rangle_{\text{eq}} \exp\,(i\omega t) = \frac{\langle v^2(t_0)\rangle_{\text{eq}}}{\bar{\gamma}(\omega) - i\omega}, \tag{19}$$

where $\bar{\gamma}\,(\omega)$ is the Fourier-Laplace transform of $\gamma\,(t)$, already defined in (5). We now need a statement on the single variable equilibrium distribution $P_1\,(v)$ to supplement the GLE for the evolution of the velocity from a *given* initial value: namely, that $P_1\,(v)$ is a Maxwellian.** Then $\langle v^2(t_0)\rangle_{\text{eq}}$ is fixed by the equipartition theorem to be equal to $k_B T/m$, and (19) coincides with the LRT result, (6).

*The minus sign on the right in (14) is an *addition*, not a subtraction, of the friction component.

**Recall the remarks in § 1. We may add the following technical points. The *ordinary* Langevin equation for v is equivalent to a Fokker-Planck equation (for P_2) of the second type in the sense of Van Kampen (1977), and the asymptotic solution of the latter is a Gaussian (the Maxwell distribution). The GLE with a stationary Gaussian $L(t)$ leads to a Fokker-Planck-like equation for P_2 (Fox 1977) whose asymptotic solution is again a Gaussian.

5. The second FD theorem: proof using the power spectra

The second FD theorem is a generalisation of the very familiar Nyquist relation between the thermal noise voltage in a resistor and its resistance. The theorem connects the auto-correlation of the random force $L(t)$ to the memory function $\gamma(t)$. The proof involves certain subtleties that appear to have been overlooked in the literature. We shall therefore present a careful derivation of the theorem. In § 6, we have thought it worthwhile to present once again a rigorous version of an alternate proof; here, too, a certain crucial point appears to have been slurred over in previous work.

As before, we begin with the GLE in the absence of an external force:

$$m\,\dot{v}(t) + m \int_{-\infty}^{t} dt'\,\gamma(t-t')\,v(t') = L(t). \tag{20}$$

Fourier analysing $L(t)$ according to

$$L(t) = \int_{-\infty}^{\infty} d\omega\,\tilde{L}(\omega)\exp(-i\omega t), \tag{21}$$

and similarly $v(t)$ too, it is seen easily that the retarded form of the memory function in (20) leads directly to the solution

$$\tilde{v}(\omega) = \tilde{L}(\omega)/m\,[\tilde{\gamma}(\omega) - i\omega] \equiv \mu(\omega)\,\tilde{L}(\omega). \tag{22}$$

Given this, one can assert that the power spectra of v and L are related (Rice 1944, 1945; Wang and Uhlenbeck 1945) according to

$$\int_{-\infty}^{\infty} dt\,\langle v(0)\,v(t)\rangle_{\text{eq}}\exp(i\omega t) = |\mu(\omega)|^2 \int_{-\infty}^{\infty} dt\langle L(0)L(t)\rangle_{\text{eq}}\exp(i\omega t). \tag{23}$$

Equation (23) is best proved by direct substitution of (22) in the left hand side, after writing each velocity variable in terms of its Fourier transform $\tilde{v}(\omega)$. When simplification is carried out, one obtains the factor $\mu(\omega)\,\mu(-\omega)$ in the penultimate step. At this stage, one invokes the first FD theorem, already established, and observes that $\mu(\omega)$ is the one-sided Fourier transform of a real function of t (namely, the equilibrium auto-correlation of the velocity). Hence $\mu^*(\omega) = \mu(-\omega)$ for real ω, and (23) is obtained.*

Now $\langle v(0)\,v(t)\rangle_{\text{eq}}$ is an even function of t (stationarity; commuting variables), so that

$$\begin{aligned}\int_{-\infty}^{\infty} dt\,\langle L(0)\,L(t)\rangle_{\text{eq}}\exp(i\omega t) &= 2\,\text{Re}\int_{0}^{\infty} dt\,\langle v(0)\,v(t)\rangle_{\text{eq}}\exp(i\omega t)\\ &= (2/\beta)\,\text{Re}\,\mu(\omega),\end{aligned} \tag{24}$$

*This is of course a special case of the symmetry property $\chi^*_{AB}(\omega^*) = \chi_{AB}(-\omega)$ provable in LRT for a generalised susceptibility.

where the final step follows from the first FD theorem. Therefore (23) becomes

$$\int_{-\infty}^{\infty} dt \, \langle L(0)\, L(t) \rangle_{\text{eq}} \exp(i\omega t) = (2/\beta) \operatorname{Re} [1/\mu(\omega)]$$

$$= (2m/\beta) \operatorname{Re} \bar{\gamma}(\omega). \tag{25}$$

Using the symmetry of the correlation function of L, we get

$$\operatorname{Re} \int_{0}^{\infty} dt \, \langle L(0)\, L(t) \rangle_{\text{eq}} \exp(i\omega t) = (m/\beta) \operatorname{Re} \bar{\gamma}(\omega). \tag{26}$$

Here is where we have to be careful. We cannot naively delete ' Re ' on both sides of (26) without a further observation. Now $\bar{\gamma}(\omega)$ is the Fourier-Laplace transform of a real function $\gamma(t)$, and it is evident from the very representation (5) that it is analytic in the upper half-plane in ω, in addition to the real axis (the latter following from the presumed existence of the integral in (5) as it stands). Exactly the same remarks apply to the integral on the left hand side in (26). Since the real parts of the two analytic functions concerned are equal, so are their imaginary parts, and hence the functions themselves.* Thus

$$m\,\bar{\gamma}(\omega)\, k_B T = \int_{0}^{\infty} dt \, \langle L(0)\, L(t) \rangle_{\text{eq}} \exp(i\omega t). \tag{27}$$

This is the second FD theorem. In the case of the ordinary LE the left-hand side reduces to $m\gamma k_B T$, and the random force *must* be δ-correlated for consistency. The usual relation between its ' strength ' and the friction constant γ is thus recovered.

We note in passing that for $\omega = ip$ (p real), (27) becomes a relation between Laplace transforms. As these have unique inversions, it follows that

$$m\,\gamma(t)\, k_B T = \langle L(0)\, L(t) \rangle_{\text{eq}}, \tag{28}$$

almost everywhere in $0 \leqslant t < \infty$ (the region in which the memory function is defined.)

6. Alternate proof directly from the GLE

The theorem embodied in (27) may also be derived from the GLE in a manner similar to that of § 4 for the first FD theorem, as follows. This route is a bit more involved, though, and one must proceed in two main steps. We first establish the theorem for the random force R, and then demonstrate its equivalence with (27) which involves the ' true ' random force L.

*The possibility of the two functions of ω differing by a pure imaginary constant is precluded, because when ω is on the positive imaginary axis (which is within the region of analyticity), both functions must be real and equal to each other.

Writing down the GLE (again in the absence of an applied force) at time t_0, we have

$$m\,\dot{v}(t_0) = R(t_0;\, t_0). \tag{29}$$

Here
$$R(t_0;\, t_0) = L(t_0) - m \int_{-\infty}^{t_0} dt'\, \gamma(t_0 - t')\, v(t'), \tag{30}$$

as in the definition of R given in (16). Multiplying both sides by $R(t_0+t;\, t_0)$,

$$m\dot{v}(t_0)R(t_0+t;\, t_0) = R(t_0;\, t_0)R(t_0+t;\, t_0)\ (t>0). \tag{31}$$

On the left hand side, we substitute for $R(t_0+t;\, t_0)$ from the GLE at time (t_0+t) (namely, (14)), and average over the equilibrium ensemble. Multiply both sides by $\exp(i\omega t)$, and integrate over t from 0 to ∞, as before. Simplification of the left-hand side is carried out using the properties

$$\langle \dot{v}(t_0)v(t_0+t)\rangle_{eq} = -\langle v(t_0)\dot{v}(t_0+t)\rangle_{eq}, \tag{32}$$

and
$$\langle \dot{v}(t_0)v(t_0)\rangle_{eq} = 0, \tag{33}$$

which follow from stationarity. After some algebra (Balakrishnan 1976), we finally arrive at

$$\int_0^\infty dt \langle R(t_0;\, t_0)R(t_0+t;\, t_0)\rangle_{eq} \exp(i\omega t) = m^2 [\tilde{\gamma}(\omega) - i\omega]\, .$$
$$\cdot \Big[\langle v^2(t_0)\rangle_{eq} + i\omega \int_0^\infty dt\, \langle v(t_0)v(t_0+t)\rangle_{eq} \exp(i\omega t)\Big]. \tag{34}$$

The integral on the right, however, has already been evaluated, in (19), while establishing the first FD theorem. Putting this in and using also the equipartition theorem for $\langle v^2\rangle_{eq}$, we get

$$m\tilde{\gamma}(\omega)k_B T = \int_0^\infty dt \langle R(t_0;\, t_0)R(t_0+t;\, t_0)\rangle_{eq} \exp(i\omega t). \tag{35}$$

As already pointed out in Kubo (1966), $R(t_1;\, t_0)$ is *not* a stationary random variable (in contrast to $L(t_1)$), because of the dependence on the fiducial instant of time t_0. However, it can be shown that

$$\langle R(t_0;\, t_0)R(t_0+t;\, t_0)\rangle_{eq} = \langle L(t_0)L(t_0+t)\rangle_{eq}, \tag{36}$$

as we shall demonstrate. It is clearly necessary to do so in order to complete the proof of the theorem. In Kubo (1966), on the other hand, one encounters a circular argument at this stage: it is argued that (36) is true because (27) and (35) hold good, and that, putting this back in (27), one obtains (35)!

Equation (36) is proved as follows. The definition of R yields

$$\langle R(t_0;\, t_0)R(t_0+t;\, t_0)\rangle_{\text{eq}} = \langle L(t_0)L\,(t_0+t)\rangle_{\text{eq}} + m^2 \int\limits_{-\infty}^{t_0} dt_1 \int\limits_{-\infty}^{t_0} dt_2 \cdot$$

$$\cdot \gamma(t_0-t_1)\gamma\,(t_0+t-t_2)\,\langle v(t_1)v(t_2)\rangle_{\text{eq}}$$

$$-m \int\limits_{-\infty}^{t_0} dt_1\, \gamma(t_0-t_1)\,\langle v(t_1)\, L(t_0+t)\rangle_{\text{eq}}$$

$$-m \int\limits_{-\infty}^{t_0} dt_1\, \gamma(t_0+t-t_1)\,\langle v(t_1)\, L(t_0)\rangle_{\text{eq}}. \tag{37}$$

But the causality condition (17) has already shown that v and L are correlated as in (18). The original form of this relation follows at once from (17), and is

$$\langle v(t_0)\, L(t_0+t)\rangle_{\text{eq}} = m \int\limits_{-\infty}^{t_0} dt'\, \gamma(t_0+t-t')\,\langle v(t_0)\, v(t')\rangle_{\text{eq}},\ (t>0). \tag{38}$$

This result (*with appropriately altered variables*) is applied to the last two terms on the right hand side in (37). These terms then add up to

$$-m^2 \int\limits_{-\infty}^{t_0} dt_1 \int\limits_{-\infty}^{t_0} dt_2\, \langle v\,(t_1)\, v\,(t_2)\rangle_{\text{eq}}\, [\gamma\,(t_0-t_1)\,\gamma\,(t_0+t-t_2)$$

$$+\gamma(t_0+t-t_1)\,\gamma(t_0-t_2)]. \tag{39}$$

With the re-labelling $t_1 \longleftrightarrow t_2$ in the second part of this expression, the above cancels exactly against the second term on the right in (37). The identity(36) is thus proved. Equation (35) then reduces to

$$m\bar{\gamma}(\omega)k_B T = \int\limits_0^{\infty} dt\, \langle L(t_0)L(t_0+t)\rangle_{\text{eq}}\, \exp\,(i\omega t), \tag{40}$$

in terms of the true random force $L(t)$. This coincides with (27), the second FD theorem.

7. Equilibrium autocorrelations from stochastic equations

In this final section, we should like to draw attention to a very simple property of consistent stochastic equations that enables the equilibrium autocorrelation of the ‘ output ’ or driven variable to be obtained practically without effort.

The method is just this. The solution to a stochastic equation such as the GLE has two terms. The first involves the initial condition, while the second is the particular integral involving the random force $L(t)$. For instance, (20) has the solution

$$v(t) = mv(o)\mu(t) + \int_0^t dt'\mu(t-t')L(t'), \tag{41}$$

where $\mu(t)$ is the inverse (Fourier-Laplace) transform of the quantity $\mu(\omega)$ defined in (4), and $v(0)$ is the (given) initial value of the velocity. To find the autocorrelation in equilibrium, one must write down the expressions for $v(t_0)$ and $v(t_0+t)$, multiply the two, take averages over the distribution of the force L (in which process the terms linear in L vanish, because L has zero mean); and then average over the distribution $P_1(v(0))$ of the initial velocity—or else, equivalently, simply let $t_0 \to \infty$. In the latter case, only the autocorrelation of L survives. This must be put in, the second FD theorem for its normalisation must be incorporated, and finally the result for the velocity autocorrelation emerges. Our observation is that as long as we *know* that the equation is consistent with the FD theorem, this lengthy process can be short-circuited—because much of it is a redundant verification all over again of the FD theorem! In (41), let us directly average over the random force (i.e., over a sub-ensemble corresponding to the given initial condition $v(0)$). The second term vanishes because L has zero mean. Denoting this partial average by an overhead bar, we have, on multiplying both sides by $v(0)$,

$$v(0)\,\overline{v(t)} \equiv \overline{v(0)v(t)} = mv^2(0)\mu\,(t). \tag{42}$$

The autocorrelation *in equilibrium* is now obtained by averaging over all values of $v(0)$ with the help of the stationary distribution $P_1 v(0)$. For a Maxwellian, the equi-partition theorem $\langle v^2(0)\rangle_{eq} = k_B T/m$ directly yields

$$\langle v(t_0)v(t_0+t)\rangle_{eq} = \langle v(0)v(t)\rangle_{eq} = m\langle v^2(0)\rangle_{eq}\,\mu(t) = k_B T\mu(t), \tag{43}$$

without further ado*. It is to be noted that we have obviated the need for an elaborate calculation; in the case of the GLE, for instance, one must expend much labour in proving that

$$\int_0^{t_2} dt'_2 \int_0^{t_1} dt'_1\, \mu(t_2-t'_2)\mu(t_1-t'_1)\,\overline{L(t'_1)L(t'_2)}$$

$$= k_B T\,[\mu(t_2-t_1) - \mu(t_1)\mu(t_2)], \tag{44}$$

for $t_2 \geqslant t_1$, which Fox (1977) has done. Similar comments apply to the ordinary Langevin equation

$$m\dot{v}(t) + m\gamma v(t) = L(t), \tag{45}$$

*This is, of course, the idea underlying Mori's equation for the correlation function.

where γ is a constant (and L of course has different statistical properties than in the case of the GLE); as also to the stochastic equation

$$m\dot{v}(t)+m\gamma(t)v(t)=L(t), \tag{46}$$

that describes a non-stationary, Gaussian, Markov process (Fox 1977). In each case, the *transient* (i.e., the solution of the homogeneous equation) that is given by

$$v(t)=v(0)\exp(-\gamma t) \tag{47}$$

in the case of (45), or by

$$v(t)=v(0)\exp\left[-\int_0^t dt'\ \gamma(t')\right] \tag{48}$$

in the case of (46), is sufficient to deduce the velocity autocorrelation in equilibrium (This quantity is dependent on *both* time arguments in the second instance.) Ultimately, this is because the systematic part of the random force embodied in the friction term has already been tailored to be consistent with the FD theorem. (This is what we meant by a ' consistent ' stochastic equation.) As a final, striking illustration of the point, let us consider the (ordinary) Langevin equation for an oscillator (Uhlenbeck and Ornstein 1930; Chandrasekhar 1943),

$$m\ddot{x}(t)+m\gamma\dot{x}(t)+m\omega^2x(t)=L(t), \tag{49}$$

where the random force must be stationary, Gaussian and δ- correlated according to

$$\langle L(t_0)L(t_0+t)\rangle = 2m\gamma k_BT\,\delta(t), \tag{50}$$

exactly as for the Langevin equation (45). The solution of (49) corresponding to the initial conditions $x=x_0$ and $v=v_0$ at $t=0$ is given by

$$x(t)=\left[\frac{(\gamma x_0+2v_0)}{2\omega_1}\sin\omega_1t+x_0\cos\omega_1t+\frac{1}{m\omega_1}\int_0^t dt'L(t')\right.$$

$$\left.\cdot\sin\omega_1(t-t')\exp(\gamma t'/2)\right]\exp(-\gamma t/2), \tag{51}$$

and $$v(t)=\left[-\frac{(2\omega^2x_0+\gamma v_0)}{2\omega_1}\sin\omega_1t+v_0\cos\omega_1t+\frac{1}{m\omega_1}\int_0^t dt'L(t')\left\{\omega_1\cos\omega_1(t-t')\right.\right.$$

$$\left.\left.-\tfrac{1}{2}\gamma\sin\omega_1(t-t')\right\}\exp(\gamma t'/2)\right]\exp(-\gamma t/2), \tag{52}$$

where $\omega_1^2=(\omega^2-\gamma^2/4)$ (underdamped case). It is evident that a brute force calculation of the velocity autocorrelation in equilibrium, using (50) for that of the force, is a tedious task in terms of the algebra involved. Our method, on the other hand, immediately yields

$$\langle v(0)v(t)\rangle_{\rm eq} = \Big[\langle v_0^2\rangle_{\rm eq}\cos\omega_1 t - \frac{1}{2\omega_1}(2\omega^2\langle x_0 v_0\rangle_{\rm eq} + \gamma\langle v_0^2\rangle_{\rm eq})\sin\omega_1 t\Big]\exp(-\gamma t/2). \tag{53}$$

The averages $\langle v_0^2\rangle_{\rm eq}$, etc. can themselves be determined from (51) and (52) once again, for instance, by using the property

$$\langle v_0^2\rangle_{\rm eq} = \lim_{t\to\infty} \overline{v^2(t)} \tag{54}$$

together with (50) for the autocorrelation of L. It is, however, simpler to use the equipartition theorem which yields

$$\langle v_0^2\rangle_{\rm eq} = k_B T/m,\ \langle x_0^2\rangle_{\rm eq} = k_B T/m\omega^2. \tag{55}$$

Further, $\langle x_0 v_0\rangle_{\rm eq}$ must vanish because of the stationarity that obtains in equilibrium. Hence

$$\langle v(0)v(t)\rangle_{\rm eq} = (k_B T/m)\left(\cos\omega_1 t - \frac{\gamma}{2\omega_1}\sin\omega_1 t\right)\exp(-\gamma t/2) \tag{56}$$

and similarly

$$\langle x(0)x(t)\rangle_{\rm eq} = (k_B T/m\omega^2)\left(\cos\omega_1 t + \frac{\gamma}{2\omega_1}\sin\omega_1 t\right)\exp(-\gamma t/2). \tag{57}$$

We have verified that the method works in more complicated cases as well. One such is a linear reactive-diffusive stochastic equation occurring in the study of fluctuations in chemical reactions (e.g., see Gardiner 1976; Grossmann 1976), that has recently been used also in the analysis of resistance fluctuations (Balakrishnan and Bansal 1978). The real power of the method, however, would seem to lie in the regime of non-linear stochastic equations. Once we are satisfied that such an equation is 'consistent' (in the sense explained above), it should be much easier to solve the *homogeneous* equation (or to find a satisfactory approximate solution) and to evaluate the equilibrium autocorrelation function using the stratagem described here with appropriate modifications. We shall report on some work in this direction elsewhere.

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