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Connection between deterministic and stochastic descriptions of nonlinear systems

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Abstract. Using the recent statistical mechanical theory for nonlinear irreversible processes of Grabert, Graham and Green, we re-examine the fluctuations in an electric circuit containing a nonlinear dissipative resistance. We explicitly establish the relationship between the nonlinear thermal fluctuations and the deterministic irreversible transport law. In particular, we verify their choice of the metric in frames where the macrovariables are sums of molecular variables. In a second part, we discuss the connection between the stochastic differential equation description and the deterministics. We show that neither the Ito-drift nor the Stratonovitch-drift coincides with the deterministic flow. By use of the example of driven Brownian motion with nonuniform damping we further demonstrate the usefulness of the nonlinear transport theory for the problem of adiabatic elimination in stochastic nonlinear equilibrium systems.

1. Introduction

At present the theory of thermal fluctuations in nonlinear systems is receiving a great deal of attention. In what follows, we will not study *steady* nonequilibrium states but rather the nonlinear relaxation of systems initially far from equilibrium. On a macroscopic level, the description of a dynamical process is either considered as stochastic or as deterministic, depending on the strength of the noise. If there is a clear-cut separation between the time-scale on which the macrovariables, a, change significantly and the time-scale of the microscopic memory characterized by the correlation time of external (relative to a) influences, the stochastic dynamics can be modeled by a Markov process. However, the deterministic and stochastic approaches are connected because they emerge from the common statistical mechanics of all microscopic degrees of freedom. For linear systems such a connection between deterministic theory of irreversible processes and stochastic theory of fluctuations has been clarified by Onsager [1–3]. A great deal of such a connection is presently also known for the class of nonlinear systems in which the dissipative part of the dynamics is given by a linear law [4–5]. The initial element of the stochastic theory for this latter class of nonlinear systems is the (linear) fluctuation-dissipation theorem (FDT) [4, 5]. For Markovian processes characterized by a Fokker–Planck equation, this relationship is given by an Einstein relation between the constant diffusion and the constant damping coefficient (Ginzburg-Landau approach) [4]. For nonlinear systems which *do* contain a nonlinear irreversible dynamic part, this connection between deterministic and stochastic formulation is much less obvious [6, 7]. The stochastic formulation of such nonlinear systems has been developed from the principles of statistical mechanics by Green [8]. He derived a generally nonlinear Fokker–Planck equation which for a single macrovariable a in the absence of a reversible drift component is of a form which intrinsically reflects detailed balance [8]

$$\dot{p}(at) = -\frac{\partial}{\partial a}\left\{\tfrac{1}{2}p_s^{-1}(a)\frac{\partial}{\partial a}(D(a)p_s(a))\right\}p(at) + \frac{1}{2}\frac{\partial^2}{\partial a^2}D(a)p(a,t). \tag{1}$$

Here p_s denotes the equilibrium probability. The main problem in irreversible thermodynamics is the identification of the kinetic coefficients like drift or diffusion in such equations. In general there are two approaches possible: the rigorous model-microscopic and a phenomenological approach. For obvious reasons, most workers in statistical mechanics do not choose the rather ambitious microscopic approach. On the phenomenological level, there have been put forward many different approaches [6, 7, 9–12] which generally lead to different results and consequently generate a lot of confusion. The problem is that in the presence of nonlinear fluctuations, the drift coefficient in (1) will contain nonlinear effects of the nonlinear noise, and it is not clear how the relationship between deterministic and stochastic evolution appears. For example, if one simply neglects the nonlinear diffusion, the corresponding (deterministic) drift approximation leads to different results in different coordinate systems.

II. A short summary of the theory in Refs. 13, 14

An attempt at solving this important problem, i.e., the question of the relationship between the deterministic and stochastic description of nonlinear systems has been put forward in two very recent publications [13, 14]. The deterministic equation is written as a generalization of Onsager's form as [13]

$$\dot{a} = L(a)\chi(a) = f(a) \tag{2}$$

which also has been shown to emerge from statistical mechanics [15]. Hereby, $L(a)$ is the (nonlinear) transport coefficient satisfying the generalized Einstein relation [13, 14]

$$D(a) = 2kTL(a), \qquad k\text{: Boltzmann constant} \tag{3}$$

$$\chi(a) = T\frac{\partial S(a)}{\partial a} = -\frac{\partial F(a)}{\partial a} \tag{4}$$

is the thermodynamic force driving the system towards equilibrium. S denotes the entropy of the equilibrium probability, whereas in this paper I prefer to work in terms of free energy $F = -TS$, which is connected with the equilibrium probability by

$$p_s(a) \propto g(a)^{-1/2}e^{-F(a)/kT}. \tag{5}$$

Thereby, $g(a)$ is the determinant of the metric in state space [13]. The connection between deterministic description ($k \to 0$) and the stochastic Fokker–Planck equation is then given in terms of the Fokker–Planck drift $v(a)$ [term in braces on right-hand side of (1)] by [13, 14]

$$v(a) = f(a) + kTg^{1/2}(a)\frac{\partial}{\partial a}(L(a)g^{-1/2}(a)). \tag{6}$$

The crucial point of this connection is of course given by the definition of the entropy S or equivalently of the metric g. In Ref. 13 the metric has been identified with the diffusion matrix. However, discussions with the advocates of these papers [13, 14] revealed that such a definition may lead to inconsistencies.[1]) A much more physical definition of the metric g has been put forward in Ref. 14.

III. Thermal fluctuations in a nonlinear electric circuit

The first purpose of this paper is to elucidate the theory of the authors of Refs. 13 and 14 by a simple example: We reconsider the old problem of the nonlinear Brownian motion, i.e., we consider an electric circuit consisting of a linear capacitance C in series with a nonlinear dissipative resistance which is in contact with a heat bath at temperature T [9]. The stochastic dynamics will be described in terms of the macroscopic charge fluctuations a on the capacitance. For the transport coefficient $L(a)$ we choose the symmetric conductance function of MacDonald [9]

$$L(a) = \frac{1}{R}(1 + \varepsilon a^2) \tag{7}$$

where R denotes the linear part of the resistance and the fixed and k-independent coefficient ε denotes the nonlinearity parameter. In terms of the voltage $U = a/C$, which constitutes the thermodynamic force $-\chi(a)$ for our problem, we can write

$$a = f(a) = -\frac{a}{RC}(1 + \varepsilon a^2). \tag{8}$$

By virtue of (4), we immediately read off the free energy of the equilibrium process

$$F = \frac{a^2}{2C} \tag{9}$$

which just represents the energy on the linear capacitance. The normalized equilibrium probability is given in terms of this energy by

$$p_s(a) = (2\pi kTC)^{-1/2} \exp - \frac{a^2}{2kTC} \tag{10}$$

which on the other hand determines via (5) the metric g to be a constant

$$g(a) = \text{const.} \tag{11}$$

[1]) For example, the definition for the metric g in Ref. 13 yields via (7) and (10) a very unphysical expression for the free energy and as a consequence an unphysical thermodynamic force $\chi(a) \neq -a/C$.

With (6), (8) and (11) we ultimately obtain for the Fokker–Planck drift $v(a)$ the result

$$v(a) = -\frac{a}{RC}(1+\varepsilon[a^2-2kTC]) \tag{12}$$

whereas the diffusion is from (1) consistently given by (see (3))

$$D(a) = \frac{2kT}{R}(1+\varepsilon a^2). \tag{13}$$

Several comments are now in order: The macroscopic charge a clearly gives a natural representation of the state of the system, i.e. the total charge a is just the algebraic sum of the microscopic charges on the capacitance. The metric for this choice of representation has been shown in (11) to be constant. This result is just in accordance with the physical definition given in Ref. 14 where the metric for a natural representation has been *defined* to be constant.

IV. Connection between stochastic differential equations and macroscopic flows

A better physical insight into the nonlinear Fokker–Planck equation is gained when we study the corresponding stochastic differential equation (SDE) or Langevin equation. With $b^2(a) = D(a)$, we obtain from (12) and (13) the Ito-SDE

$$da = -\frac{a}{RC}(1+\varepsilon[a^2-2kTC])\,dt + b(a)\,dw \tag{14}$$

where $w(t)$ denotes the standard Wiener process. Alternatively, the *equivalent* Stratanovitch-SDE is calculated to be

$$da = -\frac{a}{RC}(1+\varepsilon[a^2-kTC])\,dt + b(a)\,dw. \tag{15}$$

From (14) and (15), it is worth emphasizing the following: Neither the Ito-drift nor the Stratanovich-drift coincides with the deterministic evolution in (8). In particular, the fact that the Stratanovitch-drift does not equal the deterministic flow $f(a)$ is rather interesting and somewhat in contrast to the common opinion of many statistical physicists. Moreover, for kT approaching zero, both the Ito-drift as well as the Stratanovitch-drift reduce to the deterministic flow in (8). Thus, the common phenomenological concept of simply adding a random force to the deterministic equation and interpreting the resulting SDE, e.g. in the Stratanovitch sense, is subject to pitfalls. Independent of the underlying stochastic calculus, the corresponding drift terms will generally contain already k-dependent effects of the nonlinear fluctuations [see kT-dependent terms in (14), (15)].

Let us next consider the average of the current. From the Ito-SDE, (14), we ultimately find

$$\langle \dot{a} \rangle = -\frac{1}{RC}[\langle a \rangle + \varepsilon \langle a^2 \rangle] + \frac{2\varepsilon kT}{R}\langle a \rangle. \tag{16}$$

If the fluctuations are small in the sense that the variance $\sigma(t)$ of the process $a(t)$

remains very small compared with the nonlinearity scale σ_{nl}

$$\sigma(t) \ll \sigma_{nl} \sim \frac{df}{da} \Bigg| \frac{d^2f}{da^2} \tag{17}$$

i.e. if for *all times* t the probability $p(a, t)$ is very sharply peaked we can write as an approximation for equation (16) (neglect of, in virtue of equation (17), small effects of 2-nd, $\sigma(t)$, and higher order cumulants)

$$\langle \dot{a} \rangle \approx -\frac{\langle a \rangle}{RC}[1+\varepsilon\langle a \rangle^2] + \frac{2\varepsilon kT}{R}\langle a \rangle \tag{18}$$

Equation (18) has to be looked upon as a bare [16] 'phenomelogical law' valid only as an approximation to equation (16) when $\sigma(t) \ll \sigma_{nl}$ for all t. It is *not* the deterministic flow because any macrostate $a(t)$ within the margin set by the fluctuations would be equally acceptable. The correct way to obtain the deterministic description is by focussing on the parameter k which permits to scale down the fluctuations and studying the limit $k \to 0$ in which the fluctuations vanish. Also the result of this limiting scheme does not depend on the special choice of coordinate system [13, 14].

Also, it is obvious from the foregoing discussions that none of the drift expressions is proportional to the gradient of the free energy in (9) (invalidity of the Ginzburg–Landau hypothesis because of the nonconstant diffusion).

The nonlinear transport theory put forward in Refs. 13, 14 has very useful application to the problem of adiabatic elimination in nonlinear stochastic differential equations describing an equilibrium system. For example, let us focus on the problem of contracting the description of the Brownian motion in phase space into that of position space. In presence of a nonuniform friction $\gamma(x)$ this problem is not trivial [17]. The deterministic flow equations for a Brownian particle moving in a potential field $\phi(x)$ read in coordinate, x, and velocity, u, phase space (unit mass assumed)

$$\begin{aligned} \dot{x} &= u \\ \dot{u} &= -\gamma(x)u - \frac{\partial \phi(x)}{\partial x} \end{aligned} \tag{19}$$

In the large damping limit we can eliminate adiabatically the velocity yielding the *deterministic* contracted flow

$$\dot{x} = \frac{1}{\gamma(x)}\left(-\frac{\partial \phi(x)}{\partial x}\right) \tag{20}$$

From (20) we read off immediately the nonlinear transport coefficient $L = \gamma^{-1}(x)$ which via the generalized Einstein relation in (3) determines the diffusion coefficient $D(x)$ of the corresponding Fokker–Planck description

$$D(x) = 2kT/\gamma(x) \tag{21}$$

The Fokker–Planck or Ito-drift $v(x)$ is with the constant metric $g = \text{const.}$ readily evaluated via (6)

$$v(x)=\frac{-1}{\gamma(x)}\left[\frac{\partial\phi(x)}{\partial x}+\frac{kT\frac{\partial\gamma(x)}{\partial(x)}}{\gamma(x)}\right] \tag{22}$$

The results in (21) and (22) coincide with very recent independent studies [17, 18], which, however, utilize somewhat more complex methods. In particular, the use of nonlinear transport theory put forward in Refs. 13, 14 avoids the ambiguous stochastic calculus present in the adiabatic elimination from the stochastic differential equations. Again, neither the Ito-drift in (22) nor the corresponding Stratonovitch-drift coincide with the deterministic flow in (20).

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