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Starting with the Langevin equation for a nonlinear oscillator (the "Duffing oscillator") undergoing ordinary Brownian motion, we derive linear transport laws for the motion of the average position and velocity of the oscillator. The resulting linear equations are valid for only small deviations of average values from thermal equilibrium. They contain a renormalized oscillator frequency and a renormalized and non-Markovian friction coefficient, both depending on the nonlinear part of the original equation of motion. Numerical computations of the position correlation function and its spectral density are presented. The spectral density compares favorably with experimental results obtained by Morton using an analog computer method.

KEY WORDS: Brownian motion; nonlinear; oscillator; noise; transport.

# 1. INTRODUCTION

We investigate here an application of techniques of nonequilibrium statistical mechanics to a simple *nonlinear* system, the "Duffing oscillator." This is an anharmonic oscillator, with linear and cubic terms in the restoring force, undergoing ordinary Brownian motion as a result of interactions with a heat bath.

The purpose of the investigation is to find linear transport laws that describe the motion of the average position and velocity of the oscillator when deviations from thermal equilibrium are small but the effect of nonlinearity in the restoring force cannot be ignored. This is done by a variant of the projection operator method introduced by Zwanzig<sup>(1)</sup> in connection with the decay of correlation functions, and developed by Mori<sup>(2)</sup> in his theory of generalized Brownian motion.

245

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Mordechai Bixon and Robert Zwanzig

We believe that the results of this study illustrate two significant points in nonequilibrium statistical mechanics, the relation between linear transport laws and nonlinear microscopic equations of motion, and the role of nonlinearities in the "renormalization" of transport coefficients.

The first point was made in a somewhat different context by Van Kampen<sup>(3)</sup>:

"... linearity of the macroscopic law is not at all the same as linearity of the microscopic equations of motion. In most substances Ohm's law is valid up to a fairly strong field; but if one visualizes the motion of an individual electron and the effect of an external field E on it, it becomes clear that microscopic linearity is restricted to only extremely small field strengths. *Macroscopic linearity, therefore, is not due to microscopic linearity, but to a cancellation of nonlinear terms when averaging over all particles*. It follows that the nonlinear terms proportional to  $E^2$ ,  $E^3$ ,... in the macroscopic equation do not correspond respectively to the terms proportional to  $E^2$ ,  $E^3$ ,... in the microscopic equations, but rather constitute a net effect after averaging over all terms in the microscopic motion."

In our calculations, Van Kampen's average over all particles is replaced by an average over a Langevin fluctuating force, and nonlinear powers of the external field E are replaced by a nonlinear restoring force, but the essence of his point will be seen clearly in our results.

The other point illustrated here is the relation between transport coefficients in nonlinear transport equations and the corresponding coefficients in linear approximations to those equations. Consider, e.g., the flow of a fluid near its gas-liquid critical point. The equations of motion are the Navier–Stokes equation and the Fourier heat law, or more correctly, the Langevin form of these equations as introduced by Landau and Lifshitz<sup>(4)</sup>. These equations contain transport coefficients, the viscosity, and thermal conductivity, which are presumed to be nonsingular at the critical point; but they also contain important nonlinearities arising from dependence of local pressure and entropy on deviations from equilibrium. It appears that when the effects of nonlinearity are taken into account, e.g., by "mode–mode coupling,"<sup>(5)</sup> the resulting linearized transport laws contain *renormalized* transport coefficients which can be singular at the critical point. In our calculations, it will be seen that a Markovian transport coefficient in a nonlinear Langevin equation is replaced by a non-Markovian transport coefficient in the linear equation for the average motion.

Brownian motion of the Duffing oscillator may be described by either a Fokker– Planck equation or by a Langevin equation. The Fokker–Planck equation will be given later; the Langevin equation is

$$\ddot{x} = -(x + \beta x^3) - \alpha \dot{x} + \mathscr{F}(t) \tag{1}$$

The displacement of the oscillator at time t is x(t). (For convenience, the mass and linear spring constant are both set equal to unity.)

The fluctuating force  $\mathcal{F}(t)$  is a Gaussian random variable, with a zero mean value, and with a delta-function correlation

$$\langle \mathscr{F}(t) \mathscr{F}(t') \rangle = D\delta(t - t')$$
 (2)

The spectral density D is related to the friction coefficient  $\alpha$  by the fluctuationdissipation theorem

$$D = 2k_B T \alpha \tag{3}$$

where T is the temperature of the heat bath. (We may also set D equal to unity. This determines completely the mass, length, and time scales.)

While we do not make use of the fact here, it is worth noting that the above Langevin equation can be derived from a well-defined Hamiltonian system, in which the anharmonic oscillator interacts appropriately with a heat bath of suitably chosen harmonic oscillators. This was done by Ford *et al.*<sup>(6)</sup>

The Langevin equation determines the actual, i.e., microscopic, motion of the oscillator. In this article, we derive linear equations for the *average* motion,

$$\frac{d\langle x; t\rangle}{dt} = \langle v; t\rangle 
\frac{d\langle v; t\rangle}{dt} = -\Omega^2 \langle x; t\rangle - \alpha \langle v; t\rangle - \int_0^t ds \ K(s) \langle v; t - s\rangle$$
(4)

where  $\langle x; t \rangle$  is the average displacement at time t, and  $\langle v; t \rangle$  is the average velocity. In these equations,  $\Omega$  is an effective temperature-dependent frequency, and K(t) is an additional non-Markovian friction coefficient. We give explicit formulas for these quantities, together with some numerical results, later in this article. The only special condition required for the validity of this linear transport law is that the average displacement and velocity must be sufficiently small at some initial time.

An important property of the Duffing oscillator is the spectral density of its response to Gaussian noise. This has been measured by Morton,<sup>(7)</sup> using an analog computer, and some of his results were discussed by Morton and Corrsin.<sup>3</sup> We present numerical calculations of the spectral density, and compare them with Morton's results. In our calculations, we use a continued-fraction expansion of the spectral density, constructed so as to give exactly the first nine frequency moments of the spectral density.

# 2. DERIVATION OF THE LINEAR TRANSPORT EQUATIONS

The linear transport equations, giving the time dependence of the average displacement and velocity of the anharmonic oscillator, are derived in this section. First, we write down the Fokker–Planck equation for Brownian motion of the Duffing oscillator. Then, we introduce a projection operator that selects the part of the distribution function that is relevant to calculation of certain average values. We find a kinetic equation for this relevant part. Finally, we extract from this equation the desired linear transport equations.

As is well known, all the dynamical and statistical information that is contained in the Langevin equation (including the statistical specification of the fluctuating force)

<sup>&</sup>lt;sup>3</sup> Ref. 8a gives a description of Morton's experiments, but only limited results. Further details are presented in Ref. 8b.

#### Mordechai Bixon and Robert Zwanzig

is contained also in the Fokker-Planck equation. This is an equation of motion for the distribution function f(x, v; t) of oscillator displacements and velocities at time t. In the present case, this equation is

$$\frac{\partial f}{\partial t} = -v \frac{\partial f}{\partial x} - F(x) \frac{\partial f}{\partial v} + \alpha \frac{\partial (vf)}{\partial v} + \frac{1}{2} D \frac{\partial^2 f}{\partial v^2}$$

$$= \mathscr{D} f$$
(5)

The force on the oscillator is derived from a potential energy U(x),

$$U(x) = \frac{1}{2}x^2 + \frac{1}{4}\beta x^4, \qquad F = -\partial U/\partial x \tag{6}$$

For convenience, we denote the entire operator on the right-hand side of Eq. (5) by the symbol  $\mathcal{D}$ .

The equilibrium distribution function  $f_0$ ,

$$f_0 = Q_0^{-1} \exp\{-(2\alpha/D)[\frac{1}{2}v^2 + U(x)]\}$$
(7)

is a stationary solution of the Fokker-Planck equation. ( $Q_0$  is the normalization constant, or partition function.)

We are interested particularly in the evolution of the average displacement and velocity. This suggests that we may profitably introduce the projection operator P, defined by its effect on some arbitrary phase space function B(x, v),

$$PB = f_0 \iint dx \, dv \, B + (vf_0/\langle v^2 \rangle_0) \iint dx \, dv \, Bv + (xf_0/\langle x^2 \rangle_0) \iint dx \, dv \, Bx \quad (8)$$

Equilibrium averages denoted by  $\langle \rangle_0$  are taken with the distribution function  $f_0$ . The mean-squared velocity is

$$\langle v^2 \rangle_0 = k_B T = D/2\alpha \tag{9}$$

and the mean-squared displacement is used to define an effective frequency  $\Omega$ ,

$$\langle x^2 \rangle_0 = k_B T / \Omega^2 \tag{10}$$

It is easily verified that  $P^2 = P$ .

If we make the special choice B = f(x, v; t), then the projected part of the distribution function is "relevant" in the sense that it gives correctly the average values of x and v,

$$\iint dx \, dv \, xf = \iint dx \, dv \, xPf$$

$$\iint dx \, dv \, vf = \iint dx \, dv \, vPf$$
(11)

We denote these averages, taken with the distribution function at time t, by  $\langle x; t \rangle$  and  $\langle v; t \rangle$ . Then, the projected part of f may be written as

$$Pf = f_0[1 + (v\langle v; t \rangle / \langle v^2 \rangle_0) + (x\langle x; t \rangle / \langle x^2 \rangle_0)]$$
(12)

The rest of our discussion will be restricted to situations where the remaining "irrelevant" part of f vanishes at some initial time t = 0,

$$(1 - P)f(x, v; 0) = 0$$
(13)

Thus, the initial distribution function is assumed to have exactly the structure of the projected distribution function in Eq. (12).

It will be noticed that the projected distribution function Pf(x, v; t) can become negative for sufficiently large displacements or velocities. For the most part, this is not a reason for concern. For  $t \neq 0$ , Pf will be used only as an intermediary quantity for calculating the average x and v; and for these quantities, it gives precisely the correct values. It may not give correct values for other quantities, but that is of no interest here.

At the initial time, however, the potential negativity of Pf is of concern, because we assume that the *actual* distribution function has the structure of Eq. (12). Evidently, we must require that the initial average values are so small that Pf(x, v; 0) itself does not become negative for any physically interesting values of x and v. This is one reason why our results are restricted to small initial deviations of the averages from their equilibrium values.

Our assumption that the initial distribution function has the projected form can be justified by an argument due to Mori<sup>(2)</sup>. Suppose that at the initial time we know the average energy, the average displacement, and the average velocity. The most probable distribution function consistent with these constraints is the one that maximizes the entropy under these constraints. (Or we may insist that the initial ensemble is in thermal equilibrium, subject to these constraints.) Then, the initial distribution function is

$$f = Q^{-1} \exp[-(1/k_B T)(\frac{1}{2}v^2 + U) + av + bx]$$
(14)

where a and b are Lagrange multipliers associated with the constraints. The partition function Q depends on a and b. The initial averages are given by

$$\langle v \rangle = \partial(\log Q)/\partial a, \quad \langle x \rangle = \partial(\log Q)/\partial b$$
 (15)

By expanding the partition function in powers of a and b, and then solving for a and b in terms of the specified averages, we find

$$a = (1/\langle v^2 \rangle_0) \langle v \rangle + O(\langle v \rangle^2), \qquad b = (1/\langle x^2 \rangle_0) \langle x \rangle + O(\langle x \rangle^2) \tag{16}$$

When the average velocity and displacement are small, then so are the parameters a and b. If, finally, we expand the initial distribution function in powers of a and b, we obtain the general form that was assumed for the initial distribution. Again we see that the restriction of small average deviations from equilibrium has been imposed.

#### Mordechai Bixon and Robert Zwanzig

A kinetic equation for the projected part of the distribution function can be obtained by methods discussed, e.g., in Ref. (1). These methods are usually applied to the Liouville equation, but they can be applied just as well to the Fokker–Planck equation. The only change is to replace the Liouville operator by the Fokker–Planck operator  $\mathcal{D}$ . The result of the derivation is

$$\partial Pf(t)/\partial t = P \mathscr{D} Pf(t) - \int_0^t ds \, k(s) \, Pf(t-s) \tag{17}$$

where the kernel (operator) is

$$k(t) = -P\mathscr{D}(1-P) \cdot \left[\exp t(1-P)\mathscr{D}\right] \cdot (1-P)\mathscr{D}P.$$
(18)

Note that this equation does not contain an inhomogeneous term arising from the "irrelevant" part of the initial distribution function, because we have assumed that this vanishes.

The various contributions to the kinetic equation can be worked out without difficulty. For convenience, we introduce the notation

$$PB = f_0 B_0 + (v f_0 / \langle v^2 \rangle_0) B_v + (x f_0 / \langle x^2 \rangle_0) B_x$$
<sup>(19)</sup>

which focuses attention on the components  $B_0$ ,  $B_v$ , and  $B_x$ . Then, we find that

$$[P\mathscr{D}Pf(t)]_{0} = 0$$

$$[P\mathscr{D}Pf(t)]_{x} = \langle v; t \rangle$$

$$[P\mathscr{D}Pf(t)]_{v} = -\Omega^{2} \langle x; t \rangle - \alpha \langle v; t \rangle$$
(20)

The corresponding components of the memory term are

$$[k(s) Pf(t-s)]_{0} = 0$$

$$[k(s) Pf(t-s)]_{x} = 0$$

$$[k(s) Pf(t-s)]_{v} = \iint dx \, dv F(1-P)[\exp s(1-P) \mathcal{D}]$$

$$\times (1/\langle v^{2} \rangle_{0}) f_{0}(F + \Omega^{2}x) \langle v; t-s \rangle$$
(21)

All the information that is contained in the kinetic equation for Pf(t) is contained also in the equations of motion for the average values. These are

$$\partial \langle x; t \rangle / \partial t = \langle v; t \rangle$$
  
$$\partial \langle v; t \rangle / \partial t = -\Omega^2 \langle x; t \rangle - \alpha \langle v; t \rangle - \int_0^t ds \ K(s) \langle v; t - s \rangle$$
  
(22)

The memory kernel K(t) (now a function, and not an operator) is

$$K(t) = (1/\langle v^2 \rangle_0) \iint dx \, dv (F + \Omega^2 x) [\exp t(1 - P) \mathscr{D}] (F + \Omega^2 x) f_0$$
(23)

Langevin equation. In particular, the frequency  $\Omega$  and the kernel K(t) are functions of the nonlinearity parameter  $\beta$ . In the limit  $\beta \to 0$  corresponding to a linear system, the frequency  $\Omega$  approaches unity, and the kernel K vanishes.

Note that the final term in Eq. (22) involves a *non-Markovian* frictional behavior. If the range of the kernel, i.e., its "memory," were sufficiently short relative to the other characteristic time scales in this equation, then we could approximate K(t) by a delta function; this would convert Eq. (22) to a Markovian equation. We shall see later that under some circumstances this cannot be done. The transport law is intrinsically non-Markovian.

Equation (22) may be regarded as the average of an effective linear Langevin equation, having the same structure but with an additional fluctuating force. The mean value of the fluctuating force vanishes. Its correlation function, according to the fluctuation-dissipation theorem, consists of two terms; one its proportional to  $\alpha\delta(t)$ , and the other is proportional to K(t). Since the latter is not a delta function, the fluctuating force in this effective linear Langevin equation is not Markovian. Thus, the Markovian nonlinear Langevin equation is approximated by a non-Markovian linear Langevin equation.

# 3. CORRELATION FUNCTION AND SPECTRAL DENSITY

The methods that we have just discussed can be used also to calculate the displacement correlation function and its spectral density.

The displacement correlation function is defined by

$$C(t) = \langle x(0) | x(t) \rangle \tag{24}$$

The average is taken over the equilibrium phase space distribution function of the oscillator, and over the distribution of fluctuations due to interactions with the heat bath. The time dependence of x(t) is determined by the Langevin equation. If we average first over the randomly fluctuating force, then the stochastic Liouville operator associated with the Langevin equation of motion is replaced by the Fokker-Planck operator, and the correlation function is given by

$$C(t) = \iint dx \, dv \, x \cdot (\exp t\mathscr{D}) \cdot x f_0 \tag{25}$$

In this form, all explicit effects of the heat bath are eliminated.

It is evident that the correlation function may now be regarded as the average value of x at time t, computed with a distribution function that evolves from the initial value

$$f(x, v; 0) = xf_0 (26)$$

This has precisely the structure of the class of initial distribution functions that were

studied in the previous section of this article. Thus, the correlation function itself obeys Eq. (22), or

$$\dot{C}(t) = -\Omega^2 C(t) - \alpha \dot{C}(t) - \int_0^t ds \ K(s) \ \dot{C}(t-s)$$
(27)

We emphasize that this equation, in distinction to Eq. (22), is exact. The difference is due to the character of the two initial distributions. In deriving Eq. (22), we used an initial distribution function that cannot be entirely correct because it is negative for some positions and velocities. But in deriving Eq. (27), the initial distribution function  $xf_0$  is introduced only as a convenient artifice in calculating the correlation function. The actual distribution function used to define the average in C(t) is  $f_0$ , and this is positive.

Equation (27) is solved most conveniently by Laplace transforms. We use  $\hat{A}(\epsilon)$  to denote the Laplace transform of A(t),

$$\hat{A}(\epsilon) = \int_{0}^{\infty} dt \ e^{-\epsilon t} A(t)$$
(28)

Then the solution is the inverse Laplace transform of

$$\hat{C}(\epsilon) = \hat{G}(\epsilon)[\epsilon + \alpha + \hat{K}(\epsilon)]\langle x^2 \rangle_0$$
(29)

where

$$\hat{G}(\epsilon) = [\epsilon^2 + \Omega^2 + \epsilon \alpha + \epsilon \hat{K}(\epsilon)]^{-1}$$
(30)

Note that the initial first derivative of C(t) vanishes because it is odd in the velocity.

The quantity  $\hat{C}(i\omega)$  is a complex spectral density. Its real part is the cosine transform of C(t),

$$\operatorname{Re} \hat{C}(i\omega) = \int_{0}^{\infty} dt(\cos \omega t) C(t)$$
(31)

where Re denotes the real part. Aside from normalization constants, this is the quantity that was measured by Morton using an analog computer.

On Laplace inversion (replacing  $\epsilon$  by  $i\omega$ ), the time dependence of C(t) is found to be

$$C(t) = (1/2\pi) \int_{-\infty}^{\infty} d\omega \ e^{i\omega t} \hat{C}(i\omega)$$
(32)

(This result holds for positive t. For negative t, we must replace t by its absolute value.) Coefficients of powers of t in the series expansion

$$C(t) = \sum_{m=0}^{\infty} (C_m t^m / m!)$$
(33)

are related to moments of the complex spectral density  $\hat{C}(i\omega)$  by

$$C_m = (i)^m (1/2\pi) \int_{-\infty}^{\infty} d\omega \,\,\omega^m \hat{C}(i\omega) \tag{34}$$

They are also related to coefficients in the high-frequency expansion of  $\hat{C}(i\omega)$  by

$$\hat{C}(i\omega) = \sum_{m=0}^{\infty} \left[ C_m / (i\omega)^{m+1} \right]$$
(35)

Equations having the same structure as Eqs. (32)–(35) apply also the memory kernel K(t) and its spectral density  $\hat{K}(i\omega)$ . It is easy to see that knowledge of the first *m* terms in the power series expansion of K(t) is equivalent to knowledge of the first m + 2 terms in the power series expansion of C(t).

In the following section, we use these results to find analytic approximations for C(t). Our procedure is to compute analytically coefficients in the expansion

$$K(t) = \sum_{m=0}^{\infty} (K_m t^m / m!)$$
(36)

up to some power  $t^{M}$ . (We have actually done this up to M = 7.) From this information on the high-frequency expansion

$$\hat{K}(i\omega) = \sum_{m=0}^{\infty} \left[ K_m / (i\omega)^{m+1} \right]$$
(37)

we construct a continued fraction

$$\hat{K}(i\omega) = \frac{A(0)}{B(1) + i\omega - \frac{A(1)}{B(2) + i\omega - \frac{A(2)}{B(3) + i\omega - \cdots}}$$
(38)

which has the same high-frequency expansion. The constants A(0), A(1),..., B(0), B(1),... are determined by the coefficients  $K_0$ ,  $K_1$ ,.... We truncate the continued fraction at various levels to test convergence.

Our procedure is fully equivalent to Mori's scheme<sup>(9)</sup> for finding a continuedfraction expansion for the spectral density of any time correlation function.

To complete the calculation, we invert the cosine transform in Eq. (31), and obtain C(t).

# 4. NUMERICAL RESULTS

This section contains some numerical results on the computation of the correlation function C(t) and its spectral density. These results were obtained partly to provide some information on the structure of the memory kernel, and partly to compare our procedure with results obtained by Morton using analog computer experiments.

The power series expansion of the momery kernel is straightforward, although it rapidly becomes tedious. We simply expand the exponential operator in Eq. (23),

$$K_m = (1/\langle v^2 \rangle_0) \iint dx \, dv (F + \Omega^2 x) [(1 - P) \mathscr{D}]^m (F + \Omega^2 x) f_0 \tag{39}$$



Fig. 1. Spectral density as a function of frequency. The friction coefficient is  $\alpha = 2.0$  and the nonlinearity parameter is  $\beta = 0.25$ .



Fig. 2. Same as Fig. 1, except  $\beta = 1.0$ .



Fig. 3. Same as Fig. 1, except  $\beta = 2.0$ .

and iterate the operator  $(1 - P)\mathcal{D}$  directly. In the course of the calculation, one gets averages of various powers of the velocity; these are computed with the Gaussian distribution of velocities. Also, one gets averages of various powers of derivatives of the force F(x). All powers of the force itself can be eliminated by the identity

$$\langle FA(x) \rangle = -k_B T \langle A'(x) \rangle$$
 (40)

Explicit formulas for  $K_0$  to  $K_7$  are given in the appendix. Because the force is a polynomial in x, all averages reduce to averages of even powers of x. Further, the effective frequency  $\Omega$  also requires knowledge of the average of  $x^2$ .

It is easy to show that these averages are determined explicitly by

$$\langle x^{2n} \rangle_0 = (D/\alpha\beta)^{n/2} [\Gamma(n+\frac{1}{2})/\Gamma(\frac{1}{2})] U(n,z)/U(0,z)$$
 (41)

where

$$z = (\alpha/\beta D)^{1/2} \tag{42}$$

and U(n, x) is a parabolic cylinder function. Numerical tables of these functions are given in Ref. (10). In this way, the frequency and all coefficients  $K_m$  can be found explicitly.

As we have already pointed out, these coefficients can be used to determine a continued-fraction approximation to the spectral density of the memory kernel.

Several different levels of truncation were investigated. These are labeled by roman subscripts, and are

$$\hat{K}_{I}(i\omega) = 0$$

$$\hat{K}_{II}(i\omega) = \frac{K_{0}}{i\omega}$$

$$\hat{K}_{III}(i\omega) = \frac{K_{0}}{i\omega - A(1)/B(2)}$$

$$\hat{K}_{IV}(i\omega) = \frac{K_{0}}{i\omega - \frac{A(1)}{B(2) + i\omega - A(2)/B(3)}}$$

$$\hat{K}_{V}(i\omega) = \frac{K_{0}}{i\omega - \frac{A(1)}{B(2) + i\omega - A(2)/B(3)}}$$

$$\hat{K}_{V}(i\omega) = \frac{K_{0}}{i\omega - A(1)}$$

(It turns out that the constant B(1) vanishes, so it has been omitted.) Because of the way that the continued fractions are constructed, the constants A(m) and B(m) are the same in all approximations.

Equations (29) and (30) are used to construct the corresponding continued fraction approximations to  $\hat{G}(i\omega)$ . The real part of the spectral density is taken for comparison with Morton's experimental data. This time-dependent memory kernel and correlation function are found by Fourier inversion.



Fig. 4. Same as Fig. 1, except  $\beta = 3.0$ .



Fig. 5. Same as Fig. 1, except  $\alpha = 0.5$  and  $\beta = 0.1$ .

This sequence of calculations has been carried out for six sets of parameters  $\alpha$  and  $\beta$ . We present results in tabular and graphical form.

Figures 1-6 show the spectral density Re  $\hat{C}(i\omega)$ , computed with our best approximation  $\hat{K}_{V}(i\omega)$  to the memory kernel. These figures show also the experimental results obtained by Morton. (His values have been scaled down by a factor of two because of a difference in definition of the spectral density.)

The sequence of curves with  $\alpha = 2$  covers a wide range of nonlinearity, from  $\beta = 0.25$  to  $\beta = 3.0$ . This value of  $\alpha$  corresponds to critical damping in the limit  $\beta = 0$ .

The curves with  $\alpha = 0.5$  are for  $\beta = 0.1$  and  $\beta = 0.25$ . This value of  $\alpha$  corresponds to underdamped oscillation in the limit  $\beta = 0$ . The resonant character of the spectral density is clearly seen. The theoretical peak heights are considerably larger than the experimental ones. This may be due to Morton's use of a bandpass filter with a nonnegligible bandwidth; any averaging process will tend to lower and broaden a resonant peak.

Figure 7 shows the time dependence of the correlation function C(t) and also that of the memory kernel K(t), for the case  $\alpha = 2.0$  and  $\beta = 2.0$ . These were constructed with our best approximation  $\hat{K}_{\nu}(i\omega)$ . The correlation function oscillates at long times, with an amplitude that is too small to be shown in this figure.

Note that the decay time of the memory kernel is about half the decay time of the correlation function itself. This extra contribution to the frictional behavior is evidently non-Markovian. However, the magnitude of the memory kernel is always



Fig. 6. Same as Fig. 1, except  $\alpha = 0.5$  and  $\beta = 0.25$ .

less than 0.15, and is to be added to the original friction coefficient  $\alpha = 2.0$ . While the memory kernel is non-Markovian, it has only a rather small effect on the decay of the correlation function.

We have investigated the lower-order approximations to the memory kernel. To save space, we report some results in tabular rather than graphical form. Table I gives the zero-frequency values of the spectral density  $\hat{C}(i\omega)$  for five approximations to the memory kernel. It contains also the effective frequencies for each  $\alpha$  and  $\beta$ .

The zero-frequency behavior was chosen as a measure of convergence for the following reason. Our approximation method starts with a high-frequency expansion, which may be expected to converge only up to the singularity in the complex frequency



Fig. 7. The correlation function C(t) and the memory kernel K(t) as functions of time, for  $\alpha = 2.0$  and  $\beta = 2.0$ .

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α	β	Ω	$\hat{C}_{\mathrm{I}}$	$\widehat{C}_{\mathrm{II}}$	$\hat{C}_{\mathrm{III}}$	$\hat{C}_{IV}$	$\hat{C}_{\mathbf{V}}$	
0.5	0.1	1.10	0.335	0.335	0.337	0.366	0.337	
0.5	0.25	1.20	0.239	0.239	0.242	0.292	0.242	
2.0	0.25	1.07	0.376	0.376	0.377	0.377	0.377	
2.0	1.0	1.20	0.239	0.239	0.242	0.245	0.245	
2.0	2.0	1.32	0.168	0.168	0.171	0.175	0.173	
2.0	3.0	1.39	0.133	0.133	0.137	0.142	0.140	

Table I. Zero-Frequency Value of the Spectral Density  $\hat{C}(i\omega)$ ,<sup>*a*</sup> for Various Friction Coefficients  $\alpha$  and Nonlinearity Parameters  $\beta$ 

<sup>a</sup> The Roman subscripts refer to the approximations for the memory kernel listed in Eq. (43). The effective frequency  $\Omega$  is included.

plane that is farthest from the origin. The continued fraction is used to analytically continue the high-frequency expansion to the entire frequency plane. Thus, the value of the continued fraction at the origin is a sensitive test of the adequacy of the analytic continuation.

On inspection of Table I, it will be seen that convergence is fairly good for the highly damped case  $\alpha = 2.0$ , and less good for the underdamped case  $\alpha = 0.5$ . In all cases, the result obtained by omitting the memory kernel entirely is almost as good as the highest approximation. In a practical sense, the main effect of this theoretical treatment is the introduction of the effective frequency  $\Omega$ .

It must be mentioned that Morton and Corrsin have given an alternative theoretical treatment of this problem. They use an infinite-order perturbation expansion of the nonlinear Langevin equation, and perform resummations of selected classes of terms in this expansion. The spectral density of the correlation function is obtained by iterative solution of three coupled, nonlinear integral equations in three unknown functions. (Their method is modeled on one introduced by Kraichnan in his theory of turbulence.) The numerical results obtained by Morton and Corrsin agree with the computer experiments about as well, and perhaps a bit better, than ours. However, much more labor is involved in their treatment.

# 5. CONCLUSION

The main point of this article was to show how one can get, from a nonlinear microscopic equation of the Langevin type, a linear transport equation for an average value. The resulting linear transport equation is restricted to small initial deviations from equilibrium. It contains a renormalized oscillator frequency and a renormalized and non-Markovian friction coefficient, both depending on the nonlinearity parameters of the original microscopic equation.

A subsidiary point of the article was to present numerical calculations of the position correlation function of the Duffing oscillator. These calculations were based on a continued-fraction expansion, equivalent to precise specification of the first nine frequency moments of the spectral density of the correlation function. The results

of the numerical calculations are in fairly good agreement with Morton's analog computer experiments.

# APPENDIX

Here are given the first eight coefficients in the expansion of the memory kernel.

$$\begin{split} K_{0} &= -\Omega^{2} - \langle F' \rangle \\ K_{1} &= 0 \\ K_{2} &= \langle F' \rangle^{2} - \langle (F')^{2} \rangle \\ K_{3} &= -\alpha K_{2} \\ K_{4} &= (3D/2\alpha) \langle (F'')^{2} \rangle - \langle (F')^{3} \rangle + 2 \langle (F')^{2} \rangle \langle F' \rangle - \langle F' \rangle^{3} + \alpha^{2} K_{2} \\ K_{5} &= -5D \langle (F'')^{2} \rangle + 2\alpha [\langle (F')^{3} \rangle - 2 \langle (F')^{2} \langle F' \rangle + \langle F' \rangle^{3}] - \alpha^{3} K_{2} \\ K_{6} &= -15 (D/2\alpha)^{2} \langle F''' \rangle^{2} \rangle + 21 (D/2\alpha) \langle F'(F'')^{2} \rangle \\ &\quad - 6 (D/2\alpha) \langle (F'')^{2} \rangle \langle F' \rangle + (25/2)\alpha D \langle (F'')^{2} \rangle \\ &\quad - 3\alpha^{2} [\langle (F')^{3} \rangle - 2 \langle (F')^{2} \rangle \langle F' \rangle + \langle F' \rangle^{3}] \\ &\quad - \langle (F')^{4} \rangle + \langle (F')^{2} \rangle^{2} + 2 \langle (F')^{3} \rangle \langle F' \rangle - 3 \langle (F')^{2} \rangle \langle F' \rangle^{2} + \langle F' \rangle^{4} + \alpha^{4} K_{2} \\ K_{7} &= (105/4) (D^{2}/\alpha) \langle (F''')^{2} \rangle - (103/2) D \langle (F'')^{2} F' \rangle \\ &\quad + 13D \langle (F'')^{2} \rangle \langle F' \rangle - 28\alpha^{2} D \langle (F'')^{2} \rangle \\ &\quad + 4\alpha^{3} [\langle (F')^{3} \rangle - 2 \langle (F')^{2} \rangle \langle F' \rangle + \langle F' \rangle^{3}] \\ &\quad + 3\alpha [\langle (F')^{4} \rangle - \langle (F')^{2} \rangle^{2} - 2 \langle (F')^{3} \rangle \langle F' \rangle + 3 \langle (F')^{2} \rangle \langle F' \rangle^{2} - \langle F' \rangle^{4}] - \alpha^{5} K_{2} \end{split}$$

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