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On the superposition of relaxation spectra as an explanation for 1/f noise

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Résumé. — L'objet de ce papier est de montrer les limites dans l'interprétation des bruits en 1/f de la méthode de superposition des spectres de relaxations. On montre que cette méthode se ramène à une superposition des processus Ornstein-Uhlenbeck impliquant des phénomènes stationnaires, Gaussiens mais non Markoviens. Ceci entraîne que les phénomènes ne sont pas des processus obéissant à la Thermodynamique Irréversible d'Onsager. Ce modèle ne peut être utilisé pour une interprétation plus générale du bruit en 1/f.

Abstract. — It is investigated to what extent a suitable weighting of relaxation processes can serve as a more general explanation of 1/f noise. The usual interpretation is shown to reduce to a superposition of Ornstein-Uhlenbeck processes, yielding a Gaussian stationary and non-Markovian process. The model treats the 1/f noise as originating from a system that does not belong to Irreversible Thermodynamics on the basis of the Onsager relations. It cannot be used as a more general explanation for 1/f noise.

Introduction. — An investigation about the origins of 1/f noise should include a discussion of the McWhorter model, henceforth M-model (1). The model has had reasonable success in electronic devices. Particularly with respect to MOSFET's where the flicker noise has been theoretically analysed by many investigators. In other devices such as integrated resistors, tunnel diodes, Shottky diodes and FET's, the analyses were mostly based on physical mechanisms which were all within the broad scope of the original concepts proposed by McWhorter.

One may argue of course, that this tunneling model cannot be valid in general, because 1/f noise exists in devices and materials without an oxide layer. It has even been measured in cases which have nothing to do with solid state physics. One should nevertheless probe its statistical and physical contents in order to establish its limits of application, since the basic idea of mixing certain processes may be of value.

In this paper the M-model is treated statistically in a formal way. It provides us with some criteria about its applicability to physical processes. We shall deal with such questions as (i) Stationarity (ii) Fluctuations in noise records (iii) Gaussian and Markovian character.

For MOS or MIS structures, which are the ideal case for an application of the M-model, discrepancies arise on a number of occasions with a McWhorter type of interpretation. Statistically, since we do not allow for electron-electron correlations, electron-phonon coupling and other non-Poissonian microscopic processes. This can lead to non-Markovian processes, bunching effects and non-linear phenomena. These effects cannot be treated by the straightforward M-model. One tacitly assumes a linear, homogeneous Markov system. In the non-linear case it is then subsequently linearised by applying the G-R theorem or a simple Langevin method (white source). This implies that it is assumed that the system (in equilibrium or not) converges in its parameters to an Ornstein-Uhlenbeck process. It limits the theoretical characterisation of such a special phenomenon as 1/f noise. Physically, we tacitly assume that no interaction is taking place between the electrons and the lattice (polarons, self trapping, hopping, charged dangling bonds, localization etc.). In all theories the number of traps remains a constant and the rate constants of the various kinetics are the mean values of uncorrelated point processes. No carrier density related mobility, trap-density, capture or release is allowed in the theories we know of. It is generally accepted however,
that a random potential at the surface exists and that the oxide contains many positive and negative charges. No models exist yet for these problems. These effects may play a role in future since the general trend in Si-technology is towards smaller and subthreshold devices. In this contribution the M-model is analysed statistically.

1. The model. — A detailed description can be found in [1] and [2]. A fluctuating time dependent number is considered, which usually represents the number of trapped carriers. One therefore studies the development of a random-variable with respect to time (Langevin). The next alternative would be the study of the evolution of the probability (Master equation). For our purposes, the following steps are relevant:

(i) The starting point is a basic stochastic process with an autocovariance:

\[ C(t, \tau) = \Delta x^2 e^{-t/\tau} \]  

where the time constant \( \tau \) is determined by the process under study, and \( x \) the fluctuating number.

(ii) The second order properties are determined by simple Langevin methods (white source) and the G-R theorem [3] or Burgess' method [4].

(iii) For the spectrum, the Wiener-Khintchine theorem is applied.

(iv) The final spectrum is obtained by a weighting of the basic spectra with a predetermined 1/\( \tau \) distribution of time constants.

1.1 The basic process. — The starting point in the usual theories on the basis of the M-model is a physical process, the fluctuations and time dependency of which, are characterized by the covariance as is given by (1). For its derivation, the G-R theorem and simple Langevin methods (white source) are used. We shall show that both procedures are equivalent. However, they impose upon the physical process under study certain conditions which need not hold in practice.

For our discussion we need a suitable description of the physical system in order to set up our statistical model. Previous work on the macroscopic treatment of noise makes generally the following assumptions [5]:

1. The system is linear.
2. Microscopically the system obeys time reversibility.
3. The system is stationary and Markovian.
4. The variables have a Gaussian distribution.

Note that points one and three imply four. These assumptions appear to hold for a wide class of realistic physical systems. The M-model treats the 1/\( f \) problem as originating from a stationary physical system, which will be shown in the sequel. The question whether 1/\( f \) noise is a stationary or non-stationary phenomenon has not been settled yet in a satisfactory way. We nevertheless start with the stationarity assumption on the following grounds.

In equilibrium statistical mechanics we can find all of the thermodynamic properties of any particular system, if we can first calculate its partition function. It affords the idea, however, of ensembles and a phase space density, which leads to the Liouville operator. This is a purely dynamic quantity whose explicit form depends entirely on the Hamiltonian of the system. The study of irreversible processes on the frame of classical or quantum mechanics can also be carried out by the Liouville equation. In short, the usual starting point of physical master equations is the Liouville equation. But this implies strict stationarity (or even ergodicity), since otherwise we can not use ensemble averages or introduce a phase space distribution. (It may be interesting to note that the basis of linear response theory is the ergodic property of the system.)

The next step will be the study of the Markovian character of the system, since there exists a large literature on the mathematical analysis of stationary Markov processes. Normally, a physical system has the ability to forget quickly the initial values of the microscopic variables, since the time scale of the experiment is much larger than the one of the microscopic processes. Most systems in equilibrium behave that way [6, 7]. If we choose for its description a sufficiently complete set of variables, omitting any relevant slowly varying component then a Markovian description becomes possible. In fact, random processes associated with a complete set of variables are stationary Markovian [6]. Since the Liouville operator depends entirely upon the Hamiltonian of the system, a complete set will be in the case of Brownian motion for example, the Hamiltonian, the position, and momentum of the Brownian particle. Though it is not clear whether 1 incise satisfies these criteria as well, the basic process from the M-model does, since the macroscopic density fluctuations of the trapped or free carriers occur on a much larger time scale than the equilibration processes. The system therefore forgets quickly and the transition probability of the macroscopic variable to a future state only depends on the present state. This may not hold for disordered structures, however, since the electron-electron and lattice interactions narrow the difference between macroscopic and microscopic times. The usual Bloch-Wilson type of interpretation breaks down. Since these correlation effects have played no role in the M-model in the past, we maintain the independent particle picture and conclude that the basic process in the M-model is Markovian. (Though the covariance (1) already shows a Markov behaviour, we want to point out that the systems underlying the M-models from the past are all Markovian on purely physical grounds.)
Dealing with a stationary Markov process, the statistics can now be analysed mathematically in a formal way. After certain approximations it then should be possible to arrive at the same results as those which are given by the G-R theorem or Burgess' method and the simple Langevin approaches. This reduction of the general case should provide us then with certain conditions imposed upon the real process.

The most general description of a Markov process in continuous time and discrete state space is by Kolmogorov's forward and backward differential equations [8]. In continuous state space the arising integro-differential equation is known to physicists as the Boltzmann or Smoluchowski equation:

\[
\frac{\partial p(x, t)}{\partial t} = \int p(y, t) q(y, x) \, dy - \int p(x, t) q(x, y) \, dy.
\]

This expresses that the rate of change of the population of a cell in x-space, representing the quantity under study, is the difference of the rate of departures from the cell and the rate of arrivals. The quantity \( p(x, t) \) is the probability that the random variable \( X(t) \) takes the value \( x \) at time \( t \), and \( q(x, y) \) is the probability per unit of time that the state of the system will undergo a transition from \( y \) to a volume \( dx \) about \( x \). This equation is difficult to handle mathematically. Expansion of the transition probability yields the Kramers-Moyal expansion:

\[
\frac{\partial p(x, t)}{\partial t} = - \frac{\partial}{\partial x} \left[ \mathcal{A}_1(x) p(x, t) \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[ \mathcal{A}_2(x) p(x, t) \right].
\]

The second approximation is also caused by analytical difficulties encountered in trying to solve the parabolic equation (5). To that propose we have a closer look at \( \mathcal{A}_1(x) \) and \( \mathcal{A}_2(x) \). A more transparent way of writing (4) is the following:

\[
\mathcal{A}_n(x) = \lim_{\Delta t \to 0} \frac{\{ X(t + \Delta t) - X(t) \}^n}{\Delta t^n}
\]

or even more simply:

\[
\mathcal{A}_1(x) = \lim_{\Delta t \to 0} \frac{\Delta x}{\Delta t} \quad \text{and} \quad \mathcal{A}_2(x) = \lim_{\Delta t \to 0} \frac{(\Delta x)^2}{\Delta t}.
\]

For most physical systems the macroscopic equation contains a linear term describing the drift towards a certain equilibrium value. This term will be linear in the state variable for a small deviation and with a proportionality factor which is determined by the system. The first moment of the increment \( \Delta x \) is therefore represented by \( -\beta x \). For a stationary process a constant incremental variance \( \sigma^2 \) is assumed, so that the final process is described by:

\[
\frac{\partial p(x, t)}{\partial t} = - \beta \frac{\partial}{\partial x} \left[ xp(x, t) \right] + \frac{1}{2} \sigma^2 \frac{\partial^2}{\partial x^2} \left[ p(x, t) \right].
\]

This equation can be solved exactly [9]. The process \( X(t) \) is called an Ornstein-Uhlenbeck (O-U) process. It is the most general Gaussian, stationary and Markovian process. The covariance turns out to be:

\[
\langle X(t) \rangle \langle X(t + \tau) \rangle = \Delta x^2 \exp \left( -\frac{\tau}{\tau} \right), \quad \beta = \frac{1}{\tau}, \quad \overline{X(t)} = 0
\]

and the stationary variance:

\[
\overline{\Delta x^2} = \frac{1}{2} \sigma^2 / \beta.
\]

This shows that the variance of a system, which can be described by an O-U process, is determined by the incremental variance and the time constant of the system.

In fluctuation phenomena in solids (electrons in...
our case), usually a generation and recombination rate is defined, such that the macroscopic behaviour is described by [3]:

$$\frac{dx}{dt} = g(x) - r(x). \quad (11)$$

It should be noted that $x$ basically represents a discrete number. However, the system is assumed to be large enough in order to use the mathematically more convenient continuous state space. Returning to (6) the incremental moments are in the case of (11):

$$\begin{align*}
\alpha_1(x) &= g(x) - r(x) \\
\alpha_2(x) &= g(x) + r(x).
\end{align*}$$

Substituting this into (5) and comparing the result with equation (8) yields for $\beta$:

$$\beta = \left( \frac{\partial r(x)}{\partial x} \right)_0 - \left( \frac{\partial g(x)}{\partial x} \right)_0. \quad (12)$$

where the subscripts refer to the equilibrium values. This is only possible if the relative fluctuations around equilibrium are small enough, since the terms $(\Delta x)^n$ with $n > 2$ are neglected. We thus require once more sharply peaked transition probabilities. The O-U process therefore has as a variance:

$$\Delta x^2 = \frac{g_0 + r_0}{2} \left( \frac{\partial r(x)}{\partial x} \right)_0 - \left( \frac{\partial g(x)}{\partial x} \right)_0 \quad (13)$$

which is the wellknown result from the G-R theorem and of Burgess' method. Its derivation from first principles of the theory of stochastic processes shows under which conditions equation (13) can be applied:

(i) The underlying physical process is replaced by an O-U process, i.e. it is stationary, Markovian and Gaussian.

(ii) The system responses are linear in the forces. Nonlinear systems are linearized.

(iii) We deal with small deviations from equilibrium.

(iv) The systems are large enough to allow a diffusion approximation.

(v) Microscopically the system obeys time reversibility.

Strictly speaking, points (ii)-(v) are already imbedded in (i) since we deal with sharply peaked transition probabilities. We thus see that application of the G-R theorem or Burgess' method imply the general assumptions from noise theory, which were given at the beginning of this section. But this need not be the case for $1/f$ noise with its long time constants involved. It is not clear whether for this case the decay of the system obeys the macroscopic equation. (This property follows from (i)-(v) in particular point (ii).) If not, one of Onsager's assumptions would be violated and $1/f$ noise would not belong to the usual world of thermostatics and irreversible thermodynamics.

We now turn to the simple Langevin description (white source) in $1/f$ theories. Statistically, its origins could be described by Wold's decomposition theorem of a stationary Markovian process [10]. It states that an arbitrary stationary Markov process can be expressed as the sum of two processes uncorrelated with one another, one pure deterministic and one purely undeterministic. Its representation in the discrete time case is in terms of moving average and autoregressive processes. For a derivation of the Langevin equation, the continuous analogue of a first order autoregressive process could then be used [10]. We shall not develop this any further, since a discussion in terms of the incremental moments will be more consistent in the present context. It shows however that the artifice of a priori statistics can be accounted for rigorously in the statistical sense for processes which are stationary, Markovian and Gaussian.

As we have seen, the change in $X(t)$ in a small time interval $dt$ is a normal variate with mean $\alpha_1(x)dt$ and variance $\alpha_2(x)dt$. A small increase in the random variable $X(t)$ can then be represented as [10]:

$$dX(t) = \alpha_1(x)dt + Z(t)\sqrt{\alpha_2(x)}dt. \quad (14)$$

The purely random process $Z(t)$ with $\overline{Z(t)} = 0$ and variance equal to unity, determines whether the small amount $\alpha_2(x)dt$ is added or subtracted. Furthermore, if one constructs a diffusion limit of a simple random walk, resulting in the so-called Wiener process it follows that the incremental change $dA(t)$ of this process equals exactly the second term of the RHS of (14):

$$dA(t) = \alpha_1(x)dt + dA(t) \quad (15)$$

$A(t)$ therefore represents a Wiener process with a variance parameter of $\alpha_2(x)$.

In noise problems one usually starts with the simple Langevin equation:

$$\frac{dx}{dt} = -\beta x + H(t). \quad (16)$$

Comparing (16) with (15) it follows that $H(t)$ is the derivative of a Wiener process. (We shall not go into the matter whether this is possible or not.) It is tried to recover the incremental moments (7) from equation (16). A small change in $t$ will give a corresponding change in $x$:

$$\int_x^{x + \Delta x} dx = -\beta \int_t^{t + \Delta t} x dt + \int_t^{t + \Delta t} H(t) dt \quad (17)$$

or

$$\Delta x = -\beta x \Delta t + 0(\Delta x \Delta t) + H(t) \Delta t + 0(\Delta t^2). \quad (18)$$
Taking the ensemble averages over the incremental changes:
\[
\Delta x = -\beta x \Delta t + 0(\Delta x \Delta t) + \overline{H(t)} \Delta t + 0(\Delta t)^2.
\]  

(19)

From which it follows:
\[
\alpha_1(x) = \lim_{\Delta t \to 0} \frac{\Delta x}{\Delta t} = -\beta x + \overline{H(t)} , \quad \overline{H(t)} = 0.
\]  

(20)

Squaring both sides of (20) and taking the ensemble averages yields in the limit for \(\Delta t \to 0\):
\[
\alpha_2(x) = \lim_{\Delta t \to 0} \frac{(\Delta y)^2}{\Delta t} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \overline{H(t_1) H(t_2)} \, dt_1 \, dt_2.
\]  

(21)

For the O-U process the incremental variance was equal to \(\sigma^2 \, dt\). This follows also from (21), since \(H(t_1) \, dt_1\) can be written as \(dA(t_1)\) which is equal to \(\sigma Z(t_1) \, dt_1\) (see equations (14), (15), (16)) and because of the fact that \(Z(t)\) is a pure random process with \(Z(t_1) Z(t_2) = \delta(t_1 - t_2)\). Any macroscopic variable represented by (16) therefore has as a stationary variance \(1/2(\sigma^2/\beta)\). This shows that the simple Langevin approach and the G-R theorem or Burgess’ method are equivalent: They both replace the actual physical process by an O-U process.

This equivalence is not surprising. Both procedures consider a normal distribution at equilibrium. Non-linear cases are linearized since sharply peaked transition probabilities are assumed. In other words, the relative fluctuations have to be small enough in order to be able to characterize the macroscopic behaviour by the mean values of the quantities under study. It implies that it can be separated in a mean and fluctuating behaviour (Wold’s theorem). Both procedures are therefore imbedded in the usual classical (non) equilibrium statistical mechanics. As was mentioned before, 1/f noise does not need to satisfy these criteria. For more involved problems the next step could be the Fokker-Planck equation (5), since it considers the evolution of the probability density function itself, and not of the random variable as in the Langevin case.

Concluding, it can be said that for 1/f theories, using a basic process with a covariance as is given by (1), it is assumed that the system can be described by a stationary and Gaussian Markov process. This implies that the M-model does not work for:

(i) Non-linear cases which cannot be linearized.
(ii) Large fluctuations from a nonlinear equilibrium state (phase transitions, cooperative phenomena, bunching effects, small systems).
(iii) Non-Gaussian incremental distributions (frequency dependent friction in the Langevin case. For example, a velocity dependent cross-section).
(iv) Non-Markovian cases (Non-poissonian microscopic processes).
(v) Non-stationary phenomena (possibly with exceptions).

1.2 Superposition of Spectra:— For 1/f calculations the spectra from (1) are averaged over a 1/\(\tau\) distribution. First of all, it should be noted that the integration over an interface distance, uniformly distributed between two limits [2], is equivalent to the 1/\(\tau\) averaging in the case of an exponential weighting. To see this, we note the following.

Frequently an exponential probability of access for the states in the oxide is assumed. The distribution of time constants involves tunneling through the surface oxide over a distance \(y\) between the surface and the oxide trap: \(\tau = \tau_0 \exp(\alpha y)\), where \(\tau_0\) is the time constant associated with the surface trap, and \(\exp(-\alpha y)\) the probability of access for the oxide trap. The constant \(\alpha\) depends on the effective mass and an energy barrier, which is usually the difference between the edge of the conduction band of the SiO\(_2\) and the top of the valence band of Si. If we consider \(y\) as a uniformly distributed random variable, then the distribution of the random variable \(\tau\) becomes:
\[
g(\tau) = (\alpha y_1 \tau)^{-1}
\]  

(22) since the Jacobian of the transform turns out to be \(\alpha \tau\). The traps were assumed to be uniformly distributed between \((0, y_1)\). The normalizing constant is now \((\alpha y_1)^{-1}\). In other words, this approach is equivalent in assuming a \(A/\tau\) distribution, with
\[
A = \ln\frac{\tau_2}{\tau_1} \left|\tau_1 = \tau_0 \right.
\]  

(23)

we therefore simply discuss the averaging of a spectrum over a \(A/\tau\) distribution.

The autocovariance (1) yields a spectrum
\[
S(f) = 4 \overline{A^2} \cdot \frac{\tau}{\omega^2 \tau^2 + 1}.
\]  

(24)

Averaging over \(A/\tau\) gives:
\[
S(f) = \frac{4}{\omega} \overline{A^2} \left[\tan^{-1} \omega \tau_2 - \tan^{-1} \omega \tau_1\right],
\]  

(25)

\[
A = \ln\frac{\tau_2}{\tau_1} \left|\tau_1 = \tau_0 \right.
\]

For a realistic spectrum \(\tau_2 \gg \tau_1\) with \(\tau_2\) being large enough. The averaging implies that \(S(f)\) is in fact a random variable. It appears to be difficult to find the Jacobian of the transform which is given by (24). We therefore average the autocovariance and use this result for our discussion. The averaging of \(C(t, \tau)\) is allowed since the Fourier transform is unique:

\[
C(t, \tau) = \int_{-\infty}^{\infty} S(f) \exp(-i 2\pi ft \tau) \, df.
\]  

(26)

\[
S(f) = \frac{4}{\omega} \overline{A^2} \left[\tan^{-1} \omega \tau_2 - \tan^{-1} \omega \tau_1\right],
\]

(27) For a realistic spectrum \(\tau_2 \gg \tau_1\) with \(\tau_2\) being large enough. The averaging implies that \(S(f)\) is in fact a random variable. It appears to be difficult to find the Jacobian of the transform which is given by (24). We therefore average the autocovariance and use this result for our discussion. The averaging of \(C(t, \tau)\) is allowed since the Fourier transform is unique:
Therefore:

\[
\int_{t_1}^{t_2} \left[ \int_{-\infty}^{\infty} e^{-j\omega t} C(t, \tau) \, dt \right] \frac{A}{\tau} \, d\tau =
\]

\[
= \int_{-\infty}^{\infty} e^{-j\omega t} \left[ \int_{t_1}^{t_2} C(t, \tau) \frac{A}{\tau} \, d\tau \right] \, d\omega .
\]

Therefore:

\[
\overline{C(t)} = \int_{t_1}^{t_2} \frac{\Delta x^2}{\Delta x^2} e^{-t/\tau} \frac{A}{\tau} \, d\tau
\]

\[
= A \Delta x^2 \left[ E_1(t/\tau_2) - E_1(t/\tau_1) \right]
\]

where \(E_1(z)\) represents the exponential integral [11] :

\[
E_1(z) = \int_{z}^{\infty} \frac{e^{-t}}{t} \, dt , \quad |\arg z| < \pi .
\]

For \(z \to 0\) this integral diverges so that the M-model has a low frequency limit \((t_2\) is an upper limit). We can check whether \(C(t)\) is a real mean value. The density function of the autocovariance \((1)\) can be calculated explicitly since the density function of \(r\) is assumed to be \(A/\tau\). Carrying out the transform:

\[
P(C) = A \left[ C \ln \left( \frac{\Delta x^2}{C} \right) \right]^{-1} , \quad C = C(t, \tau)
\]

with \(C_1 = \Delta x^2 \exp(-t/\tau_1)\) and \(C_2 = \Delta x^2 \exp(-t/\tau_2)\) after normalization. It is now straightforward to show:

\[
\int_{C_1}^{C_2} C p(C) \, dC = \int_{t_1}^{t_2} C(t, \tau) p(\tau) \, d\tau .
\]

The LHS is the true mean of the random variable \(C\), and the RHS represents the averaging of the autocovariance. The superposition of the spectra is therefore equivalent to the Fourier transform of the mean of the autocovariance density.

The variance has been treated as a constant in the averaging procedure. It is usual practice, whenever the M-model is applied [1, 2]. This is a little surprising, since the variance necessarily contains the time constant to be averaged. The stationary variance of an O-U process contains the incremental variance and also the time constant of the process under study, see equation (10). Including the variance in the averaging procedure does not result in a 1/\(f\) spectrum in general. In the simplest case (rate equation describing a time dependent Poisson process), a 1/\(f^2\) spectrum is obtained. The superposition of spectra therefore represents a weighting of autocorrelation functions, rather than autocovariances.

It also follows from (30) that the superimposed O-U processes are assumed to be independent. In the probabilistic sense, the averaging procedure uses the total probability theorem which considers the occurrence of the processes with different autocorrelation functions (normalized autocovariances) as being mutually exclusive events, the sum of which equals the certain event.

Concluding, the averaging of the spectra in the M-model represents a weighting of autocorrelation functions from independent, stationary and Gaussian Markov processes.

1.3 AVERAGED PROCESS. — The results from the previous section can be used for a discussion of the character of the final process after averaging. We first study its stationarity. For stationarity in the wide sense the process has a mean which is a constant and its autocovariance depends only on the time difference. It should be kept in mind that for a wide sense stationarity a Gaussian process automatically implies strict sense stationarity. Here, the only information about the process is the averaged autocovariance (27). According to a theorem of Doob [12] this enables us to establish whether the final process has a mean or not.

The time average

\[
\overline{X(t)} = \lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} X(i) \, dt
\]

exists only if:

\[
\lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} | \overline{C(t, \tau)} - \overline{X(t)}^2 | \, dt = 0 .
\]

Substituting (27) into (32) gives the integral:

\[
\int_{0}^{T} \overline{C(t, \tau)} \, dt = A \Delta x^2 \left[ T[E_1(T/\tau_2) - E_1(T/\tau_1)] + \tau_2(1 - e^{-T/\tau_2}) - \tau_1(1 - e^{-T/\tau_1}) \right].
\]

Using the fact that [11] :

\[
\lim_{z \to \infty} E_1(z) \quad \text{tends to} \quad \lim_{z \to \infty} \frac{e^{-z}}{z}
\]

yields

\[
\frac{1}{T} \int_{0}^{T} \overline{C(t, \tau)} \, dt \to \frac{\tau_2 - \tau_1}{T} A \Delta x^2 .
\]

Substituting (34) into (32) therefore shows that the mean of the averaged process exists. It also follows from (27) that the autocovariance only depends on the time difference (arbitrary origin) so that the final result is at least stationary in the wide sense. We now turn to its Gaussian character.

What is termed, the superposition of relaxation spectra, basically represents a randomisation or mixing [8] of the underlying O-U processes. A new distribution is then defined in the \((x, \tau)\) plane, serving as a sample space. In the M-model only the autocorrelation function, not the autocovariance, is
averaged. It means that the O-U processes are only weighted with respect to their decaying properties (constant variances in equilibrium). The question is now whether a mixing of autocovariances (or autocorrelation functions) implies a mixing of the density function of the underlying O-U processes. From (27) it follows:

$$C(t, \tau) = \int_{t_1}^{t_2} C(t, \tau) p(\tau) \, d\tau = \int_{t_1}^{t_2} \bar{X}(t) \bar{X}(t + \tau) p(\tau) \, d\tau$$

where the mean is suppressed for convenience. Since \( \bar{X}(t) \) is stationary in the strict sense (Gaussianity plus wide sense stationarity) we can take the ensemble average and the autocovariance can be written as:

$$\bar{X}(t) \bar{X}(t + \tau) = \int_0^\infty x_1 x_2 p(x_1, x_2) \, dx_1 \, dx_2$$

where \( x_1 \) and \( x_2 \) represent the values \( X(t) \) takes at times \( t \) and \( t + \tau \) respectively and \( p(x_1, x_2) \) is their joint probability density function. Substituting (36) into (35) and using the conditional relationship

$$p(x_1, x_2) = p(x_2 | x_1) p(x_1)$$

while interchanging the integrals yields for (35):

$$C(t, \tau) = \int_0^\infty x_1 x_2 \left[ \int_{t_1}^{t_2} p(x_2 | x_1) p(\tau) \, d\tau \right] \, dx_1 \, dx_2 .$$

This shows that mixing \( C(t, \tau) \) with \( p(\tau) \) is equivalent to the mixing of the transition probability \( p(x_2 | x_1) \), which is Gaussian and can be obtained explicitly from (8) [9]:

$$p(x_2, t | x_1, 0) = \left[ 2 \Delta x^2 (1 - e^{-2\beta t}) \right]^{1/2} \times \exp[-(x_2 - x_1 e^{-\beta t})^2/2 \Delta x^2 (1 - e^{-\beta t})].$$

The problem is now reduced to the question whether the Gaussianity of the transition probability is preserved after mixing. It thus needs to be demonstrated that the outcome \( f(t; \tau_1, \tau_2) \) remains normal after mixing of a Gaussian density function \( f(t, \tau) \), which is our notation for the transition probability

$$f(t; \tau_1, \tau_2) = \int_{t_1}^{t_2} f(t, \tau) p(\tau) \, d\tau.$$  

To proof this we interpret the integral in the Riemann sense and write:

$$f(t; \tau_1, \tau_2) = \lim_{N \to \infty} \frac{\tau_2 - \tau_1}{N} \times \sum_{k=1}^{N} f(t, k \frac{\tau_2 - \tau_1}{N}) p(k \frac{\tau_2 - \tau_1}{N}).$$

Equivalently:

$$f = \lim_{N \to \infty} (a_1 f_1 + a_2 f_2 + \cdots + a_n f_n)$$

with \( f_n \) being independent and Gaussian random variables with the condition that \( \lim \sum a_n = 1 \).

Defining a characteristic function for \( f \) and using the property of independence for \( f_n \) shows that the result is an \( N \)-variant Gaussian density function [13]. By means of the central limit theorem we then get to our final result, which is a Gaussian density for \( f(t; \tau_1, \tau_2) \). Unfortunately, the averaged process lost its Markovian character, since a normal, stationary Markov process must have an exponential autocorrelation function [14], which is not the case here.

The M-model therefore averages the autocorrelation functions of Gaussian, stationary Markov processes, yielding a Gaussian, stationary non-Markovian process.

In experiments it may be worthwhile to know the speed of convergence of the noise records. The variance of a single record in \((0, 2T)\) is given by [13]:

$$\sigma_{\tau} = \frac{1}{T} \int_0^{2T} \left( 1 - \frac{t}{2T} \right) \bar{C}(t, \tau) \, d\tau, \quad \bar{X}(t) = 0$$

where the record is defined as a time average:

$$n_T = \frac{1}{2T} \int_{-T}^{T} X(t) \, dt.$$  

A measure for the speed of convergence of the record variance is then

$$\sigma_{\tau} \leq \frac{1}{T} \int_0^{\infty} \bar{C}(t, \tau) \, d\tau .$$

Substituting (27) yields:

$$\sigma_{\tau} \leq A \Delta x^2 \frac{\tau_2 - \tau_1}{T}$$

where we have used [11]:

$$\int_0^p E(\alpha x) \, dx = p E(\alpha p) + (1 - e^{\alpha p})/\alpha ,$$

$$E_1(-x) = -E_1(x) .$$

As a contrast, the variance of an O-U record is calculated. This can be done exactly. Using (1) in (42):

$$\sigma_{\tau_0} = \Delta x^2 \frac{\tau}{T} \left[ 1 - \frac{\tau}{2T} (1 - e^{-2T/\tau}) \right] .$$
For a small relaxation time $\tau \ll T$:

$$\sigma_{x0} \approx \frac{\Delta x^2}{T^2}. \quad (48)$$

The same result is obtained if the measure for the speed of convergence, given by (44), is used. Particularly for white noise, which can also be represented by an O-U process with a relaxation time equal to the mean time between two collisions (mean free path assumption), it can be seen from (48) that the variance of a noise record is negligible small. This is not the case for the averaged process in the M-model, see equation (45). Its autocovariance approaches the time axis much slower. It appears also that the upper bound (44) is too high. For a realistic spectrum of, say, eight decades the lower limit for the time constant will be of the order of days, so that according to (45), the measurements are not reproducible for reasonable record lengths. The approximation $t \ll T$ is therefore not accurate enough and the extension of the integration to infinity for the upper bound of $\sigma$ is probably not allowed since the autocovariance levels off too slowly. Nevertheless equation (45) shows clearly that the $1/f$ records within the context of the M-model are very noisy: the lower the low-frequency limit, the larger the fluctuations.

1.4 Discussion. — The G-R theorem in the multivariate case was derived in [3, 4] along similar lines. It was our purpose to show in a coherent way that the Langevin and G-R methods lead to an O-U process, which is the most general Gaussian stationary Markov process. This is important in our case since those physical processes which do not satisfy these criteria cannot be treated with Langevin or G-R methods. In [3, 5] a phenomenological relaxation matrix is defined which already implies small deviations from an equilibrium value. Processes non linear in their state variable are therefore linearized. This leads to difficulties for the case where the relaxation back towards the equilibrium state cannot be described by the macroscopic equation. In equilibrium the variance of the G-R theorem [3, 5] is identical with (13) in the one dimensional case. We have used a somewhat different vocabulary however. Smoluchowski’s equation in [3] is termed the Chapman-Kolmogorov equation since the former has been rediscovered rigorously by the latter authors within the context of the theory of stochastic processes. The same holds for what is termed the master equation in [3] where we have used Kolmogorov’s system of differential equations. What are termed the Fokker-Planck moments in [3, 5] are in the stochastic literature the derivative, or infinitesimal or incremental moments, where we have used the latter (one may get the impression from Fokker-Planck moments that they only belong to a Fokker-Planck type of description). Finally, the scepticism from [3] about the foundations of the Langevin procedure is unfounded for at least the white source case. One always can describe with a differential equation a first order autoregressive process and show by Wold’s theorem that an arbitrary stationary Markov process has an autoregressive or moving average representation [10].

The derivation of the one dimensional result from [4] differs at first sight from the multivariate approach of [3] and [5]. The origins and the used concepts are quite similar however. The generalized birth and death process, which was the starting point, represents the equilibrium result of Kolmogorov’s forward equation for a Markov process with local changes, so that we already dealt with a stationary Markov process. The normal assumption [4] at equilibrium then leads to the final result, which is the O-U process.

Up to now before averaging of the basic processes the statistical description refers to processes which are classical in the thermodynamic sense. In equilibrium we may assume that a time shift has no impact upon the $n$-joint density function, or in the weaker case, that a mean exists and the covariance only depends on the time shift (arbitrary origin). The stationarity assumption can be accounted for in a large majority of cases. This also holds for the Gaussian approximation. It has an almost universal validity. Almost all sufficiently large systems can be linearized (small deviations from equilibrium) so that a normal approximation becomes highly accurate. Particularly in thermostatistics where the equilibrium theory is approached through the method of the Gibbs ensembles. The application of Liouville’s theorem (phase space picture) assures the stationarity assumption, where as the application of the partition function assures small relative fluctuations (Lagrange multipliers). From the theory of stochastic processes [10] it then follows that the system is also Markovian since a strictly stationary Gaussian process is automatically Markovian for linear processes (or those which can be linearized). For irreversible thermodynamics the O-U process is also of great importance, since Onsager’s relationships require a linear stationary Gaussian Markov process [15]. In short, a large number of realistic physical processes converge in their parameters to a system which is describable by the Fokker-Planck equation (8). Even in the nonlinear case the system is supposed to be large enough to ensure a rapid converging of some expansion, sharply peaked transition probabilities, and additive rate processes (Master equation expansion, path integral representation and other perturbation approximations). Finally, the result of fluctuation-dissipation theory is obtained from the master equation treatment in the thermodynamic limit. All these examples show how accurate the O-U process is as a description for various systems, which are large enough and have a small relative fluctuation.

This does not mean that $1/f$ noise also belongs to this group. Questions like stationarity, Gaussianity, Markovian or equilibrium behaviour, have not been
resolved yet rigorously. There seems to be some evidence that it is an equilibrium effect [16] (2), which contradicts the assumption of a stationary Gaussian Markov process (SGMP) [15] since this process automatically leads to an exponential auto-correlation function. As we have seen, after averaging, the M-model yields a [14] non-Markovian process. Non-Gaussian stationary and linear Markov processes will not be discussed here since we are interested in the second order properties (spectrum) and for those linear processes which have a non-Gaussian distribution (Bose Einstein for instance) the autocovariance from the G-R theorem or from Langevin methods is still exact. If now the M-model is needing a non-Markovian system for a derivation of its spectrum, then this implies that 1/f noise originates from a system not in equilibrium, since linear irreversible thermodynamics imply SGMP processes and thus exponential autocorrelation functions [14]. This does not mean that linear response theory and the fluctuation dissipation theorem do not work far from equilibrium. For those cases where these approaches are still accurate, the M-model therefore also breaks down for non-equilibrium situations, unless we deal with a system with a memory (non-white source in the Langevin picture). We thus conclude that the M-model treats 1/f noise as a Gaussian stationary non-Markovian process, which is not in equilibrium. This contradicts recent developments [16], treating 1/f noise as an equilibrium phenomenon, but it is consistent with the experimental fact that its spectral density can difficultly be related to the admittance of the system.

It will be shown elsewhere that the application of the M-model in devices, on the basis of the derived conditions from this paper, becomes a rather delicate matter. In other words, it is too simple to explain such a specific phenomenon as 1/f noise in such a complex system as a simple surface. It breaks down for a system with a strong electron phonon coupling.

This does not rule out that the basic idea of mixing certain processes can be of great value for explaining a certain type of 1/f noise. (It has been suggested in [17] that the 1/τ superposition could serve as a more general explanation for 1/f noise.) Though the M-model only deals with stationary processes, the idea of averaging (mixing) certain processes can also be applied to nonstationary processes. For this case the time and ensemble average cannot be interchanged and the autocovariance is determined from a single record, which is then subsequently averaged over its ensemble. For infinite truncation time a constant spectral density can be obtained in a number of cases (simplest example: the Wiener process). The averaging and its physical interpretation is now more difficult.

2. Conclusion. — For a correct application of the M-model, utilizing SHR statistics, the G-R theorem and simple Langevin methods, a system is required which can be described by an O-U process.

The question whether a superposition of relaxation spectra could serve as a more general explanation for 1/f noise, showed the following:

(i) The M-model mixes independent, Gaussian and stationary Markov processes, yielding a Gaussian, stationary but non-Markovian process.

(ii) It treats the 1/f noise as a non-equilibrium effect.

(iii) It does not work for systems which cannot be linearized e.g., various non-Markovian processes and nonlinear (small) systems.

(iv) A suitable mixing (not necessarily 1/τ) of O-U processes can serve as a prediction for 1/f noise on some occasions.

References


(2) This will be discussed elsewhere since a complete phenomenological theory of irreversible processes could be based upon SGMP’s [15].