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SOME PROPERTIES OF THE PHENOMENOLOGICAL RELAXATION MODES OF G–R NOISE

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Synopsis

Some properties are derived for the eigenvalues of the phenomenological relaxation matrix. The normal mode expressions for a thermal and steady state g–r process are discussed and partly improved. The tacid assumptions in the literature that the eigenvalues are always real and the plateau constants of the autovariance modes are positive are shown to be incorrect. Various forms for the relaxation matrix and their connections are discussed for systems with particle conservation (charge neutrality).

1. *Introduction.* Generation–recombination (g–r) noise in a semiconductor with s participating energy levels can be described as an $s - 1$ dimensional Markov process if there is a charge neutrality constraint. Accordingly, the correlation function is generally a sum of $s - 1$ exponentials, with decay times τ_k ($k = 1, 2 \ldots s - 1$), which are the reciprocal eigenvalues of the phenomenological relaxation matrix M of the system of linearized rate equations. The spectral densities of the electron or hole fluctuations can be written as the sum of $s - 1$ modes, $\sum_k A_k/(1 + \omega^2\tau_k^2)$. Expressions for these modes can be derived with a master-equation approach (van Vliet, Fassett[1]; Lax[2]) or with a Langevin procedure (Wessels[3]). It has been tacidly assumed by most investigators in this field that the τ's are real and that the A's are positive. Computer calculations showed that this is not always correct. For the nonthermal equilibrium steady state (Wessels and Kruizinga[4]) it was clear that both complex lifetimes τ_k and negative plateau constants A_k can occur. For the thermal equilibrium state more can be said. The eigenvalues are in that case real and positive semidefinite as will be shown here. The claim of ref. 4 that the plateau constants must be positive is incorrect, however, as is apparent from the particular three-level

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models considered by Colligan and van Vliet [5]) for gold-doped silicon. Nevertheless, in view of the fact that the integral over the spectral density represents a carrier variance or covariance, certain limitations on the *sum* of the normal modes must apply.

In this paper, which is based on Wessels's Ph. D. thesis with some extensions, we shall briefly state some properties of the eigenvalues of the phenomenological relaxation matrix. We shall do this for the matrix with charge neutrality constraint, M, as well as for a similar matrix in which this constraint is ignored, $\hat{M}$. The properties of the latter are more simple. For thermal equilibrium, the results will be found to be in harmony with the general considerations of irreversible thermodynamics stated by de Groot and Mazur [6]). The steady state results indicate that the τ_k's can be complex with positive real parts.

The normal mode expressions of ref. 1 will be corrected for the steady state when the τ_k's are not necessarily real. Further, asymptotic forms for the normal mode sum for small and large ω will be stated. The notation of ref. 1 will be followed.

2. *Properties of the relaxation matrix.* We consider transition rates $p_{ij}(\boldsymbol{n})$ between s energy levels $\varepsilon_1, \ldots \varepsilon_s$ with electron occupancies $n_1, \ldots n_s$. The rate equations for the conditional averages are

$$\mathrm{d}\langle n_i\rangle_{\mathrm{cond}}/\mathrm{d}t = \sum_{j=1}^{s} [\langle p_{ji}(\boldsymbol{n})\rangle_{\mathrm{cond}} - \langle p_{ij}(\boldsymbol{n})\rangle_{\mathrm{cond}}]. \tag{2.1}$$

These equations must be linearized for the fluctuations, which are generally subject to a charge constraint, $\sum_{i=1}^{s} \langle \Delta n_i\rangle_{\mathrm{cond}} = 0$, as is apparent from the form of the p_{ij}. In the literature this has usually been affected by elimination of the variable $\Delta n_s(t)$. It is advantageous, however, for some considerations, to carry along this dependent variable. Thus, we can write the linearized equations in two forms. Let $p_{ij}(\boldsymbol{n})$ denote the rates expressed in the vector variable $\boldsymbol{n} = \{n_1, \ldots n_{s-1}\}$ and let $p_{ij}(\mathfrak{n})$ denote the rates expressed in the vector variable $\mathfrak{n} = \{n_1, \ldots n_s\}$. Then

$$\frac{\mathrm{d}\langle\Delta n_i\rangle_{\mathrm{cond}}}{\mathrm{d}t} = -\sum_{j=1}^{s-1} M_{ij}\langle\Delta n_j\rangle_{\mathrm{cond}} \qquad (i = 1, \ldots s-1) \tag{2.2}$$

with

$$M_{ij} = \frac{\partial}{\partial n_j} \sum_{k=1}^{s} [p_{ik}^0(\boldsymbol{n}) - p_{ki}^0(\boldsymbol{n})], \tag{2.3}$$

where the super zero stands for the value evaluated at $\boldsymbol{n} = \langle\boldsymbol{n}\rangle$; alternately

$$\frac{\mathrm{d}\langle\Delta n_i\rangle_{\mathrm{cond}}}{\mathrm{d}t} = -\sum_{j=1}^{s} \hat{M}_{ij}\langle\Delta n_j\rangle_{\mathrm{cond}} \qquad (i = 1, \ldots s) \tag{2.4}$$

with

$$\hat{M}_{ij} = \frac{\partial}{\partial n_j} \sum_{k=1}^{s} [p_{ik}^0(\mathfrak{n}) - p_{ki}^0(\mathfrak{n})]. \tag{2.5}$$

We write this also in a slightly different form. Let

$$\sum_{k=1}^{s} [p_{ik}^0(\mathfrak{n}) - p_{ki}^0(\mathfrak{n})] \equiv F_i(\mathfrak{n}). \tag{2.6}$$

Then

$$\hat{M}_{ij} = \frac{\partial F_i(\mathfrak{n})}{\partial n_j} \equiv \partial_j F_i \qquad (i, j = 1, \dots s); \tag{2.7}$$

$$M_{ij} = \frac{\partial F_i(\mathfrak{n})}{\partial n_j} + \frac{\partial F_i(\mathfrak{n})}{\partial n_s} \frac{\mathrm{d}n_s}{\mathrm{d}n_j} =$$

$$= \partial_j F_i - \partial_s F_i = \hat{M}_{ij} - \hat{M}_{is} \qquad (i, j = 1, \dots s - 1). \tag{2.8}$$

Further, because of the charge constraint

$$\sum_i F_i = 0 \qquad \text{and} \qquad \sum_i \hat{M}_{ij} = 0. \tag{2.9}$$

From the latter property it follows that $\det(\hat{\mathbf{M}}) = 0$, so that one eigenvalue is zero. We now state some further properties.

a) The other eigenvalues of $\hat{\mathbf{M}}$ are identical with those of $\mathbf{M}$. We consider the secular determinant for the eigenvalues of $\hat{\mathbf{M}}$, *i.e.*

$$|\hat{\mathbf{M}} - \lambda \mathbf{I}| = 0.$$

We subtract the last column from the other columns. The result can be written in the partitioned form

$$\left| \begin{array}{c|c} \mathbf{M} - \lambda \mathbf{I} & \begin{matrix} \hat{M}_{1s} \\ \vdots \\ \hat{M}_{s-1,s} \end{matrix} \\ \hline \hat{M}_{s,1} - \hat{M}_{ss} + \lambda \dots M_{s,s-1} - M_{s,s} + \lambda & \hat{M}_{ss} - \lambda \end{array} \right| = 0.$$

Next we add the first $(s - 1)$ rows to the last one. Because of (2.9) the result is

$$\left| \begin{array}{c|c} \mathbf{M} - \lambda \mathbf{I} & \begin{matrix} \hat{M}_{1s} \\ \vdots \\ \hat{M}_{s-1,s} \end{matrix} \\ \hline 0 \; 0 \; \dots\dots \; 0 & -\lambda \end{array} \right| = 0. \tag{2.10}$$

Accordingly, the eigenvalues of $\hat{\mathbf{M}}$ are the $s - 1$ eigenvalues of $\mathbf{M}$, in addition to the eigenvalue zero.

b) For one-electron transitions all eigenvalues are positive or have a positive real part.

In order to prove this, we notice that generally for an electron gas the rates $p_{ij}(\mathfrak{n})$ are monotonically increasing functions of n_i and decreasing functions of n_j (for one electron transitions $i \to j$). Accordingly from (2.6) we find

$$\partial_i F_i \geq 0 \qquad \text{and} \qquad \partial_j F_i \leq 0 \qquad (j \neq i). \tag{2.11}$$

Whence with (2.7) and (2.9)

$$\hat{M}_{ii} \geq 0, \tag{2.12}$$

$$\sum_{i \neq j} |\hat{M}_{ij}| = - \sum_{i \neq j} \hat{M}_{ij} = \hat{M}_{ii} \geq 0. \tag{2.13}$$

Moreover, the equal signs in these inequalities cannot hold for all i, since only few rates are quasi-independent of the occupancies (like band to band transitions). Now according to Gerschgorin's theorem[7]) the eigenvalues of $\hat{M}$ are within the domain formed by the union of all circles with centers $\hat{M}_{ii}$ and radii $\sum_{i \neq j} |\hat{M}_{ij}|$. Hence, they lay within the circle with diameter OA where O is the origin and A is the point $2 \max_i \hat{M}_{ii}$ on the real axis. Hence, the real parts are positive.

Whenever there are impact ionization processes or Auger transitions, the above result still holds for rates that involve two electrons from the same level, *e.g.* $i + i \to j$ or, $i \to j$ conditional to $i \to k$. However, for other processes, such as $i + j \to k$ or $i + j$ conditional to $k \to l$, the second inequality of (2.11) cannot be proved. We have not been able to find a domain in the positive half plane to which the eigenvalues are confined in the general case.

c. The sum of the squares of the (conjugate complex) eigenvalues is positive. This can be seen as follows:

$$\begin{aligned} \sum_{k=1}^{s} \lambda_k^2 &= (\sum_k \lambda_k)^2 - 2 \sum_{i<j} \lambda_i \lambda_j = \\ &= (\sum_i \hat{M}_{ii})^2 - 2 \sum_{i<j} (\hat{M}_{ii}\hat{M}_{jj} - \hat{M}_{ij}\hat{M}_{ji}) = \\ &= \sum_i \hat{M}_{ii}^2 + 2 \sum_{i<j} \hat{M}_{ij}\hat{M}_{ji} > 0, \end{aligned} \tag{2.14}$$

where eq. (2.11) has been used.

This property gives further restrictions on the location of the eigenvalues. For instance, in a three level system, $\lambda_1 = 0$ and $\lambda_{2,3} = \mu \pm i\nu$, with $-\pi/4 <$ argument $\lambda_{2,3} < \pi/4$.

d) In thermal equilibrium when detailed balance applies the eigenvalues are real and positive (except for $\lambda = 0$).

This statement holds for any thermal Markov process[6]) and follows from irreversible thermodynamics. We can then write

$$M = R^{-1} \mathsf{s}^0, \qquad \hat{M} = \hat{R}^{-1} \hat{\mathsf{s}}^0 \tag{2.15}$$

where R^{-1} (or $\hat{R}^{-1}$) is the generalized Onsager coefficient matrix and $-\mathbf{s}^0$ (or $-\hat{\mathbf{s}}^0$) consists of the second order entropy derivatives with respect to $n_1, \ldots n_{s-1}$ (or $n_1, \ldots n_s$). The form for R and $\hat{R}$ is the same, *i.e.*,

$$(\overset{(\wedge)}{R}{}^{-1})_{ii} = \sum_{j=1}^{s}{}' \, p_{ij}^0/k,$$
$$(\overset{(\wedge)}{R}{}^{-1}{}_{ij}) = -\, p_{ij}^0/k \qquad (i, j = 1, \ldots s-1 \text{ or } s), \tag{2.16}$$

where k is Boltzmann's constant. This symmetric matrix has real eigenvalues and by statement 2 is positive definite. The symmetric matrix $\overset{(\wedge)}{\mathbf{s}}{}^0$ is likewise positive semidefinite. This proves the statement. The form of $\hat{\mathbf{s}}^0$ is diagonal, contrary to that of $\mathbf{s}^0$. The elements are given by (compare ref. 1, eq. (221)):

$$s_{ij}^0 = k\left[\frac{1}{\xi_s n_s^0} + \frac{\delta_{ij}}{\xi_i n_i^0}\right]; \tag{2.17}$$

$$\hat{s}_{ij}^0 = k\delta_{ij}/\xi_i n_i^0; \tag{2.18}$$

where $\xi_i = 1 - n_i/N_i$ for N_i impurity levels, and ξ_i is a ratio of Fermi integrals for degenerate bands (ref. 1, eqs. (218)–(220)).

3. *Properties of the plateau constants.* For the computation of the spectra according to the correlation function method it is necessary to work with the restricted variables, $n_1, \ldots n_{s-1}$. Setting $\Delta n_i = \alpha_i$, the general steady state result for the spectra can be given in the matrix form (ref. 1, eq. (67)):

$$(M + \mathrm{j}\omega I)\, S(\tilde{M} - \mathrm{j}\omega I) = 2\langle\alpha\alpha\rangle\, \tilde{M} + 2M\langle\alpha\alpha\rangle = 2B(\boldsymbol{n}_0). \tag{3.1}$$

From the Langevin equation procedure, a similar result is also readily obtained for the unrestricted set of variables $n_1, \ldots n_s$ (ref. 3; see also eq. (2.4)):

$$(\hat{M} + \mathrm{j}\omega I)\, S(\tilde{\hat{M}} - \mathrm{j}\omega I) = 2\hat{B}(\mathbf{n}_0). \tag{3.2}$$

The elements of the matrices B and $\hat{B}$ are identical except that the latter has an extra row and column which convey no information. As always,

$$B = 2kR^{-1}; \qquad \text{likewise} \qquad \hat{B} = 2k\hat{R}^{-1}. \tag{3.3}$$

The elements of the spectral matrix $\hat{S}$ are identical with those of S except that an extra row and column is to be added, subject to the conditions $\sum_{i=1}^{s} \hat{S}_{ij} = \sum_{j=1}^{s} \hat{S}_{ij} = 0$*. Simple algebra shows that (3.1) and (3.2) are consistent taking account of relationship (2.8). However, a general in-

* It is to be noted that integration of $\hat{S}$ over all frequencies yields the *restricted* covariance matrix $\langle\alpha\alpha\rangle$. This is so because the $\hat{B}$ matrix, as well as the B matrix (as given by eqs. (2.16) and (3.3)), accounts automatically for the charge constraint.

version of (3.2) is impossible because $\det(\hat{M}) = 0$*. On the contrary, the inversion of (3.1) is immediate. For all ω:

$$S = 2(M + j\omega I)^{-1} B(\tilde{M} - j\omega I)^{-1}. \tag{3.4}$$

The asymptotic forms for small and large ω are:

$$S(\omega \text{ small}) \approx 2M^{-1}B\tilde{M}^{-1}; \tag{3.5}$$

$$S(\omega \text{ large}) \approx 2B/\omega^2. \tag{3.6}$$

Normal mode expressions are possible for the general case that $\det(M) \neq 0$. Let $G = \text{Re } S$, and let c^{-1} be the matrix composed of the eigenvectors of M (*i.e.*, cMc^{-1} is diagonal). For thermal equilibrium the result has been correctly stated before (ref. 1, eq. (85)):

$$G_{mn} = 2 \sum_{i,k=1}^{s-1} c_{mi}^{-1} c_{ik} B_{kn} \tau_i^2/(1 + \omega^2 \tau_i^2). \tag{3.7}$$

For the steady state case we must also consider the possibility that τ_i is complex. Let $\tau_i^{-1} = \mu_i + j\nu_i$. The correct result is then [cf. ref. 1, eqs. (87)–(89)]:

$$G_{mn} = 2 \,\text{Re} \sum_{ihkl} \left\{ \frac{c_{mi}^{-1} c_{nh}^{-1} c_{ik} c_{hl} B_{kl}}{[\mu_i + j(\nu_i + \omega)][\mu_h + j(\nu_h - \omega)]} \right\}. \tag{3.8}$$

Generally, the matrix c has complex elements. Likewise, in terms of the variances [cf. ref. 1, eqs. (90)–(92)]:

$$G_{mn} = 2 \,\text{Re} \sum_{kl} \left\{ \frac{\langle \alpha_l \alpha_n \rangle \, c_{mk}^{-1} c_{kl}}{\mu_k + j(\nu_k + \omega)} + \frac{(\alpha_l \alpha_m) \, c_{nk}^{-1} c_{kl}}{\mu_k + j(\nu_k - \omega)} \right\}. \tag{3.9}$$

(This expression is symmetrical in m and n as we see by replacing j by $-j$, and by noticing that c^{*-1}_{nk} occurs in conjunction with the complex conjugate eigenvalue for which $\nu_k \to -\nu_k$.)

A priori, we can say nothing about the sign of the elements of the eigenvectors which make up c_{kl}^{-1}. Simple examples have shown that even in thermal equilibrium the plateaus of each normal mode can have either sign. The total spectrum of a self variance (like G_{mn}) must be positive definite, however. One easily recovers the sums (3.5) and (3.6) from either expression (3.7), (3.8) or (3.9), by eliminating the factors τ by

$$\sum_k c_{ik} M_{kj} = \lambda_i c_{ij} = c_{ij}/\tau_i,$$

* The only published method which uses the complete set of Langevin equations, without elimination of n_s, is that of Champlin[8]). Thus, for an s-level problem, he constructs an s-terminal R–C equivalent network, of which, in the absence of dielectric relaxation, one R–C time is zero.

and

$$\sum_k M_{jk}^{-1} c_{ki}^{-1} = c_{ji}^{-1}/\lambda_i = c_{ji}^{-1}\tau_i.$$

For instance, for the expression (3.8) the high frequency asymptote is immediately seen to be equal to (3.6); we note that the diagonal elements of B are positive. The low frequency limit is

$$G_{mn} = 2 \sum_{ijklpq} c_{ik}c_{jl}B_{kl}M_{mp}^{-1}c_{pi}^{-1}M_{nq}^{-1}c_{qj}^{-1} = 2 \sum_{qp} M_{mp}^{-1}B_{pq}M_{nq}^{-1},$$

in accord with (3.5). Some algebra shows that the diagonal elements ($m = n$) are again positive.

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Note added in proof. Recently Kleinpenning of this laboratory showed that the plateau constants A_k in a three-level system in thermodynamic equilibrium must be positive. The result, which has not yet been published, is in contradiction to the results of Colligan and Van Vliet (*loc. cit.*).