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NOTE

Chaotic Algorithms: A Numerical Exploration of the Dynamics of a Stiff Photoconductor Model

The photoconducting property of semiconductors leads, in general, to a very complex kinetics for the charge carriers due to the non-equilibrium processes involved. In a semiconductor with one type of trap, the dynamics of the photoconducting process are described by a set of ordinary coupled non-linear differential equations given by [1]

$$\frac{dn}{dt} = G - n\alpha_1(N_t - m) + \gamma_1 m - c_1 n$$
$$\frac{dm}{dt} = n\alpha_1(N_t - m) - \delta_0 mp - \gamma_1 m \qquad (1)$$
$$\frac{dp}{dt} = G - \delta_0 mp - c_2 p,$$

where n and p are the free electron and hole densities, and m the trapped electron density at time t. A physical description and values for the seven parameters are given in Refs. [1, 2], respectively.

So far, there is no known closed form solution for the set of non-linear differential equations (1), and therefore, numerical integration techniques have to be employed, as, for example, the standard procedure of the Runge–Kutta (RK) method. Now then, each one of the mechanisms of generation, recombination, and trapping has its own lifetime, which means that different time constants are to be expected in the time dependent behavior of the photocurrent. Thus, depending on the parameters of the model, the system (1) may become stiff if the time scales between n, m, and p separate considerably. This situation may impose a considerable stress upon a fixed step numerical algorithm as the RK, which may produce then unreliable results, and other methods have to be considered.

Therefore, the purpose of this note is to examine, for a critical range of parameters, the results of the numerical integration of the stiff system (1) obtained by standard numerical schemes, such as the single-step fourth-order Runge–Kutta method and the multistep Gear method [3], the latter being appropriate for a rigid system of equations.

It was found that, in general, both integrators lead to the same solution, see Fig. 1, but for certain parameters, for which the separation of time scales is considerable, the results begin to differ drastically. Even though both integration schemes lead almost always to the same asymptotic state for system (1), the main difference was found at the transient response with the results depending very sensitively on the size of the RK integration step.

Figure 2 shows the results of (1) according to the 4-RK integration scheme, where it is possible to see the underlying irregular transient, with ''turbulent'' or chaotic regions alternating with ''laminar'' or periodic ones. This intermittent behavior is followed by a reverse period doubling process through which the system finally reaches an equilibrium or steady state. On the contrary, for the same set of parameters, integration with the Gear scheme yields a very regular behavior similar to that of Fig. 1.

The amazing behavior of Fig. 2 could be explained by taking into account the unavoidable discretization in time of (1) by the numerical method. In the RK method the iteration array sets explicitly the x_{k+1} variable as a non-linear function of x_k [3]. Now, the chaotic transient with its period-doubling bifurcation of Fig. 2 closely resembles other period-doubling processes, as for instance, the well-known logistic map [4], $x_{k+1} = \mu x_k(1 - x_k)$.

Before looking for the common features between the standard discretization of the RK scheme and the logistic map, let us quickly set the differences. First, the chaotic map produced by the logistic map is not in time, as in Fig. 2. It is a plot of the steady state of x_k versus the parameter μ. Second, the onset of chaos exhibited by the logistic equation is reached through period-doubling bifurcations [4], while the present system (1) suppresses chaos through reverse period-doubling bifurcations.

Now, since the chaotic transient occurs in the time domain, apparently the time should have to appear explicitly into Eqs. (1), which is not the case for the autonomous dynamical system (1). If instead the numerical algorithm itself is examined, some similarities between the logistic map and the RK method may become apparent. But the time t does not appear explicitly in the RK discretized version either, and it should be expressed as the iteration factor n times the integration step, $h = t_{k+1} - t_k$, that is, a factor nh multiplying the non-linear term for x_k in order

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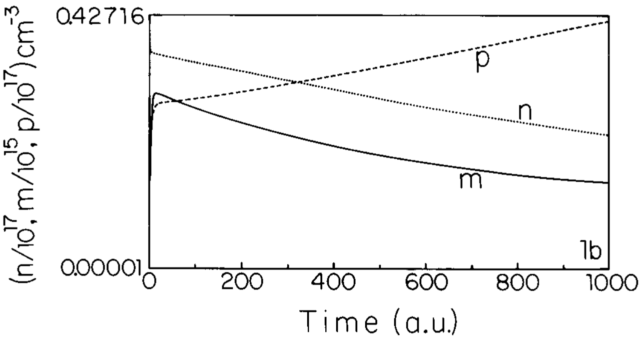

FIG. 1. Numerical integration of the photoconductor equations for $\alpha_1 = 2.5 \times 10^{-15}$ cm^{-3} sec^{-1} and $N_t = 5 \times 10^{14}$ cm^{-3}. The results with the fourth order Runge–Kutta and the Gear algorithms are identical for $h \leq 0.01$.

to play the same role in the time domain as the parameter μ of the logistic map in the parameter domain [4]. Nevertheless, such a factor nh could be found in the iteration of the RK scheme as follows.

Consider a simple non-linear differential equation,

$$dy/dx = \lambda y^2. \tag{2}$$

Discretization of (2) through the forward Euler algorithm [3] (which is the fundamental algorithm for the RK formulas) produces

$$dy/dx = \lambda y^2 \approx (y_{k+1} - y_k)/h \Rightarrow y_{k+1} = y_k(1 + \lambda h y_k), \tag{3}$$

where h is the integration step. Similarly, it can be shown that the second order RK scheme over (2) yields

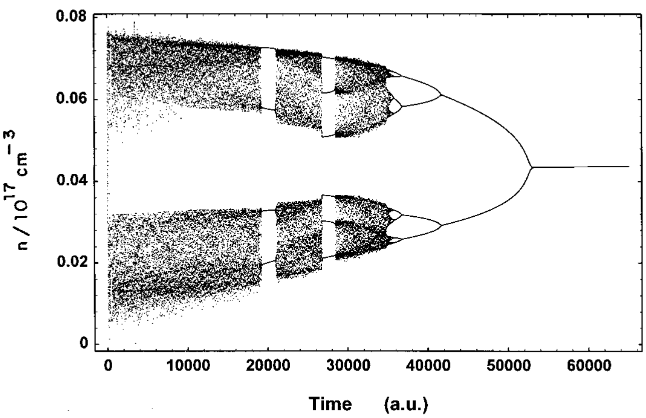

FIG. 2. Complete transient of the free electrons obtained with the 4-RK algorithm for $\alpha_1 = 4.64 \times 10^{-14}$ cm^{-3} sec^{-1} and $h = 0.01$. The lines joining the successive points generated by the numerical integration were removed to reveal the underlying intermittent chaotic behavior and the breakdown through reversal bifurcations to the steady state.

$$y_{k+1} = y_k(1 + \lambda h y_k + (\lambda h)^2 y_k^2 + (1/4)(\lambda h)^3 y_k^3). \tag{4}$$

For $\lambda h < 1$, Eq. (4) tends to Eq. (3). Also, for $\lambda < 0$ and after simple linear transformations, it is clear that (3) is equivalent to the logistic map in terms of the parameter λh; yet time, as in $(nh)\lambda$, is not explicit in (3), nor in (4). Now, y_{k+1} is a non-linear function of y_k which in turn can be expressed as a function of the initial condition y_0 when iterating back to $k = 0$. Moreover, it can be shown for a successive few iterations of Eq. (3) that terms of the form $(1 + \lambda h y_0 w)^n$ where $w = (1 + \lambda h y_0)$ will appear. This corresponds to an expression of the form $(a + b)^n$, with $a = 1 + (\lambda h y_0)^2$ and $b = \lambda h y_0$ and, if $a^2 > b^2$, which is the present case, it is possible to expand according to

$$(a + b)^n = a^n + (n/1!)a^{n-1}b + (n(n-1)/2!)a^{n-2}b^2 + ..., \tag{5}$$

where it is clear the presence of terms involving nb, $n(n-1)b^2$, etc., that is, $nh\lambda y_0$, $n(n-1)(\lambda h y_0)^2$, etc. In this way, factors of the form nh will emerge through the iterations of the discrete version of (2), and for extension, in the non-linear model (1). Interestingly, the application of an implicit algorithm as, say, backward Euler [3] (which is the fundamental algorithm for the Gear formulas) to the example (2), does not produce binomial expressions as those described in (5); that is, transient chaos is not to be expected since the time factor nh will not appear explicitly. Therefore, discretization of (1) through explicit algorithms such as forward Euler or RK should lead to a non-linear iterative structure resembling that of the logistic map, with an explicit "parameter" involving the factors nh; so that, as time progresses, the possibility of observing chaos in the time series becomes plausible.

As the photoconductor equations involve more non-linear terms than the simple test equation (2), a much complex dynamical behavior is to be expected for the resulting discrete version of (1). Therefore, the numerical outcome will be strongly problem dependent, as found by some investigators on the dynamics of numerical methods [5, 6].

In a study by M. Ablowitz *et al.* [5] it has been demonstrated that standard discretization through a RK routine of the cubic non-linear Schrödinger equation may lead to numerical induced chaos related to the homoclinic structure associated with the equation. Similarly, in a study by H. C. Yee *et al.* [6], spurious steady states were reported when integrating non-linear differential equations models with standard explicit solvers. At this point, it is important to stress the similitude of the photoconductor set of equations (1) with the well known Lorenz equations, for which its homoclinic structure [4] has been extensively studied. Considering that the Lorenz equations are comparatively simpler than the set (1), it is clearly to be expected that a more complex underlying homoclinic structure for the photoconductor exists, yet remains to be studied, and thus, with consequences in the unstable behavior regarding standard explicit numerical computations. In the present study, however, the results go beyond just spurious numerical behavior, as it is seen how the photoconductor time series undergoes intermittent chaotic behavior that breaks down through well defined reverse bifurcations, according to an antimonotonic structure described by some authors, see Ref. [7].

In this context of a complex model with a possible homoclinic structure together with the stiffness of (1), and contrary to the implicit Gear scheme, the RK iteration of system (1) may induce numerically the observed chaotic transient and the reverse bifurcation process; this may be achieved as a result of the discretization through deterministic non-linear iterative rules specific for explicit standard algorithms. This is a speculative approach: the intention of this work is to present for the first time such remarkable phenomena and to indicate some possible sources of such peculiar behavior.

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