Toroidal Oscillation in a 3-Variable Abstract Reaction System

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An example of a chemical reaction system producing a type of oscillation that is close to a quasi-periodic oscillation is presented. Such system may help clarify the relationship between quasiperiodicity and chaos.

Introduction

Abstract reaction kinetics is dynamically universal \(^1,2\). It not only allows for 3-variable chaos, as shown recently \(^3,4\), but also for 3-variable toroidal oscillations \(^5\). These oscillations, of which “quasi-periodic oscillations” form a structurally unstable special case \(^6\), are characterized by trajectories that form spirals in close neighborhood to a torus in state space. The time-behavior of the variables hereby looks like a periodically amplitude-modulated oscillation plus a DC-component.

An Example

A first chemical example system is depicted in Figure 1. The dashed arrows correspond to catalytic couplings. The corresponding rate equations are, under the usual assumptions of well-stirredness, isothermy, and an appropriate concentration range:

\[
\begin{align*}
\dot{x} &= ax - y \frac{x}{x + K_1} + c \\
\dot{y} &= bx - z \frac{y}{y + K_2} \\
\dot{z} &= dx - e(x^2 + f) \frac{z}{z + K_3},
\end{align*}
\]

where \(a = a' - 1 - d\) and \(f = f' c_0/e\).

The equation is written in the usual non-explicit convention, that is, fast-reacting intermediates have been eliminated via a Michaelis-Menten type steady state approximation (cf. \(^7\)).

Simulation Results

In Fig. 2, a stereoscopic view of a segment of trajectory flow in state space is presented. The trajectories form a coil \(^8\) on the surface of a torus. The time-behavior of the 3 variables is shown in Figure 3. The system has been allowed some time to relax toward the asymptotic regime, after starting from nearby, but non-selected, initial conditions.

The flow of Fig. 2 looks very much like a quasi-periodic flow, that is, the trajectories do not close over the time span of the simulation. Nonetheless, none of the criteria for equations with truly quasi-periodic behavior (existence of a first integral of...
motion, vanishing divergence, or certain symmetry properties, respectively \(^6\)) applies to Eq. (1) if \(K = 0\). However, for \(K \to 0\) and \(a \to b\), Eq. (1) does possess truly quasi-periodic behavior \(^9\) in the limit. In that case, a whole 1-parameter family of invariant tori exists \(^9\).

It is to be expected that even simpler reaction schemes than the one of Fig. 1 will be able to produce the same type of behavior. The reason is, simply, that all the (formidable) nonlinearities of Michaelis-Menten type involved in Eq. (1) are not essential for the main result.

**Discussion**

Toroidal oscillations are of interest presently in nonlinear physics \(^{10-12}\) and economics \(^{13}\). In both fields (especially in hydrodynamics and economy) very large recurrence times are the rule. In turbulence theory the problem whether toroidal oscillation is a necessary — or at least frequent — step toward “chaos” is still an open question (see \(^{12}\)).

Chaos is possible in 3-variable reaction systems \(^3,4\), as well as in 3-variable models in hydrodynamics \(^4\) and lasers \(^{15,16}\). (Near-)quasiperiodic behavior, however, of 3-variable Euclidean systems has not yet been described in reaction kinetics. So far it was anticipated that chaos is easier to obtain than quasiperiodicity. The above example of a basically simple 3-variable “quasiperiodic” system of non-distributed type shows that such systems are not necessarily more complicated than the chaos-producing 3-variable systems. The essential component is a single nonlinear term of second order. Equations of the very type of Eq. (1) can also yield chaos \(^9\). In three dimensions, therefore, one way to obtain chaos is via an invariant torus. The underlying Poincaré map then is a “contracting ring map”. Thus, the two basic types of chaos (horseshoe map chaos and sandwich map chaos; see \(^{17}\)) can be complemented by a third type: ring map chaos \(^4,9\). However, it seems that toroidal oscillations are not a necessary (although, perhaps, a sufficient) condition for chaos.

In concrete chemical and biochemical systems (for example, in the glycolysis system \(^{18}\)) the occurrence probability for chaos is still greater than that for toroidal oscillation. While almost any double-loop reaction system (and even single-loop system) is likely to be capable of chaotic oscillations, especially of it contains a so-called double-periodicity, see \(^{19}\), toroidal oscillation seems, at the time being, to require more constituents (namely, a double-loop structure and a combination of catalytic influences of both first and second order on the same variable), if it is to occur in a network of strongly coupled chemical reactions. Nonetheless it is possible that toroidal oscillations will be observed in one cuvette some day. In two cuvettes (that is, with 2 independent oscillators), quasiperiodicity is, of course, unavoidable.

To conclude, another type of “exotic” oscillation has been found in 3-variable reaction kinetics, toroidal oscillation.

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