Two-dimensional spatiotemporal pattern formation in the double barrier resonant tunnelling diode

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Abstract. We present computer simulations of the spatio-temporal dynamics of the charge and current density distributions in a semiconductor nanostructure, the double barrier resonant tunnelling diode (DBRT), in the strongly nonlinear transport regime. Complex bifurcation scenarios, including bistability of stationary and oscillating space-time patterns, a subcritical Hopf bifurcation, a bifurcation by condensation of paths of spatially inhomogeneous limit cycles, and spatio-temporal period-doubling cascades to chaos, are revealed. Stable breathing, spiking, or partially homogeneous filamentary patterns are found in the dependence of the time-scale separation of the two dynamic variables. Our model is representative for a large class of globally coupled bistable reaction–diffusion systems of activator–inhibitor type in two spatial dimensions.

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1. Introduction

The double barrier resonant tunnelling diode (DBRT) is a semiconductor device which has received broad interest since the effect of resonant tunnelling was first observed in double barrier semiconductor structures [1]. Its nonlinear conduction properties are based upon quantum-mechanical phenomena [2] which entail the occurrence of negative differential conductance (NDC) due to resonant tunnelling [3]–[5]. This, together with charge accumulation in the quantum well between the energy barriers, results in a Z-shaped current–voltage characteristic [6] associated with bistability in a range of applied voltages. Depending upon the initial conditions, a state of high- or low-current density is observed. Such a bistability can lead to a variety of interesting phenomena, especially the lateral spatiotemporal pattern formation of the current density [6]–[11]. Consequently various spatiotemporal scenarios have been observed in the DBRT [12, 13]. In addition, complex spatiotemporal dynamics has been predicted by numerical simulations [14]–[16]. Even without consideration of the lateral re-distribution of charge, complex and chaotic oscillations have been found due to the inherent nonlinearity which results from the self-consistent treatment of the charge accumulation in the double barrier resonance [17]–[21]. In those models, as in the model studied in the present paper, which includes lateral charge re-distribution, the nonlinearity results from a mean-field approximation of the exact many-body quantum problem [22, 23].

From the viewpoint of nonlinear dynamics the model of the DBRT is a bistable, spatially extended reaction–diffusion system with global coupling [2, 24]. With the restriction to one (lateral) spatial degree of freedom the spatiotemporal scenarios occurring in this model have been studied extensively [14], even under the influence of time delayed feedback [25] or random fluctuations [26] or both [27]. If two lateral spatial dimensions, both perpendicular to the current flow, are considered, even richer spatio-temporal dynamics is possible. Self-organized patterns in the form of current filaments are expected to occur, and have indeed been found for a variety of nonlinear charge transport mechanisms in semiconductors [28]–[31]. While such spatio-temporal patterns have been studied in reaction–diffusion systems with local diffusive coupling, e.g., [32]–[34], much less is known for reaction–diffusion systems with global coupling. In this paper, we present an overview of complex dynamical scenarios which can occur in spatially two-dimensional systems with global coupling and Z-shaped current–voltage characteristics like the DBRT. The stability features of these patterns are complementary to systems with S-shaped current–voltage-characteristics [35, 36].

2. The model

Although modern experimental techniques provide ways and means to observe current filamentation in electronic devices [37]–[41], the measurement of the local current density distribution in nanostructure devices is still a very complicated task. Mathematical modelling remains one of the basic methods to study pattern formation involving the charge carrier dynamics in semiconductor nanostructures. For this purpose, we use a model for the DBRT suggested in [14] with two spatial degrees of freedom

\[
\frac{\partial a(x, y, t)}{\partial t} = f(a, u) + \nabla \cdot (D(a)\nabla a),
\]

\[\text{(1)}\]
\[ \frac{du(t)}{dt} = \frac{1}{\varepsilon} (U_0 - u - rJ(a, u)). \]  

(2)

All quantities in this model are dimensionless. In terms of nonlinear dynamics, this is a reaction–diffusion model of activator–inhibitor type, where \( a \) is the activator and \( u \) is the inhibitor. The dynamical variable \( a(x, y, t) \) describes the charge carrier density inside the quantum well, which depends on space and time. The second variable \( u(t) \) is the voltage drop across the device and depends only on time. The nonlinear function \( f \) models the net tunnelling rate of the electrons through the two energy barriers into and out of the quantum well, and \( D(a) \) is the effective diffusion coefficient, describing the lateral re-distribution of the electrons within the quantum well along the \( x-y \)-directions perpendicular to the current flow. The global term \( J = \frac{1}{L_x L_y} \int_0^{L_y} \int_0^{L_x} j \, dx \, dy \) gives the total current through the device, where \( j(a, u) = \frac{1}{2} (f(a, u) + 2a) \) describes the local current density in the device. The system is assumed to satisfy no flux Neumann boundary conditions and its lateral lengths are fixed at the values \( L_x = L_y = 30 \). Equation (1) is the local balance equation of the charge in the quantum well, and the equation (2) represents Kirchhoff’s law of the circuit in which the device is operated. The external bias voltage \( U_0 \), the dimensionless load resistance \( r \), and the timescale ratio \( \varepsilon \) of the dynamics of \( u \) and \( a \) are parameters; \( \varepsilon \) plays the role of a bifurcation parameter which determines the stability of the fixed points in the system [25]. Physically, \( \varepsilon = RC/\tau_a \) is related to the load resistance \( R \), and the parallel capacitance \( C \) of the attached circuit, normalized by the tunnelling time \( \tau_a \). The explicit form of the functions \( f(a, u) \) and \( D(a) \) can be found in the appendix A, and a discussion of the various deterministic bifurcation scenarios restricted to only one spatial degree of freedom, i.e., \( L_y \ll L_x \), is given in [14, 25].

3. Homogeneous and inhomogeneous steady states

Depending on the lateral dimensions \((L_x, L_y)\) of the DBRT device, different types of fixed points can exist. Whereas for small system sizes only spatially homogeneous steady states can exist, in larger systems it is possible to find stationary spatially inhomogeneous charge carrier density profiles, i.e., current filaments [6, 35]. In this work we study a device with a quadratic cross-section, in which three types of current filaments can be stable, namely hot corner filaments, cold corner filaments, and edge filaments, reflecting the spatial positions where the charge carriers are concentrated (figure 1).

In figure 2 the null isoclines of the system are plotted in the current–voltage projection. If the system is prepared in a completely homogeneous initial state \( a(x, y, 0) = a_0 \) and no spatially inhomogeneous fluctuations are taken into account, the system (1), (2) loses its space-dependence and can be reduced to a set of two ordinary differential equations for which the null isocline \( \dot{a} = 0 \) under this condition of homogeneity can be calculated analytically from the zeros of \( f(a, u) \). The intersection with the load line (null isocline \( \dot{u} = 0 \)) determines the homogeneous fixed point marked ‘H’ in figure 2(b). If we drop the condition of space-independence and return to the original full system, the additional null isoclines \( \dot{a} = 0 \) with inhomogeneous carrier density \( a(x, y, t) \) can be calculated numerically. The intersection of the load line with the null isocline of the cold corner filamentary states gives a second, inhomogeneous, fixed point in the neighbourhood of the first, spatially homogeneous, one (‘CC’ in figure 2(b)).

States on the middle branches of the \( J(u) \) characteristics are unstable in a passive external circuit with effective resistance \( r > 0 \) [6]. By choosing \( r < 0 \), which can be realized by an active
Figure 1. Spatially inhomogeneous distributions of the charge carrier density $a(x, y)$ (current filaments). These distributions represent stable steady states of the system (1), (2) for parameters $\varepsilon = 6.2, r = -35$, and (a) $U_0 = 100$, (b) $U_0 = -30$, (c) $U_0 = -84.285$.

Figure 2. (a) Null isoclines $\dot{a} = 0$ (current–voltage characteristics) for two-dimensional homogeneous (black) and inhomogeneous (coloured) carrier density profiles $a(x, y)$ in the spatially distributed system (1), (2). The lines for the filamentary density profiles correspond to the three different types of filaments shown schematically in figure 1. (b) Enlargement of (a) with the additional null isocline $\dot{u} = 0$ (load line). H marks the location of the spatially homogeneous fixed point whereas CC is the position of the filamentary cold corner fixed point. System parameters: $L_x = L_y = 30, r = -35, U_0 = -84.285$.

circuit, i.e., by applying an additional control voltage proportional to the device current $J$ in series with the bias $U_0$ [5], it is in principle possible to stabilize the middle branch of the stationary $J(u)$ characteristic and access it experimentally, but for large enough $\varepsilon$ (for $R < 0$, $C < 0$) Hopf bifurcations of ‘H’ and ‘CC’ can occur, leading to oscillations of the current and voltage [2].

4. Spatiotemporal patterns

The timescale separation $\varepsilon$ determines the stable spatio-temporal patterns, just as in the system with only one spatial degree of freedom [25].

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Figure 3. Transition from the unstable homogeneous fixed point to the cold corner filament in the system (1), (2) for $\varepsilon = 6$. At $t = 0$ the system is prepared in the homogeneous fixed point $u(0) = 266.47$, $a(x, y, 0) = 10.02$ (‘H’ in figure 2(b)) with a very small spatially inhomogeneous initial random perturbation. (a) Trajectory in the $u-J$-projection of the phase space (solid, black), null isoclines as in figure 2(b) (dotted, coloured), the arrow indicates the direction of the dynamics along the trajectory. (b) Time series of the dynamical variable $u(t)$. The vertical red lines mark the times $t$ for which the two-dimensional charge carrier density distributions are shown in (c). (c) Colour coded charge carrier density distribution $a(x, y, t)$ for five different values of $t$ as indicated. Parameters as in figure 2. (See also movie 1 in the supplementary material.)

Figure 3 demonstrates that for $\varepsilon = 6$ the cold corner filamentary state (‘CC’ in figure 2(b)) is stable. Here, the system has been prepared in the homogeneous steady state (‘H’ in figure 2(b)) with a very small inhomogeneous random perturbation. The trajectory moves away from the homogeneous fixed point and spirals into the inhomogeneous one (figure 3(a)). In figure 3(b) the corresponding time series of the dynamical variable $u(t)$ is shown and figure 3(c) provides snapshots of the spatial distribution $a(x, y, t)$ at five different times as indicated. This series illustrates the development of the spatially inhomogeneous cold corner filamentary state out of the almost homogeneous initial condition.

Recording local maxima and minima of the dynamical variable $u(t)$ under variation of $\varepsilon$ one obtains the bifurcation diagram shown in figure 4. From this one can see that the spatially inhomogeneous steady state is stable for $\varepsilon < 14.9$. Furthermore, one finds a regime of bistability in the range $14.1 < \varepsilon < 14.9$ where both the inhomogeneous fixed point and a surrounding limit cycle is stable. This situation is illustrated in figure 5 which depicts transient trajectories for two different initial conditions (figure 5(a)), one of them starting in the vicinity of the homogeneous
Figure 4. (a) Bifurcation diagram of the full spatially extended system (1), (2) (black) and of the reduced system without any spatial degree of freedom (red). In both systems local maxima and minima of the dynamical variable $u(t)$ are collected over a long time period ($T_{\text{scan}} = 5000$, after discarding a transient time $T_{\text{trans}} = 2000$) in dependence of the bifurcation parameter $\varepsilon$. (b) Enlargement of (a) with only the local maxima of $u(t)$ shown. Parameters as in figure 2.

fixed point and approaching asymptotically the inhomogeneous limit cycle (black curve), and the other one starting near the inhomogeneous fixed point and spiraling slowly inwards towards this stable focus (red curve in the centre). The series of spatial charge carrier distributions in figure 5(c) shows that the limit cycle corresponds to a breathing cold corner filament.

Around $\varepsilon = 14.1$ a limit cycle bifurcation by condensation of paths occurs, where a stable limit cycle with larger growing amplitude and an unstable limit cycle with subsequently shrinking amplitude are generated. The latter separates the basins of attraction of the stable limit cycle and the stable focus. This inhomogeneous fixed point remains stable up to $\varepsilon = 14.9$ where it undergoes a sub-critical Hopf bifurcation and becomes unstable. The larger, stable limit cycle undergoes a first period-doubling bifurcation at $\varepsilon = 14.7$ from which a stable period-2 orbit emerges. This period-2 spatio-temporal limit cycle is depicted in figure 6. Figure 6(c) shows that the general shape of the period-2 breathing filament remains almost the same as of the period-1 filament. With increasing $\varepsilon$ a period-4 limit cycle is born by a subsequent period-doubling bifurcation around $\varepsilon = 14.8$ (figure 7, here, we have omitted the series of spatial distributions since they do not provide essentially new information). Finally, the subsequent cascade of period-doubling bifurcations leads to chaos.

From figure 4(b) one can clearly see the typical periodic windows within the chaotic regime, e. g., a period-3 window at $\varepsilon = 15$. The corresponding dynamics shown in figure 8 confirms this. In contrast to the previous limit cycles and their corresponding spatio-temporal patterns (figures 5(c) and 6(c)) in this case the spatial distribution of the charge carrier density becomes almost homogeneous around the peak value of the $u$-variable (figure 8(c) for $t = 10109$). This feature becomes more and more pronounced as the bifurcation parameter is increased. For instance, a typical chaotic scenario corresponding to $\varepsilon = 18$ is depicted in figure 9. The $u$–$J$-projection of the trajectory reveals two essentially different parts of the chaotic dynamics. One part of the trajectory rotates mainly around the homogeneous fixed point, and the other part circles mainly around the inhomogenous fixed point. Consequently, the spatial distributions...
of the $a$-variable show homogeneous states corresponding to times where the trajectory is close to the homogeneous fixed point, interrupted by inhomogeneous states while encircling the inhomogenous fixed point.

Spatio-temporal pattern formation with only one spatial degree of freedom has been classified into spatio-temporal breathing or spiking scenarios [25]. Due to the more complex spatio-temporal dynamics in two dimensions, such a clear separation of breathing or spiking patterns is no longer possible here. However, as explained above, the chaotic attractor for larger values of the bifurcation parameter contains two types of oscillations, one predominantly around the inhomogeneous fixed point, which resembles breathing, and one partly around the homogeneous fixed point, the latter being a typical feature of spatio-temporal spiking.

Finally, in figure 4(a) one can see the Hopf bifurcation of the unstable homogeneous fixed point (‘H’ in figure 2(b)) around $\varepsilon \approx 16.5$. From this point emerges a spatially homogeneous

Figure 5. Bistability: stable limit cycle and stable focus, $\varepsilon = 14.5$. Simulation of the system (1), (2) initially prepared (i) in the vicinity of the cold corner filamentary steady state ‘CC’ (red trajectory) and (ii) in the vicinity of the unstable homogeneous fixed point ‘H’ (black trajectory), cf figure 2(b). (a) Trajectories in the $u$–$J$-projection of the phase space. The red trajectory is not well resolved due to its very slow spiraling into the inhomogeneous fixed point, and the black trajectory approaches the stable limit cycle, null isoclines as in figure 2. (b) Time series of the dynamical variable $u(t)$ for both time series coloured as in (a). The vertical red lines mark the times $t$ for which the two-dimensional charge carrier density distributions are shown in (c). (c) Colour coded charge carrier density distribution $a(x, y, t)$ of the limit cycle trajectory (black curve in (a)) for five different values of $t$ as indicated. Parameters as in figure 2. (See also movie 2 in the supplementary material.)
Figure 6. Period-2 orbit, $\varepsilon = 14.75$. Plots as in figure 3. (See also movie 3 in the supplementary material.)

Figure 7. Period-4 orbit, $\varepsilon = 14.83$. Plots as in figures 3(a) and (b). (See also movie 4 in the supplementary material.)

limit cycle which is of course unstable with respect to spatial fluctuations. But for large values of $\varepsilon > 20.2$ this homogeneous period-1 limit cycle finally becomes globally stable causing the disappearance of all chaotic dynamics from thereon. The corresponding transient trajectory and time series are shown in figure 10 where the system has been prepared in the inhomogeneous fixed point for $t = 0$. With time running the trajectory spirals outwards from the steady state (which for $\varepsilon = 21$ is an unstable focus) and approaches the stable homogeneous limit cycle around $t = 450$. The last two snapshots in figure 10(c) illustrate that the limit cycle is completely embedded in the manifold of spatially homogeneous states of the system.
Figure 8. Period-3 orbit, $\varepsilon = 15$. Plots as in figure 3. (See also movie 5 in the supplementary material.)

Figure 9. Chaotic dynamics, $\varepsilon = 18$. Plots as in figure 3. (See also movie 6 in the supplementary material.)
Figure 10. Transition from the unstable inhomogeneous fixed point to the homogeneous limit cycle, $\varepsilon = 21$. At $t = 0$ the system is prepared in the inhomogeneous fixed point (‘CC’ in figure 2(b)) with a very small spatially inhomogeneous initial random perturbation. Plots as in figure 3 with the stable limit cycle indicated by the solid red line in (a). (See also movie 7 in the supplementary material.)

5. Conclusions

We have investigated two-dimensional spatio-temporal scenarios in a globally coupled reaction-diffusion system modelling a semiconductor nanostructure. The time scale parameter $\varepsilon$, which describes the time scale separation of the activator and inhibitor variables of the dynamic system (1), (2), crucially determines the bifurcations and the stability of the spatio-temporal patterns. Starting from a situation where one stable inhomogeneous fixed point (cold corner filament) exists in the vicinity of an unstable homogeneous fixed point, we have varied the bifurcation parameter and observed different kinds of complex spatio-temporal patterns combining breathing and spiking filamentary, and homogeneous oscillating features. The bifurcation analysis and the different time series and spatial snapshots obtained from the numerical simulation have revealed richer scenarios than those obtained for one-dimensional simulations [25], including bistability of stationary and oscillating space-time patterns, a subcritical Hopf bifurcation, and a bifurcation by condensations of paths of spatially inhomogeneous limit cycles. With increasing bifurcation parameter the stable filamentary state loses its stability, and additionally the stable limit cycle undergoes a period-doubling cascade finally resulting in chaotic behaviour. The associated spatio-temporal patterns resemble a breathing cold corner filament. At the same time the dynamics becomes more and more influenced by the originally unstable homogeneous fixed point and the homogeneous limit cycle born from it. The latter becomes less unstable with increasing bifurcation parameter, and is finally stabilized globally.
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Appendix A

The dimensionless voltage variables $u$, $U_0$ are scaled into physical quantities by multiplying with a factor of 0.35 mV. The electron density $a$ is scaled by $10^{10}$ cm$^{-2}$, current density $j$ by 500 A cm$^{-2}$ and the units of time and space correspond to 3.3 ps and 100 nm for typical device parameters at 4 K [14].

The effective transverse diffusion coefficient $D(a)$ results from the inhomogeneous lateral re-distribution of carriers and from the change in the local potential due to the charge accumulated in the quantum well by Poisson’s equation [11]

$$D(a) = a \left( \frac{d}{r_B} + \frac{1}{1 - \exp(-a)} \right), \quad \text{(A.1)}$$

where $r_B = (4\pi\epsilon\epsilon_0\hbar^2)/(e^2m)$ is the effective Bohr radius in the semiconductor material, $\epsilon$ and $\epsilon_0$ are the relative and absolute permittivity of the material, and $d$ is the effective thickness of the double-barrier structure.

The function $f$ is obtained from microscopic quantum mechanical considerations as the difference of the tunnelling currents from the emitter into the quantum well, and from the quantum well to the emitter [14]

$$f(a, u) = \left[ \frac{1}{2} + \frac{1}{\pi} \arctan \left( \frac{2}{\gamma} \left( x_0 - u + \frac{d}{r_B} a \right) \right) \right] \left[ \ln \left( 1 + \exp \left( \eta_e - x_0 + u - \frac{d}{r_B} a \right) \right) - a \right] - a. \quad \text{(A.2)}$$

$x_0$ and $\gamma$ describe the energy level and the scattering-induced broadening of the electron states in the quantum well, and $\eta_e$ is the dimensionless Fermi level in the emitter, all in units of $k_B T$. Throughout the paper we use values of $\gamma = 6$, $d/r_B = 2$, $\eta_e = 28$ and $x_0 = 114$.

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