# Quasi-Particles in a Three-Dimensional Three-Component Reaction-Diffusion System

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**Abstract.** We investigate a reaction-diffusion system which consists of a set of three partial differential equations. Due to the reaction kinetics the system can be referred to as a 1-activator-2-inhibitor system. We show, that such systems are capable of supporting localized moving structures, so called quasi-particles. For certain parameters it is possible to predict the propagation speed of these solutions as well as their behaviour in scattering processes. In more general cases we have carried out simulations which reveal different scattering results depending on the parameters. We find annihilation, reflection and merging of particles.

## 1 Introduction

In 1952 Turing [1] introduced a two-component reaction-diffusion model for the morphogenesis of a growing organism in order to describe the formation of spatially inhomogeneous structures from an initially homogeneous state. Since then, reaction-diffusion equations have been widely used to describe pattern formation phenomena in very different biological [2,3], chemical [4,5] and physical [6–8] systems. Though a lot of phenomena, like pulse propagation in one-dimensional systems or the formation of stationary spatially inhomogeneous structures, can be explained by two-component reaction-diffusion equations, there are certain phenomena, like the destabilization of the homogeneous state by a travelling wave, that require three components. This work deals with moving, particle-like solutions of such a system described by the following set of equations

$$\dot{u} = D_u \Delta u - v - \kappa_3 w + f(u) + \kappa_1, \tag{1}$$

$$\tau \dot{v} = D_v \Delta v + u - v, \tag{2}$$

$$\theta \dot{w} = D_w \Delta w + u - w, \tag{3}$$

with $u = u(r,t)$, $v = v(r,t)$ and $w = w(r,t)$ and $r \in G \subset \mathbb{R}^n$ with $n = 2, 3$ and $\Delta$ denoting the Laplacian. For analytical considerations it is useful to assume an infinite domain $G$. For numerical simulations periodic boundary conditions or Neumann boundary conditions on box-shaped domains $G$ are used. The above equations can be regarded for example as a qualitative model for the description of pattern formation processes in a two-dimensional gas-discharge system [7], but similar phenomenological models can also arise in other systems [8]. The function $f(u)$ represents the only nonlinear term and

is chosen such that near $(u, v, w) = (0, 0, 0)$ $u$ can be referred to as an activator and that its nonlinear part prevents a blow-up of the solutions. The simple choice $f(u) = \lambda u - u^3$ fulfills these two conditions and will be used throughout this paper, though in principle different nonlinearities could be used. Following the structure of the reaction terms in Eqs. (1)-(3) the component $u$ is called activator, because it acts as a source for $v$ and $w$ and at least in a certain amplitude range for itself, too. The components $v$ and $w$ are referred to as inhibitors. They suppress their own production as well as the production of the component $u$. Apparently, if the time constants $\tau$ and $\theta$ and the diffusion constants $D_v$ and $D_w$ are of the same magnitude, it is possible to omit one inhibitor equation. Thus we expect new features, as compared to a two-component model only if the inhibitors have significantly different parameters. In the following we will usually choose $\tau > \theta$, $\tau > 1$ and $D_w > D_u$. Corresponding to this choice we call $v$ the slow inhibitor and $w$ the fast or the diffusing inhibitor.

In order to solve the Eqs. (1)-(3) numerically a finite difference scheme is used. The domain $G = [0, L_x] \times [0, L_y] \times [0, L_z] \subset \mathbb{R}^3$ is discretised with a fixed length $\Delta x$. For the time discretisation we implemented the Crank-Nicolson scheme, due to advantages in stability and accuracy properties. The resulting system is solved iteratively using the successive-overrelaxation method which provides a reasonably fast convergence. For the task of parallelisation the domain $G$ is divided into boxes of equal size and, as far as possible, cubic shape to reduce the ratio between boundary points and interior points. Every node on the parallel computer is assigned to one box and after each change of the components $u$, $v$ and $w$ the boundary points are updated using the Message Passing Interface (MPI). The computational effort strongly depends on the discretisation and on the parameters of the simulation. Calculations with a grid of about $35 \times 35 \times 35$ have been used to check existence, stability and speed of single solutions. Typically we have used 64 nodes for about one hour per node on the Cray T3E-900 in such cases. Simulations regarding scattering processes had to be performed on rather large domains with up to $120 \times 160 \times 120$ grid-points and with parameters leading to partially separated time-scales, which slowed down our algorithm considerably. Thus the most extensive calculations have been carried out on 256 nodes for about 8 hours per node.

## 2 Single Quasi-Particles

In reaction-diffusion systems a variety of different patterns can be observed. A very interesting phenomenon is the formation of stable localized current density filaments, e.g. in gas-discharge systems [9,10]. These quasi-particles can move through the system and interact with the boundaries or with each other. While stationary filaments can be described by two-component reaction-diffusion models, it was not possible to find moving localized spots

in these systems until now. In two-component systems with one activator and one inhibitor there are two possible cases: If the inhibitor is fast and diffusing, stationary structures can organize. If the inhibitor is slow, dynamical structures, spirals or scroll-waves, appear. To keep a structure moving and localized in more than one dimension, two inhibitors are at least helpful [11]. Regarding the behaviour of moving quasi-particles in two-dimensional systems different scattering phenomena have already been observed and described analytically. The interaction with each other, with inhomogeneities and the system boundaries has been studied. The following work therefore deals with different phenomena in three-dimensional space.

Figure 1 a) shows a three-dimensional solution moving from the left to the right. The iso-surfaces of activator $u$ and slow inhibitor $v$ are drawn red and green, respectively. The direction of motion of such a solution is determined by the direction of the shift of the slow inhibitor with respect to the activator. In Fig. 1 b) the profile of components $u$, $v$ and $w$ in the direction of motion of this three-dimensional solution is plotted. The slow inhibitor is shifted with respect to the activator and gives the impression to push the activator peak. The fast inhibitor surrounds this peak and controls the size of the spot. If the spot grows or shrinks, the fast inhibitor immediately reacts and stabilizes the size of the activator distribution. For a single spot the task of controlling the size can be performed by an integral feedback as well [12–14]. However, for multiple spots this approach fails, because antisymmetric fluctuations are not noticed by such a mechanism.

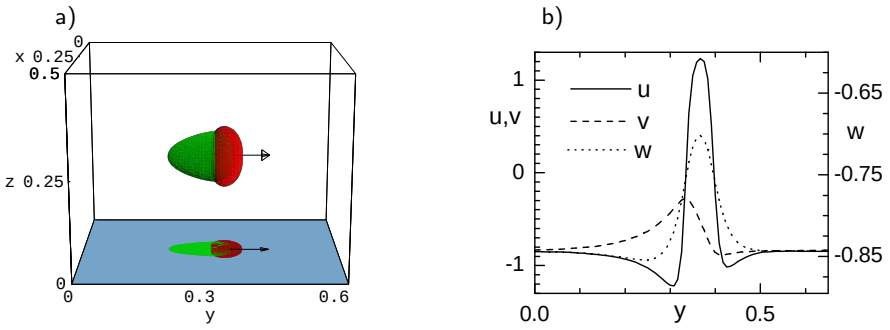


**Fig. 1.** a) Iso-surfaces of activator $u$ (red) and slow inhibitor $v$ (green) of a moving spot solution. b) The components $u$, $v$ and $w$ at $x = 0.25$ and $z = 0.25$ as a function of $y$ of the spot of Fig. a) show the different behaviour of the two inhibitors. Parameters are $G = [0, 0.5] \times [0, 0.65] \times [0, 0.5]$, $D_u = 1.5 \times 10^{-4}$, $D_v = 1.5 \times 10^{-4}$, $D_w = 9.6 \times 10^{-2}$, $\kappa_3 = 8.5$, $\lambda = 2$, $\kappa_1 = -6.92$, $\theta = 1$, $\tau = 48$ and the discretisation in space and time was $\Delta x = 0.009$ and $\Delta t = 2 \times 10^{-3}$.

In the case $D_v = 0$ and $\theta = 0$ it is possible to derive analytical results regarding the propagation speed of these structures [15]. If there exists a stationary structure $(\bar{u}, \bar{v}, \bar{w})$ for $\tau = 0$ on an infinite domain $G$, in any case the onset of propagation will occur at $\tau = 1$ and the speed of the propagating solution is given by

$$c^2 = (\tau - 1)\frac{\langle \bar{u}_x^2 \rangle}{\langle \bar{u}_{xx}^2 \rangle}, \tag{4}$$

where an index $x$ indicates the partial derivative $\partial/\partial x$ and $\langle \ldots \rangle$ denotes integration over $G$. It is even possible to show, that the onset of propagation is the primary bifurcation. Figure 2 b) shows numerical results for the speed of a travelling solution in three-dimensional space. The numerically estimated bifurcation point is at $\tau = 0.992$ and the slope of the speed deviates about 25 % from the theoretical result. The errors are due to the finite discretisation length and the fact, that $\theta = 0.01 \neq 0$. To reduce the dimension and thus the computational effort these computations have been performed using a cylindrical geometry. The stability of the moving spot for the parameters in Fig. 2 was checked by a three-dimensional calculation. The above description of the onset of propagation assumes, that there exists always a stationary solution which is unstable beyond the travelling bifurcation. This is not necessary, however. But this analysis holds only in the vicinity of the bifurcation point. For different parameters (very high values of $\tau$, or $D_v \neq 0$) it is possible to find a moving stable solution, without a stationary counterpart.

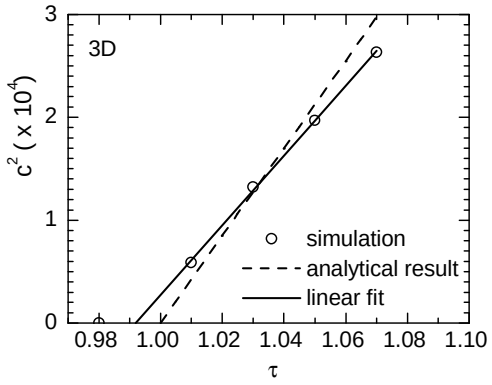


**Fig. 2.** Square of the speed $c$ of a moving spot as a function of the parameter $\tau$. The remaining parameters are $D_u = 4.67 \times 10^{-3}$, $D_v = 0$, $D_w = 10^{-2}$, $\kappa_3 = 3.33$, $\lambda = 5.67$, $\kappa_1 = -1.126$, $\theta = 0.01$. Spatial discretisation was $\Delta x = 0.02$ and for the time we used $\Delta t = 1 \times 10^{-3}$.

## 3 Interaction of Two Quasi-Particles

The equations (1)-(3) do not contain any global feedback terms. So, if the existence of a single moving spot is guaranteed, it is possible to construct solutions to the differential equations with two or more moving particles,

at least if the individual patterns are well separated in space. As two spots approach each other, there will be an interaction process, which can lead to a variety of different scattering phenomena. In the following we will present four different cases that can result from a collision processes and discuss the relevant mechanisms.

### 3.1 Deflection of Quasi-Particles

The first phenomenon which we discuss are scattering processes, that lead to a mere deflection of the particles. In this case the shape of the two localized solutions does not change significantly during the process. Typically there will be a repulsive interaction between two spots as they approach. This is due to the fast inhibitor, which surrounds the particles and inhibits the propagation of the activator distribution of the other spots.

This case can be described analytically starting with the assumptions $D_v = 0$ and $\theta = 0$. According to Eq. (4) the onset of propagation occurs at $\tau > 1$. The dynamics of a quasi particle in this regime near the bifurcation point can be described by two quantities: The position $\boldsymbol{p}_i$ of a spot $i$, and the amplitude and direction of the shift $\boldsymbol{\alpha}_i$ of the slow inhibitor with respect to the activator. While the first quantity $\boldsymbol{p}_i$ results from the translational invariance of the equations, the second quantity describes the internal degree of freedom of a solution which is decisive for the propagation speed and direction of a particle. A value of $\boldsymbol{\alpha}_i = 0$ corresponds to a stationary, and for $\tau > 1$ unstable, solution. Using a singular perturbation approach it is possible to derive equations for the time evolution of these quantities. For analytical details refer to [16] and [17]. For a system of two particles 1 and 2 the following differential equations can be deduced for the motion of particle 1:

$$\partial_t \boldsymbol{p}_1 = \boldsymbol{\alpha}_1 - W(|\boldsymbol{p}_2 - \boldsymbol{p}_1|)(\boldsymbol{p}_2 - \boldsymbol{p}_1), \tag{5}$$

$$\partial_t \boldsymbol{\alpha}_1 = (\tau - 1)\boldsymbol{\alpha}_1 - \frac{\langle \bar{u}_{xx}^2 \rangle}{\langle \bar{u}_x^2 \rangle} |\boldsymbol{\alpha}_1|^2 \boldsymbol{\alpha}_1 - W(|\boldsymbol{p}_2 - \boldsymbol{p}_1|)(\boldsymbol{p}_2 - \boldsymbol{p}_1). \tag{6}$$

The function $W(d)$ is the interaction law between two particles with the distance $d$ and is equal to zero for $d \to \infty$. It can be calculated numerically from the shape of a single spot solution $\bar{u}$. In the following we will restrict ourselves to the case of a repulsive interaction law. Obviously for $d = |\boldsymbol{p}_2 - \boldsymbol{p}_1| \to \infty$ the above system reduces to Eq. ( 4). The stationary solution $\boldsymbol{\alpha}_1 = 0$ becomes unstable for $\tau > 1$.

In Fig. 3 the trajectories of two interacting quasi-particles (spot 1 and 2) are sketched. The solid lines are from a fully three-dimensional calculation. The dashed line was calculated from (5) and (6). As initial conditions two approaching spots with an angle of about 90 degrees between their velocities have been used. As the spots approach each other the repulsive force leads to a deflection. After the collision there is a slight divergence between the

three-dimensional numerical and the simplified numerical results, but the agreement is still satisfying. As long as $\tau$ is small enough the perturbation approach (5) and (6) is valid, and thus elastic scattering can be expected in these cases.

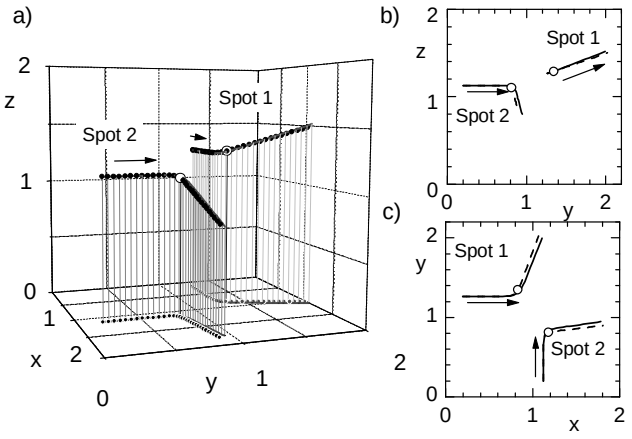


**Fig. 3.** Trajectories of two interacting quasi-particles. The solid lines indicate the results of the three-dimensional equations, the dashed lines are from the simplified model. a) Trajectories in three-dimensional space. b) and c) show the projections of the trajectories on the ground and on the back plane. Parameters were chosen as $D_u = 4.67 \times 10^{-3}$, $D_v = 0$, $D_w = 0.01$, $\lambda = 5.67$, $\kappa_1 = -1.126$, $\kappa_3 = 3.333$, $\kappa_4 = 3.333$, $\tau = 1.03$, $\theta = 0.01$ and $L = 2.25$. Space and time discretisation was $\Delta x = 0.0288$ and $\Delta t = 10^{-3}$.

### 3.2 An Overview of Typical Scattering Processes

In the previous section we have restricted the range of parameters to the case $D_v = 0$, $\theta = 0$ and $\tau \approx 1$. Thus we have been able to give an analytical description of the collision process. But since the shape and stability of the moving spots is important for this analysis certain cases are automatically excluded: The annihilation, generation or the mergence of two spots.

Before the other examples are discussed in detail Fig. 4 shall give a survey of the qualitative behaviour of two moving spots. It was not possible to define exact parameters separating different areas of qualitative behaviour in parameter space, nevertheless the basic behaviour can be described. In the following we will assume the existence of a sufficiently stable spot. Two quantities can be used to characterize the behaviour in the course of a collision process: The speed of the structure, which can be controlled by the time constant $\tau$, and the strength of the interaction force between two particles,

which can be reduced for example by decreasing the ratio of the diffusion constants $D_u/D_w$. Of course, changing other system parameters can equally effect the scattering phenomena, but the above mentioned can be regarded as the most important ones. The deflection process (I.) has been described already. This case can be found if the speed of the single particles is very low or if the strength of particle interaction is rather strong. Thus the particles cannot merge, but will be deflected. For slow particles, a reversal of speed is typically possible and leads to elastic scattering. For different parameters, e.g. if there exist only spot solutions with a certain minimal speed, one or both spots can be annihilated (II.) because the activator distribution cannot proceed due to the repulsive force and the slow inhibitor catches up and suppresses the activator. This type of annihilation process hasn't been examined yet in the three-dimensional case. In two-dimensional systems this mechanism has already been observed. If the repulsive forces between two quasi particles are weaker or the speed of the solutions is high, the propagation cannot be stopped and the activator of the two particles merges to an intermediate activator spot. This may happen due to very high speed of the particles (e.g. $\tau \gg 1$) or due to a very flat fast inhibitor distribution $w$ ($D_w \gg D_u, D_v$). In this situation there are two possibilities: either the activator spot is destroyed by the inhibitor $v$ (III.), or the activator is fast enough to escape transverse to the original direction of motion (IV.). Note that in highly excitable media the generation of new particles from remaining perturbations is possible after an annihilation process. The two cases (III.) and (IV.) are described in the next section in more detail.

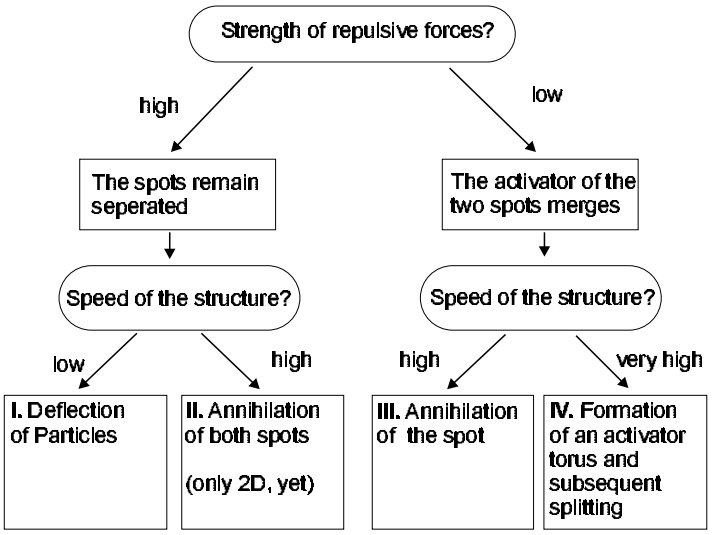


**Fig. 4.** Depending on the system parameters different scattering phenomena occur.

### 3.3 Mergence and Annihilation of Spots

In Fig. 5 the process of mergence of two spots after a head-on collision is shown. The activator $u$ (red) and the slow inhibitor $v$ (green) have been depicted as iso-surfaces. The spots approach each other in a head-on collision in (a) and (b). The inhibitor is clearly located behind the activator. In (c) the activator distribution merges. For the parameters given in Fig. 5 the activator is suppressed by the slow inhibitor in (d) and the spots vanish (e), corresponding to Fig. 4 (III.). Figure (f) shows the normalized activator integral $\langle u\rangle/|G|$ in the course of the process. The points in time corresponding to pictures (a)-(e) are marked with circles in this plot. The number of particles present in the system corresponds to the value of $\langle u\rangle/|G|$. At $t = 0$ there are two particles ($N = 2$), at $t > 100$ there remains only the homogenous state ($N = 0$). For $t \approx 52$ an intermediate state forms, which can be interpreted as a transient particle, formed by the activator and the fast inhibitor.

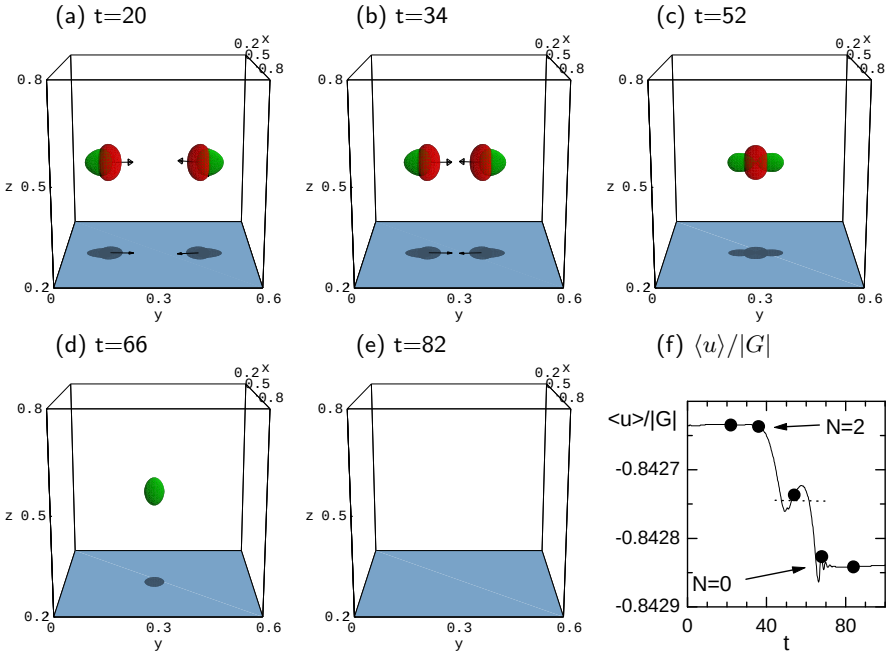


**Fig. 5.** Pictures (a)-(e) show an annihilation process between two particles. The iso-surfaces of the activator $u$ are red, those of the inhibitor $v$ are green. The normalized activator integral $\langle u\rangle/|G|$ is plotted in (f). The parameters used are $D_u = 1.5 \times 10^{-4}$, $D_v = 1.86 \times 10^{-4}$, $D_w = 9.6 \times 10^{-3}$, $\lambda = 2$, $\kappa_1 = -6.92$, $\kappa_3 = 8.5$, $\theta = 1$, $\tau = 25$. Discretisation was chosen as $\Delta x = 0.085$ and $\Delta t = 2 \times 10^{-2}$.

Starting from the annihilation process the time constant $\tau$ was increased from 25 to 48. Thus the shift of the inhibitor $v$ with respect to the activator $u$ is increased. This leads to a faster propagation of the spot. In Fig. 6 the results of this calculation are presented. Figures (a)-(e) show the iso-surfaces, (f) the normalized activator integral $\langle u \rangle / |G|$. Compared to Fig. 5 the inhibitor tails are longer, which reflects the higher time constant $\tau$. After the mergence (b) the activator is fast enough to escape transverse to the direction of motion. Due to the cylindrical symmetry of the collision process a transient activator torus forms. In Fig. 6 (c) the symmetry is already broken and two new particles have been created. This case corresponds to (IV.) in Fig. 4. The plot of the normalized activator integral again shows the formation of an intermediate transient one-particle solution, before it breaks up and the two new particles form. The value of $\langle u \rangle / |G|$ at the end of the calculations was slightly higher than in the beginning, because the particles have still not reached their final shape yet. These simulations are similar in some sense to two-dimensional results of different groups [12,13], that were related to the collisions of spots in two-component models with an inhibiting global feedback . However, the asymptotic solution is unstable in the two-component case. In a three-dimensional space transversal scattering has to break the initial cylindrical symmetry, even if multi-particle solution are asymptotically stable. There even is a possibility that more than two particles emerge from the intermediate state. A further increase of the activation potential of $u$ could lead to such a situation, but this was not observed until now.

## 4 Discussion

We have presented moving localized solutions of the three-dimensional partial differential equations (1)-(3), that can be regarded as a simple example for the complex dynamical behaviour in reaction-diffusion systems. The mechanisms that are necessary for the propagation of such solutions have been identified and it was possible to give an analytical description of the propagation and interaction properties in certain regions of the parameter space. Different scattering phenomena like annihilation and intermediate mergence of particles have been observed. The knowledge of these basic properties provides a basis for the study of multi-particle solutions by means of two complementary approaches: Fast parallel computers and, in suitable parameter ranges, effective interaction equations. – We gratefully acknowledge the support of the HLRS in Stuttgart and of the DFG.

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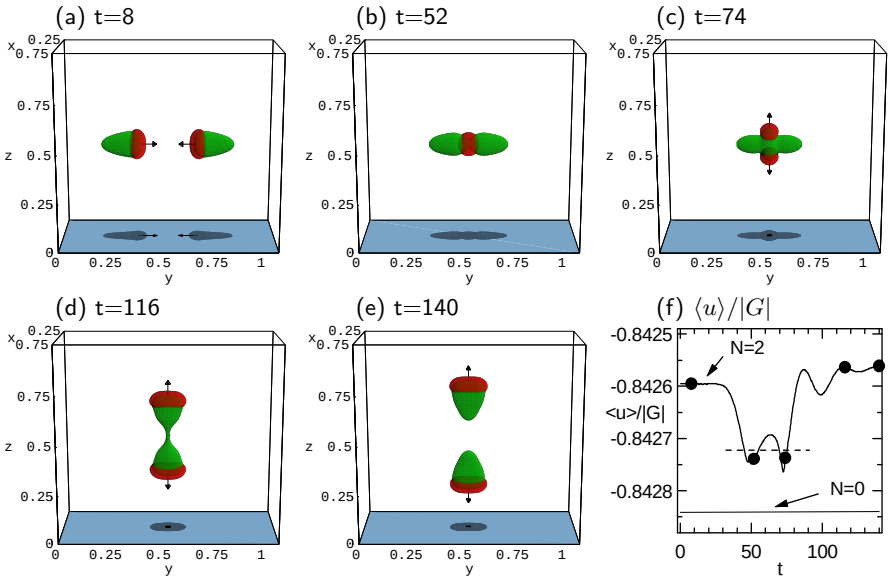


**Fig. 6.** After the mergence of two particles, the activator escapes transverse to the original direction, which can lead to the formation of two new particles. The parameters are chosen like in Fig. 5, but $\tau$ was increased to 48. (a)-(e) shows the iso-surfaces of the activator $u$ (red) and inhibitor $v$ (green). (f) is the normalized activator integral as a function of time.

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