

Drift of Spiral Waves on Nonuniformly Curved Surfaces

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SUMMARY: The evolution of spiral waves on nonuniformly curved surfaces is theoretically investigated in the framework of kinematic approach. We predict the existence of the drift proportional to the gradient of Gaussian curvature of the surface. In the excitable media with equal diffusion coefficients of activator and inhibitor the direction of the drift is perpendicular to the gradient of Gaussian curvature. If the diffusion coefficients are different the component of the velocity drift parallel to the gradient of Gaussian curvature appears. In the particular case of the paraboloid of revolution the spiral wave will “climb up” onto the top of the paraboloid. This theoretical prediction is confirmed by computer simulations. The drift of spiral waves towards the top of parabolic surface was observed in experiments with BZ reaction. The experimental results are also presented.

Introduction.

Excitable media are characterized by their tendency to organize themselves into spatio-temporal structures ¹⁾. Among these, one of the most general and important are vortices or spiral waves. Rotating spiral waves have been observed in numerous physical, chemical and biological systems ²⁾. One of the most important and well investigated chemical excitable systems is the famous Belousov-Zhabotinsky reaction.

The possibilities to control characteristics of spiral waves attract considerable interest of scientists from different fields related to nonlinear dynamics. In this paper we discuss the influence of geometrical properties of 2-D curved surfaces on spiral wave evolution. Namely, the drift of spiral waves on nonuniformly curved surfaces is investigated theoretically (in the framework of kinematic approach ³⁾) and numerically. This drift caused by the gradient of the

curvature of surface was observed in experiments with B-Z reaction initiated on the paraboloid of revolution.

Theory

Excitable media are often described by nonlinear reaction-diffusion equations. On curved surface the equations for two-variable system can be written in form:

$$\begin{aligned}\frac{\partial u}{\partial t} &= F_1(u, v) + D_u \frac{\partial}{\sqrt{g} \partial x^i} (g^{ik} \sqrt{g} \frac{\partial u}{\partial x^k}) \\ \frac{\partial v}{\partial t} &= F_2(u, v) + D_v \frac{\partial}{\sqrt{g} \partial x^i} (g^{ik} \sqrt{g} \frac{\partial v}{\partial x^k})\end{aligned}\quad (1)$$

where u, v are the activator and inhibitor variables respectively, D_u, D_v are their diffusion coefficients. Nonlinear functions F_1, F_2 specify reactions in the system, x_k are coordinates on the surface, and g is the determinant of the metric tensor g_{ik} . Analytical study of the spiral wave drift using “microscopic” equations (1) is impossible. We shall use so called “kinematic approach”^{3,4)}. In the framework of the kinematic theory autowave is completely determined by specifying the line of its front. The form and evolution of the autowave front can be described by its natural equation $k_g = k_g(l, t)$, where k_g - geodetic curvature, l - arclength, t - time. Each section of the front moves in the normal direction with the velocity $V = V_0 - D_u k_g$, where V_0 - the velocity of the front with zero geodetic curvature, D_u - the diffusion coefficient of the activator. The free end of broken front can grow or contract with tangential velocity $c = \gamma(k^* - k_{g0})$, where k_{g0} is the geodetic curvature of the front near the tip, and k^* is the critical curvature of the broken front. The coefficient $\gamma \sim D_u - D_v$, where D_v is the diffusion coefficient of the inhibitor. Note that $\gamma = 0$ in the excitable media with equal diffusion coefficients of the activator and inhibitor. The main kinematic equation for the evolution of the front on curved surface has the following form:

$$\frac{\partial k_g}{\partial t} + \left(\int_0^l k_g V d\xi + c \right) \frac{\partial k_g}{\partial l} + k_g^2 V + \frac{\partial^2 V}{\partial l^2} = -\Gamma V \quad (2)$$

where Γ is the Gaussian curvature of the surface. As it was shown in⁵⁾ a spiral wave on the spherical surface rotates faster than on the plane and the additional term is proportional to Γ :

$$\omega = \omega_0 \left(1 + \frac{V_0 \Gamma}{2\xi^2 D_u (k^*)^3} \right) \quad (3)$$

where ω_0, ω are the angular velocities of a spiral wave on a plane and on a sphere respectively and $\xi = 0.685$. If spiral wave rotates on nonuniformly curved surface it will drift. We consider this effect in the framework of so called quasi-steady approximation. In the quasi-steady regime the shape of the front near the core of a spiral adjusts itself adiabatically to the instantaneous value of the curvature at a free end (the tip), and this curvature in turn slowly varies because of growth and contraction. The condition for the applicability of the quasi-state approximation is following: $\frac{\gamma}{D_u} \ll \sqrt{\frac{V_0}{D_u k^*}}$. For weakly excitable media ($D_u k^* / V_0 \ll 1$) this condition is nearly always satisfied and the quasi-steady approximation is valid³⁾ and all properties of a spiral wave are determined by the motion of its tip.

Consider first an auxiliary problem of a spiral wave dynamics on a sphere whose radius oscillates in time according to the equation: $R = R_0 + R_1 \cos(\omega t)$, $R_1 \ll R_0$. The equations describing the tip motion are following:

$$\frac{d\vartheta}{dt} = -\frac{V \sin(\alpha) + \cos(\alpha)}{R}, \quad \frac{d\varphi}{dt} = \frac{V \cos(\alpha) - c \sin(\alpha)}{R \sin(\vartheta_0)} \quad (4)$$

where ϑ, φ are the spherical coordinates of the tip, ϑ_0 is the polar angle of the center of the core and α is the angle between the tangent vector to the autowave front near the tip and the meridian of the sphere. For convenience we choose the polar axis of the spherical coordinate system so that the core center is near equator ($\pi/2 - \vartheta_0 \ll 1$).

In this case the following effects lead to the drift of the spiral:

- variation of an angular velocity;
- variation of the geodetic curvature (and tangential velocity) near the tip;
- variations of the core radius.

Using (3), (4) we obtain after averaging the following expressions for the angular velocities of the center of the core in weakly excitable media in quasi-steady approximation:

$$\frac{d\vartheta_0}{dt} = -\frac{\gamma k^* R_1}{2R_0^2}, \quad \frac{d\varphi_0}{dt} = -\frac{V_0 R_1}{2R_0^2 \sin \vartheta_0} \quad (5)$$

Consider now the spiral wave on a sphere whose surface is slightly deformed so that the Gaussian curvature is a function of polar angle: $\Gamma = \Gamma(\vartheta)$. In this case the tip passes

successively through a region with different values of the Gaussian curvature. Therefore it moves as if the Gaussian curvature of the surface were time dependent:

$$\Gamma = \Gamma_0 + \left(\frac{d\Gamma}{d\vartheta}\right)_{\vartheta=\vartheta_0} \frac{r_0}{R_0} \cos(\omega t) \quad (6)$$

where r_0 is the radius of the core. From the other hand expression (6) can be written in the following form:

$$R = R_0 + R_1 \cos(\omega t), \quad \text{where } R_1 = -\frac{R_0^2 r_0}{2} \frac{d\Gamma}{d\vartheta} \quad (7)$$

One can see that the evolution of a spiral wave on a nonuniformly curved surface can be found by calculating the motion of a spiral wave core on a spherical surface with a periodically varying radius, which was considered above. Using (5), (7) we obtain the following expressions for corresponding angular velocities:

$$\frac{d\theta_0}{dt} = \frac{\gamma k^* r_0}{4} \frac{d\Gamma}{d\theta}, \quad \frac{d\varphi_0}{dt} = \frac{V_0 r_0}{4 \sin \theta_0} \frac{d\Gamma}{d\theta} \quad (8)$$

As it follows from (8) the theory predicts the velocities of the drift proportional to the gradient of the Gaussian curvature. For paraboloid or prolate ellipsoid $d\Gamma/d\theta < 0$. Thus we predict the climbing of the spiral wave to the “top” of paraboloid or prolate ellipsoid with the velocity proportional to $D_u - D_v$. The velocity of the motion perpendicular the gradient of the Gaussian curvature (along the parallel) does not depends directly on $D_u - D_v$. We can expect that the trajectory of the core center will have a spiral-like shape. In particular case of the equal diffusivities the spiral wave will drift along the parallel of paraboloid or ellipsoid. This case was considered in ⁶⁾. We estimate now the drift velocity for a medium with a BZ reaction. Suppose that the spiral wave rotates on the surface of paraboloid $z = Ar^2$ with $A = 0.7 \text{ mm}^{-1}$. The Gaussian curvature of the paraboloid is given by the following expression: $\Gamma = 4A^2/(1 + 4A^2r^2)^2$. We assume the values $r_0 = 0.1 \text{ mm}$, $\gamma k^* \approx V_0$ and $r = 0.4 \text{ mm}$. Using (8) one can obtain the values of the angular velocities ($V_0 \approx 0.017 \text{ mm/s}$, $\sin \vartheta_0 = 0.29$): $\frac{d\vartheta_0}{dt} \approx 1.8 \cdot 10^{-4} \text{ rad/s}$, $\frac{d\varphi_0}{dt} \approx 6.2 \cdot 10^{-4} \text{ rad/s}$.

Computer simulations

The essential features of the B-Z reaction can be simulated by use of the Oregonator model ⁷⁾

$$\begin{aligned}\frac{\partial u}{\partial t} &= \Delta u + \frac{1}{\varepsilon} \left[u - u^2 - f v \frac{u - q}{u + q} \right] \\ \frac{\partial v}{\partial t} &= \sigma \Delta v + u - v\end{aligned}\quad (9)$$

In our computations we fixed the values of the constants in this model as the following: $f = 3$ and $q = 0.002$. The ratio between the diffusion coefficients $\sigma = D_v / D_u$ was taken as $\sigma = 1$ (in this case $\varepsilon = 0.05$) or $\sigma = 0$ ($\varepsilon = 0.08$) as specified below. In order to simulate wave processes on a surface of a paraboloid determined by the expression $z = A r^2$, we used a polar coordinate system (s, ϕ) , where s is the arclength from the top of the paraboloid and ϕ is the longitude. In terms of these special coordinates the two-dimensional Laplasian on the parabolic surface writes

$$\Delta u = \frac{\partial^2 u}{\partial s^2} + \frac{1}{d \sqrt{1 + 4A^2 d^2}} \frac{\partial u}{\partial s} + \frac{1}{d^2} \frac{\partial^2 u}{\partial \phi^2} \quad (10)$$

where d is the distance from the paraboloid axis. The Laplasian was calculated by using a quasiuniform computational grid proposed earlier⁸⁾ with the time step $\delta t = 0.005$ and $\delta s = 0.25$. In all computations the no-flux boundary conditions are imposed for $s = s_R = 20$.

For the given coefficients the system (9) has a spatially uniform steady-state $u = u_s > 0$ and $v = v_s > 0$. To create a spiral wave one has to take a specific nonuniform distribution of the variables as initial conditions for (9). In our computations these were:

$$\begin{aligned}u(s, \phi) &= \begin{cases} 1, & \text{if } s_0 < s < s_R \text{ and } 0 < \phi < \phi_0 \\ 0, & \text{otherwise} \end{cases} \\ v(s, \phi) &= \begin{cases} v_0, & \text{if } 0 < s < s_0 \\ v_{in}(\phi), & \text{if } s_0 < s < s_R \text{ and } 0 < \phi < \phi_0 \\ v_{out}(\phi), & \text{if } s_0 < s < s_R \text{ and } \phi_0 < \phi < 2\pi \end{cases}\end{aligned}$$

with

$$v_{in}(\phi) = v_b - (v_b - v_f)\phi / \phi_0, \quad v_{out}(\phi) = v_f + (v_b - v_f)(\phi - \phi_0) / (2\pi - \phi_0)$$

In accordance with these initial conditions the variable u exceeds an excitation threshold within a thin stripe ($\phi_0 \ll 2\pi$) located along a meridian. The values of the second variable v increase within this stripe in the west direction from $v = v_f < 0.003$ up to $v = v_b = 0.05$. The central part of the paraboloid surface, where $s < s_0$, is placed in a refractory state determined by a constant $v_0 = 0.01$. Such a distribution of the second variable v predetermines an initial

movement of the excited stripe in the east direction⁹⁾. The induced wave with an open end evolves into a spiral wave. Variations of s_0 allows to control the initial location of the spiral wave core with respect to the top of paraboloid.

For given initial conditions the boundary of the excited stripe consists of two parts which are the front (here $du/dt > 0$) and the back (here $du/dt < 0$) of the wave. The tip of the wave is determined as the point at which $du/dt = 0$. The trajectory of this point is registered during integration of the system (9), that is one of the most important characteristics of the spiral wave dynamics.

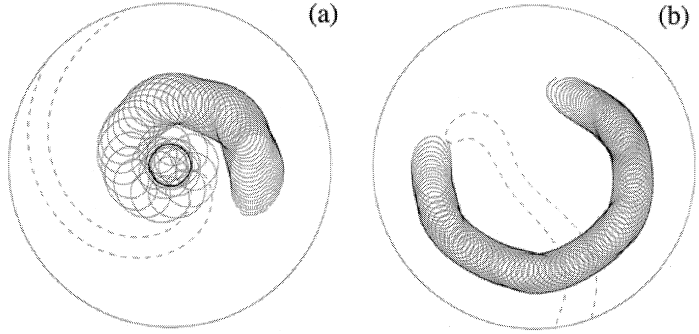


Fig 1. Trajectories of the spiral wave tip on the surface of a paraboloid with $A = 0.15$ computed for the system (9) with: (a) $\sigma = 0$ and $\varepsilon = 0.08$; (b) $\sigma = 1$ and $\varepsilon = 0.05$. Dashed curve indicates position of excited region ($u > 0.05$) at the end of the integration interval

In computations performed with $\sigma = 0$ and $A = 0$ a circular pathway of the spiral wave tip was registered. It means that a spiral wave induced on a plane described by (9) rotates rigidly around a fixed center. However on the surface of paraboloid with $A = 0.15$ a similarly induced spiral wave starts to drift. The corresponding trajectory of the spiral wave tip is shown in Fig.1 (a) in the (s, ϕ) coordinate system and can be interpreted as a circular motion around a slowly moving center. It can be seen that the spiral wave core, initially located on a distance about $s_R/2$ from the top of the paraboloid, moves mainly towards the east and there is a small component of its velocity directed towards the top. Finally the trajectory approaches a circular pathway around the top of the paraboloid. It is interesting to compare this result with a trajectory of the spiral wave tip computed on a paraboloid with the same shape, but with $\sigma = 0$ and $\varepsilon = 0.05$. This trajectory is shown in Fig.1 (b). In this case the spiral wave core is moving towards the west and practically does not drift in the perpendicular direction. Note that this case has been earlier analyzed numerically by use of quite different model of excitable media¹⁰⁾ and the same direction of the drift has been observed. Thus the

variation of the diffusion coefficient of the inhibitor results in strong influence on the spiral wave core drift. The role of the paraboloid shape was also investigated. Thus it was shown that when one will decrease the parameter A (it reduces the Gaussian curvature and its gradient), the drift of the spiral wave core will become slower as the theory predicts.

Experiment

The drift of spiral waves on parabolic surface was observed in BZ reaction by use of mesoporous glass as reaction medium¹¹⁾. We used the following solution: 0.3 M NaBrO₃, 0.3 M malonic acid, 0.3 M sulfuric acid. The temperature was 20° C. Mesoporous glass was used not only for controlling diffusion but to obtain a well-defined 2-dimensional active medium. We prepared a bullet made of mesoporous glass the head of which was paraboloid ($z = -0.69r^2$ (in mm)) with the diameter 3.52 mm and height 2.14 mm. The lower part was cylindrical (diameter 3.52 mm, height 1.7 mm). This bullet was soaked in an aqueous ferroin solution (25 mM) for very short period (5 sec.) to prepare a catalyst-immobilized curved surface. For optical measurements we made the bullet stand on its flat bottom where ferroin was not immobilized. The dynamics of spiral wave was observed from the bottom through a microscope. In the beginning of the experiment the spiral center existed at $r = 0.5$ mm, and the core radius was 0.1 mm. During its evolution the spiral wave showed very complex dynamics. After rather long and complicated transition process the spiral started drifting towards the top of the paraboloid. This drift lasted about 30 min. The measured average velocities of the drift had the following values: $d\phi_0/dt = 3.4 \cdot 10^{-4}$ rad/s, $dz_0/dt = 3 \cdot 10^{-5}$ mm/s. Note that the measured velocity dz_0/dt corresponds to the angular velocity $d\theta_0/dt = 1.64 \cdot 10^{-4}$ rad/s. In average the core of the spiral drifted about 70 degrees for one hour. At the final stage the spiral showed clear meandering of almost five-fold symmetry. Although during our experiments the drift towards the top of the paraboloid was observed and the measured velocities are in good qualitative agreement with the kinematic theory the process of the drift was not regular. Moreover in contradiction with the theory the drift on the cylindrical surface was also observed. No doubt we need more precise experiments in order to make final conclusions.

Conclusion

The drift of spiral wave on nonuniformly curved surface was studied theoretically, numerically and experimentally. The computational results correspond very well with the theoretical predictions. The experimental results, however, partly are not clear, although the drift towards the top of the paraboloid was observed. We plan to continue our experiments paying maximal attention to the homogeneity of the medium.

Acknowledgements

This work was supported partly (VSZ) by Deutsche Forschungsgemeinschaft.

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