Scroll wave meandering induced by phase difference in a three-dimensional excitable medium

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We investigated scroll waves in an inhomogeneous excitable 3D system with gradient of excitability. The gradient promotes twisting of the scroll waves. Sufficiently large excitability gradient enhances the twisting and causes simple scroll waves to transition to meandering scroll waves. For the twist-induced instability of scroll waves, we analyzed the stability of 2D spiral waves sliced from the twisted scroll in the vertical direction. The 3D problem is simplified by taking into account the diffusive coupling in the third direction as a time-delayed perturbation to the 2D spiral wave. An additional "negative mass" term measuring the twist thus arises in the 2D system and induces the transition from simple rotation to meandering. A further increase in the gradient ruins partially the unity of the meandering scrolls and generates semiturbulence, the analogs of which were observed in the Belousov-Zhabotinski reaction. We also generated the phase diagram in the parameter space by adjusting the threshold for excitation of the media.

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I. INTRODUCTION

As a prototype of spatiotemporal pattern formation in oscillatory and excitable media, spiral waves appear ubiquitously in a wide range of systems, such as chemical reactions [1], nonlinear optics [2], liquid crystal [3], magnets [4], subcellular biology [5], cardiac muscle [6], etc. In 2D systems, spiral waves can breakup through Doppler instability [7,8] and the convective Eckhaus instability [9]. The 3D analogs of spiral waves are scroll waves characterized by the shape and motion of the filament [10], i.e., the line around which the scroll rotates. Scroll waves are thought to play an important role in ventricular fibrillation [11], and this has motivated detailed examinations of their instabilities. The ways for the scroll waves to lose their stability include twist-induced instability known as "sproing" [12], negative tension instability [13–15], which gives rise to "Winfree turbulence" [11,16,17], and 3D form of meandering [18]. For all three types of instabilities, linear stability analysis of scroll waves in isotropic and homogeneous media has been reported [19]. In more recent experiments, the application of optical tomography, which permits spatial and temporal resolved observation, has allowed detailed studies of scroll waves dynamics [20,21].

The dynamics of scroll waves in the presence of parameter gradient has been investigated considerably in the past 20 years. Experiments in 3D systems with thermal [22,23], chemical [20], and illumination [24,25] gradients have been carried out. The externally applied gradients can drive the scroll waves to drift and twist [22,26], control the spatial orientation and lifetime of scroll rings [23], and promote scroll wave instability [22,27]. Numerical results showed that the instabilities can be controlled by applying a suitable periodic forcing [16,28] or simply noises [29]. In regimes of simple oscillation, the media with gradients of control parameters were demonstrated to exhibit line defects that were usually found in 2D complex oscillatory media [30].

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As scroll waves and their instabilities in homogeneous and isotropic media have been considered in detail, the situation in more complex media with spatial inhomogeneity are less analyzed [31]. In this respect, a semiquantitative ribbon model of twisted scroll waves has recently been formulated for media with spatially varying excitability [32]. In this paper, we numerically simulate the instability of scroll waves in a heterogeneous medium with gradient of excitability using the piecewise linearized FitzHugh-Nagumo model [33]. In equivalence to that reported in Ref. [19], we present an alternative treatment of the twist-induced instability. For the experimentally relevant system, we analyze the instability of 2D spiral wave sliced from the twisted scroll and take the diffusive coupling in the vertical direction into account as a time-delayed perturbation to the 2D spiral wave. This permits us to simplify the problem to 2D. The effective 2D system contains an additional "negative mass" term. It measures the twist and induces the instability.

In our simulations, the phase of meandering scroll wave gives way to a more "disordered" phase as the gradient is tuned to high levels. Simulation results are comparable to the experimental observations in the Belousov-Zhabotinski (BZ) reaction. The irregular state that we called semiturbulence has its counterpart in the BZ reaction. In the following, we will first give a description of our numerical findings in the inhomogeneous 3D system. The transition from the simple rotation to meandering is then analyzed. A brief discussion is given at the end of the text.

II. MODEL

We consider the two-species model for excitable media, which is a modified version of the FitzHugh-Nagumo model [33]. It is described by the following equations:

$$\frac{\partial u}{\partial t} = \nabla^2 u + f(u,v), \tag{1}$$

$$\frac{\partial v}{\partial t} = g(u) - v, \tag{2}$$

where u and v represent the concentrations of two reactants. The functions $f(u,v)$ and $g(u)$ are defined by

$$f(u,v) = \frac{1}{\varepsilon}u(1-u)\left(u - \frac{v+b}{a}\right) \tag{3}$$

$$g(u) = \begin{cases} 0 & u \leqslant \frac{1}{3} \\ 1 - 6.75u(u-1)^2 & \frac{1}{3} \leqslant u < 1 \\ 1 & u \geqslant 1. \end{cases} \tag{4}$$

The mass of species v is assumed to be large and is effectively nondiffusive. a, b, and ε are control parameters for the local dynamics. In excitable regimes of this model, simple spiral waves and meandering spiral waves are supported in 2D systems [33].

Here we are interested in the 3D situation of this model in which the third dimension is constrained by the gradient of a control parameter ε. We consider that the values of a and b are all equal in the whole system, and the value of ε is uniform in the x-y plane but is decreasing linearly in the third dimension z:

$$\varepsilon(z) = \varepsilon_0 + \Delta\varepsilon\left(1 - \frac{z}{h}\right), \tag{5}$$

where h is the thickness of the system, and $\Delta\varepsilon$ measures the gradient of reaction parameter ε in z direction. The 3D system is discretized into $512 \times 512 \times 15$ lattice with spacial step 0.39. The system consists thus of 15 diffusively coupled layers of 2D reaction-diffusion systems. Simulations using finer discretization with more pixels in the vertical direction produce consistent results. Parameters $a = 0.084$, $\varepsilon_0 = 0.02$, and $h = 5.46$ are fixed, and $\Delta\varepsilon$ and b are tunable parameters in our simulations. The value of ε in the 15th layer denoted as $\varepsilon(15) = 0.02$ is fixed while the values for lower layers obey Eq. (5). The Eqs. (1)–(5) are integrated numerically using the Euler algorithm with no-flux boundary condition. For each layer of the system, initial conditions for spirals are appropriately applied so that a spiral is automatically generated in the layer. For each set of parameters used in our simulations, we let the system evolve for a long time and consider only the asymptotic behaviors.

III. PHASE DIAGRAM

The parameters b and ε that we tune in our simulations are decisive for the excitable system: b determines the excitation threshold, ε determines the time scale of the fast variable and its inverse is a measure of the excitability. Equations (1)–(4) are excitable when b is positively small and $a < 1 + b$. Pattern formations in the system described by Eqs. (1)–(5) in the $\Delta\varepsilon - b$ parameter space are summarized in Fig. 1(a). The patterns that dominate the phase diagram are successively simple scrolls, meandering scrolls, and semiturbulence phase as the gradient of ε is increased. In the regime of simple scroll waves, the spirals in each layer perform simple rotations, each with its tip moving in a small periodic circle. The filament formed by the tips of the spirals' waves is a nearly vertical straight line [Fig. 2(c)]. The pattern in this regime is thus identical to normal scroll waves in homogeneous 3D systems. When the gradient of ε exceeds a critical value, the filament is no longer straight [Fig. 2(d)], and the system enters into the regime of meandering scrolls. The filament is twisted

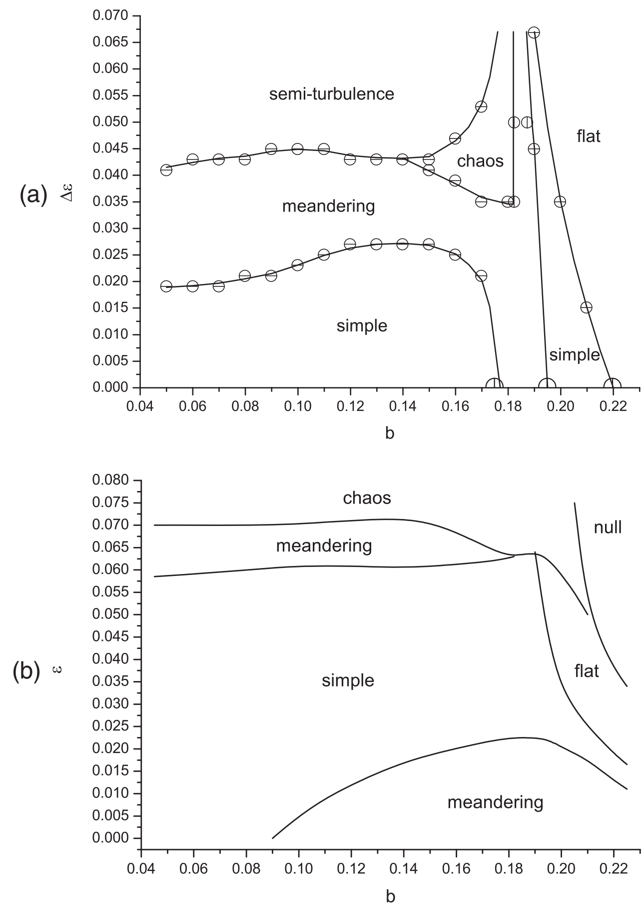

FIG. 1. (a) The phase diagram of the inhomogeneous 3D excitable system. 3D pattern formations that are possible in $\Delta\varepsilon - b$ space include simple spirals, meandering spirals, semiturbulence, chaos, and flat waves. (b) The phase diagram of the homogeneous 2D system [33]. Parameters: $a = 0.84$, $\varepsilon(15) = 0.02$.

gradually, which rotates as the time proceeds. The patterns in the top of Fig. 2 represent the "total concentration" obtained by summing up v in all 15 layers. The simple scroll is demonstrated in the top left. The meandering scroll (top right) shows a blur wave crest due to the out-of-phase meandering of spirals in each layer.

As the gradient of ε is increased further, more complex patterns appear in this inhomogeneous 3D system. For instance, as $\Delta\varepsilon$ is increased to 0.044 with b fixed at 0.13 [Figs. 3(a), 3(b), and 3(c)], the scroll waves exhibit some irregularities. The spiral in the 15th layer is almost regular due to the fact that $\varepsilon(15)$ is fixed at 0.02. As ε grows linearly down the layers and the excitability decreases, the wave crest becomes indistinct. The seemingly "turbulent" pattern is in fact partially disordered. We denote this pattern with irregularities in Fig. 1 as "semiturbulence." The filament, which is integral in the simple spiral region, bends into a wiggly spiral shape [Fig. 3(d)]. The most prominent character of this phase lies in that the majority of filament is still connected, and the pattern is partially coherent. It takes on a wiggly and irregular spiral shape, with only several fractured filaments attached on the boundary. See Supplemental Material at Ref. [34] for the movie of filament movement of this partially disordered turbulence [34]. The semiturbulence will turn into full turbulence when

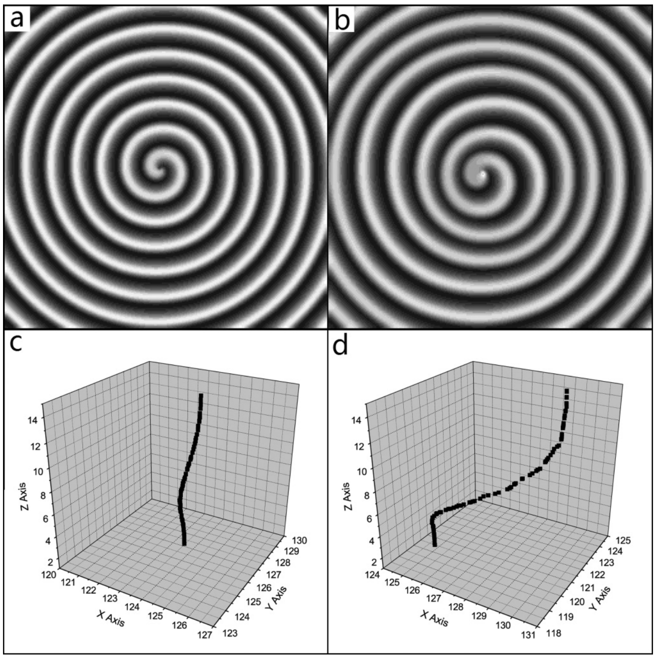

FIG. 2. The patterns of simple (a) and meandering (b) scrolls generated by summing up the v fields in all 15 layers. The filaments formed by planar spiral tips are demonstrated in (c) and (d), respectively. The former for simple scroll is almost a straight line and it is a twisted curve for the meandering spiral scroll. Parameters: $\Delta\varepsilon = 0.018$ for (a, c) and for $\Delta\varepsilon = 0.03$ for (b, d). Other parameters: $a = 0.84$, $b = 0.11$, $e(15) = 0.02$.

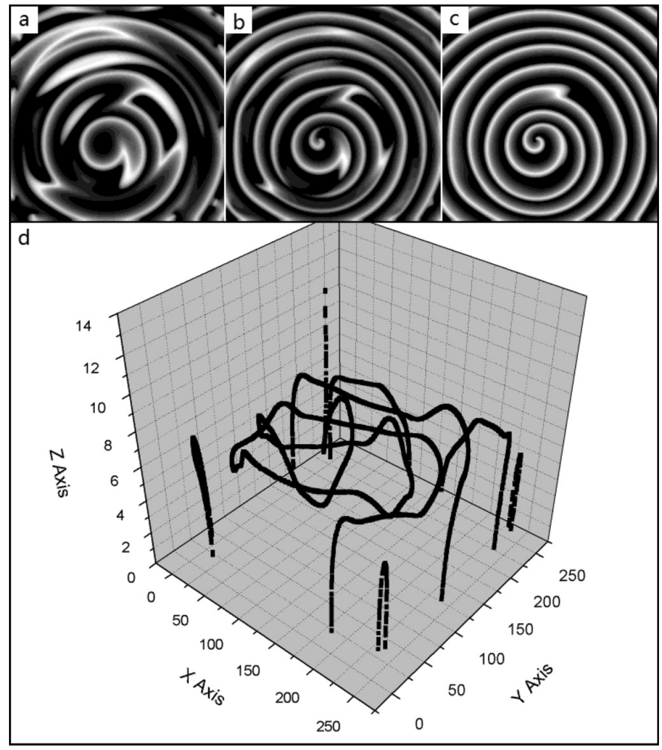

FIG. 3. The pattern denoted as semiturbulence phase. (a, b, c) The planar patterns in the 1st, 8th, and 15th layers, respectively, at a same instance of time. The filaments for this pattern is demonstrated in (d). Parameters: $a = 0.84$, $b = 0.13$, $\varepsilon(15) = 0.02$, $\Delta\varepsilon = 0.044$. Refer to the movie supplemented for the filament motion [34].

the gradient of ε is tuned high enough [not included in Fig. 1(a)].

Another full turbulence phase emerges when the excitation threshold is changed by tuning b to above 0.15, which is labeled as "chaos" in Fig. 1(a). Figures 4(a)–4(c) demonstrate the time evolution of the 2D pattern to turbulence in the 8th layer. The turbulence is generated when $\Delta\varepsilon$ is increased to 0.036 with b fixed at 0.17. During the process to turbulence, the defects of the meandering spiral wave become sources of target waves, which are unstable and continuously divide. Due to boundary effects and interference between the waves, no complete target exists in the medium when the system arrives at the asymptotic full turbulent state. In contrast to the fact that semiturbulence is partially disordered, the filament [Fig. 4(d)] of turbulence breaks into pieces and the pattern is completely disordered. See Supplemental Material at Ref. [34] for the movie of filament movement of full turbulence [34].

The simulation results obtained with $b < 0.14$ are comparable to the experimental observations in the BZ reaction as depicted in Fig. 5. The BZ experiment is carried out in a spatial open reactor (refer to Ref. [27] for the setup). We have chosen $[H_2SO_4]^{I}$ as the control parameter. It is varied from 0.40 M to 0.80 M with precision 0.1 M. Other parameters are kept fixed: $[H_2SO_4]^{II} = 0.3$ M, $[NaBrO_3]^{I,II} = 0.2$ M, $[CH_2(COOH)_2]^{I} = 0.6$M, $[KBr]^{I} = 60$ mM, and $[Ferroin]^{II} = 1$ mM. The reaction temperature is 25 ± 0.2°C. As the concentration of $[H_2SO_4]^{I}$ is tuned, the simple scroll wave [Fig. 5(a)] undergoes successive transitions to meandering scroll wave [Fig. 5(b)], to "semiturbulence" [Fig. 5(c)], and to full turbulence [Fig. 5(d)]. The experimental results in the BZ reaction are in qualitative agreement with the simulation results with increasing gradient in ε and not very large b value. For example, the"semiturbulent" spiral pattern that we simulate in our model (Fig. 3) has its analog in our experiment of BZ reaction [Fig. 5(c)]. The "semiturbulent" spiral comes out when $[H_2SO_4]^{I}$ is increased to 0.6 M. The pattern in Fig. 5(c) is seemingly turbulent but is relatively stable and presents a good experimental counterpart of our simulations.

IV. TRANSITION FROM SIMPLE ROTATION TO MEANDERING

When comparing the phase diagram in Fig. 1(a) with that of the homogeneous 2D system Fig. 1(b), one finds that the feature of 2D picture is qualitatively inherited in 3D. Nevertheless, except for the existence of more complicated phases in the 3D system, the transition point from simple to meandering spirals in both systems differs dramatically. For instance, simple spirals in the 2D system undergo the transition to meandering spirals when a and b are fixed at 0.84 and 0.07 and ε is around 0.06 [33]. While in the 3D case we consider, the system undergoes the transition when $\varepsilon(1) = 0.036$ and $\varepsilon(15) = 0.02$; both of them are far below the transition point in the corresponding 2D system. Furthermore, when ε is less than 0.06, the pattern must be the simple spiral wave in the 2D system. The transition from simple scrolls to meandering scroll waves should be caused by the 3D effect of the gradient, i.e., twist-induced instability of scroll waves.

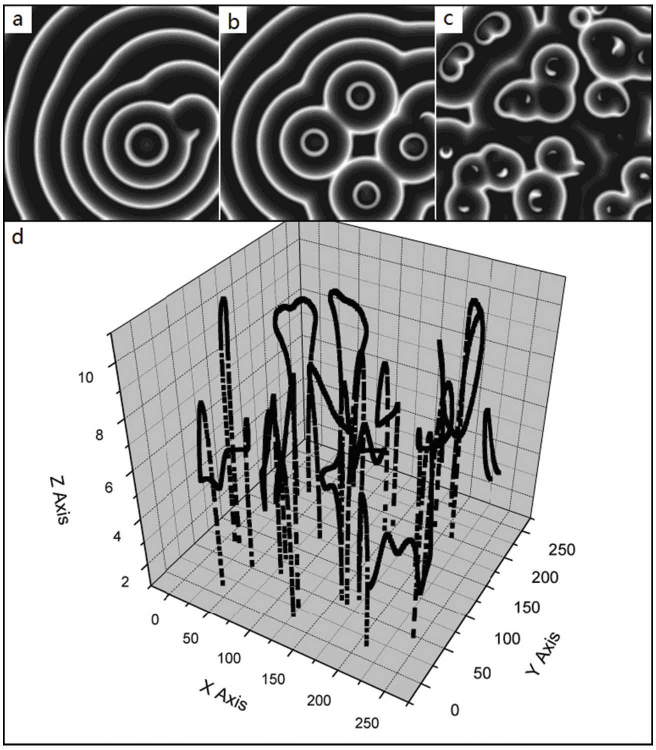

FIG. 4. The development of disordered patterns (denoted “chaos” in Fig. 1) when the gradient in ε is relatively large. The patterns are recorded from the 8th layer in three successive instances of time: (a) shows the state when the system just passes the transition point; (b) is progressing toward disordered state; (c) depicts the asymptotic state; (d) is the filament for the fully developed 3D pattern. Parameters: $a = 0.84$, $b = 0.17$, $\varepsilon(15) = 0.02$, $\Delta\varepsilon = 0.036$. Refer to the movie supplemented for the filament motion [34].

The gradient induces twisting in the scroll waves. Figure 6(a) demonstrates the time evolutions of variable u of different layers at a location with same x-y coordination. The oscillations, which are in identical form, have just phase differences. The oscillation in upper layers can be obtained from a lower layer by a time delay. In the following, we show that the time delay between lower and upper layers can lead to the transition from simple scrolls to meandering scrolls.

As the twist-induced instability of scroll waves in inhomogeneous media has been analyzed with a nonequilibrium ribbon model [32], we present here an alternative treatment that is equivalent to that in Ref. [19]. The twisted scroll wave can be considered as 2D spirals of phase lags that are stacked along the filament. The twist-induced instability is closely related to the stability of 2D spiral sliced from the twisted scroll wave in the vertical direction. As the embedded 2D spiral wave is diffusively coupled with neighboring spiral waves in the vertical direction, the problem could be simplified by taking into account the diffusive coupling in the third direction as a time-delayed perturbation to the 2D spiral wave. It is reasonable to assume that

$$u(x,y,z,t) = u(x,y,t'), \tag{6}$$

where $t' = t - \Phi(z)$ and $\Phi(z)$ is the time delay between $u(x,y,z,t)$ and $u(x,y,0,t)$. Substituting Eq. (6) into Eq. (1), one obtains the equations for the 2D spiral wave sliced

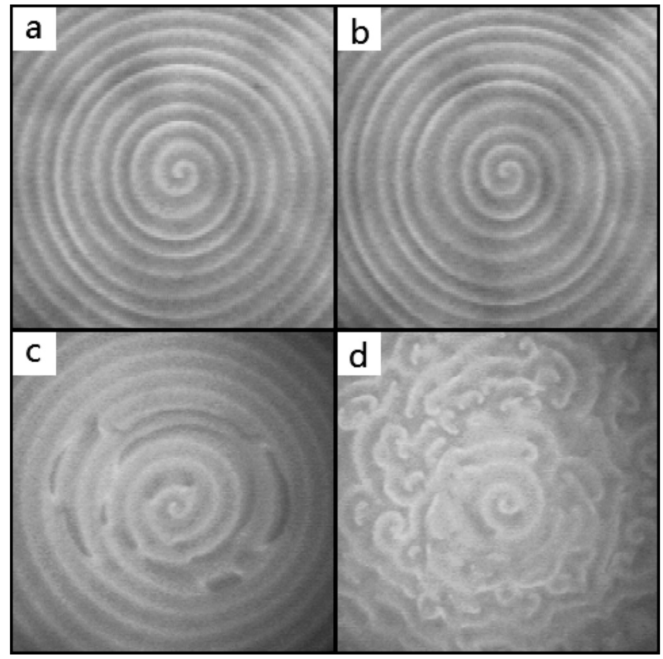

FIG. 5. Experimental observations in the BZ reaction as the concentration of $[H_2SO_4]^I$ is tuned from 0.4 M to 0.8 M. The simple scroll wave (a) undergoes successive transitions to meandering scroll wave (b), to “semiturbulence” (c), and to full turbulence (d). Control parameters: $[H_2SO_4]^I = 0.4$ M (a), $[H_2SO_4]^I = 0.5$ M (b), $[H_2SO_4]^I = 0.6$ M (c), $[H_2SO_4]^I = 0.8$ M (d).

at z,

$$\frac{\partial u(x,y,t')}{\partial t'} = \nabla^2 u(x,y,t') - \frac{d^2\Phi(z)}{dz^2}\frac{\partial u(x,y,t')}{\partial t'} + \left(\frac{d\Phi(z)}{dz}\right)^2 \frac{\partial^2 u(x,y,t')}{\partial t'^2} + f(u,v), \tag{7}$$

$$\frac{\partial v(x,y,t')}{\partial t'} = g(u,v). \tag{8}$$

The second and third terms in the right-hand side of Eq. (7) come from the diffusive coupling in the vertical coordinate. For the system we considered, the phase lag of different level is approximately linearly dependent on z except for layers near the boundary $z = 1$ and $z = 15$ [Fig. 6(b)]. $\frac{d\Phi(z)}{dz}$ is thus approximately a constant and $\frac{d^2\Phi(z)}{dz^2}$ is zero. The approximation is similar to the situation where the twist is homogeneous in z [19]. The term $\{\frac{d\Phi(z)}{dz}\}^2\partial^2 u(x,y,t)/\partial t^2$ in Eq. (7) could play a significant role. As $\{\frac{d\Phi(z)}{dz}\}^2$ is always positive, it can be considered as a “negative mass” term, which would inevitably lead to instability in mechanics. It is actually the twist that causes the simple scroll wave to lose its stability and transit to meandering spiral preceding the same transition in 2D systems.

In polar coordinates, $\frac{\partial u(r,\theta,t')}{\partial t'} = \omega\frac{\partial u(r,\theta,t')}{\partial \theta}$, where ω is the rotating rate of the twisted scroll wave, and Eqs. (7) and (8) take the form,

$$\frac{\partial u(r,\theta,t')}{\partial t'} = \nabla^2_{2D} u(r,\theta,t') + \beta^2\frac{\partial^2 u(r,\theta,t')}{\partial \theta^2} + f(u,v) \tag{9}$$

$$\frac{\partial v(r,\theta,t')}{\partial t'} = g(u,v), \tag{10}$$

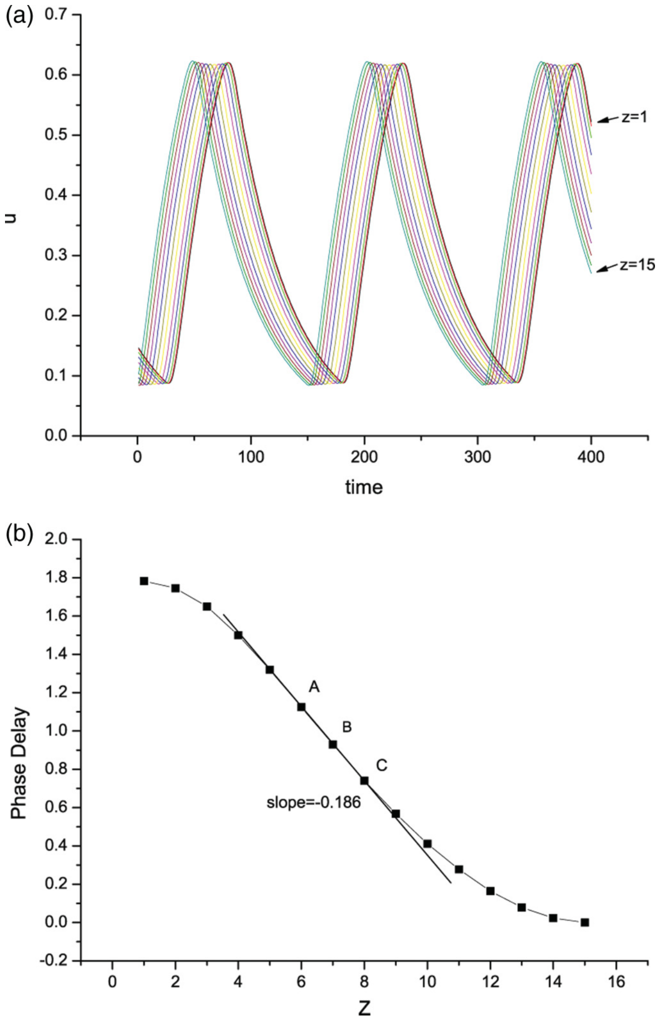

FIG. 6. (Color online) (a) The oscillations of the variable u in different layers at a location with same x-y coordination. They share the same oscillation form but have successive phase lags from the lower to upper layers. The results are obtained with parameters in the regime of simple spiral: $a = 0.84, b = 0.07, \varepsilon(1) = 0.036, \varepsilon(15) = 0.020$. (b) The phase delay as a function of the z coordination calculated from (a). The gradient of phase delay reaches the maximum at point A at the sixth layer, which is about 0.186.

where $\beta = \omega\frac{d\Phi}{dz}$ is equivalently the twist of the scroll wave.

The behaviors of the 3D system, Eqs. (1)–(5), in the neighborhood of simple spiral to meandering spiral transition can now be probed with the 2D system, Eqs. (9) and (10). The equations are simulated numerically from an initial spiral with parameters $a = 0.84$, $b = 0.07$. $\varepsilon = 0.03$ is fixed, which is the intermediate value of ε in the third direction at the transition point. We find that when the control parameter β is tuned to the critical value $\beta_c = 0.22$, the simple spiral wave of the effective 2D system described by Eqs. (7)–(9) undergoes a bifurcation from simple rotation to meandering. Figure 7 demonstrates the paths of the spiral tip as β is adjusted, in which the simple periodic circle is turned into a cycloid curve whose amplitude is amplified gradually as β is increased. Therefore, with parameters that support only simple spirals in 2D systems, meandering spirals can be induced by the phase difference in 3D systems with gradient.

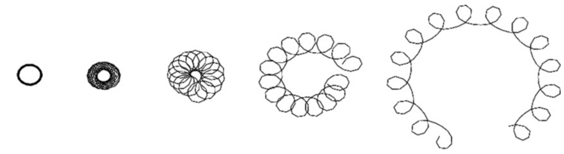

FIG. 7. The traces of spiral tip in the effective 2D system when $\beta = 0.21, 0.22, 0.23, 0.24, 0.25$, respectively (from left to right).

The transition point β_c in Eqs. (7) and (8) can be also estimated in our phase-delay model. At $\varepsilon = 0.03, a = 0.84, b = 0.07$, near the transition, β_c is close to the square of the maximum gradient of phase delay [Fig. 6(b)], which is calculated as $\beta_c = (0.186/0.39)^2 = 0.23$, where 0.39 is the spacial step of the lattice. This is quantitatively in agreement with direct simulations of the effective 2D system, with $\beta_c = 0.22$.

The linear stability analysis of the twist-induced instability has been given by Henry *et al.* [19]. Equations (9) and (10) presented here are similar to Eqs. (3) and (4) in Ref. [19] but have some differences. In Ref. [19], a transformation that takes into account both the rotation of the scroll wave and the twist in the vertical direction was made, and the homogeneous 3D system was reduced to purely 2D due to the translation symmetry along the z axis. The system we consider is inhomogeneous in z, which imposes an inherent twist on the scroll wave. In comparison to Ref. [19], Eqs. (7) and (8) describe a sliced spiral wave from the scroll, which are coupled with neighboring spiral waves that are time-delayed in z due to the twist. The scheme is basically equivalent to that reported by Henry *et al.* [19]. In fact, the control parameter β that determines the "negative mass" term in Eq. (7) or (9) is actually the twist that induces the instability.

V. CONCLUSION

In summary, we have explored the dynamics of scroll waves in the inhomogeneous 3D system with the modified FitzHugh-Nagumo model in which planar spiral waves are coupled diffusively and are constrained by a gradient of excitability in the third dimension to form twisted scroll waves. As the gradients in ε are increased, the twisting is enhanced to cause a transition from simple rotation to meandering scrolls. For the twist-induced meandering of scroll waves, we take the diffusive coupling in the vertical direction into account as a time-delayed perturbation. This permits the simplification of the 3D system to 2D. The effective 2D system contains an additional "negative mass" term, which is the twist that causes instability. Although the instability of scroll waves in complex media with spatial inhomogeneity (gradient) has been studied in several experiments and simulations, it has not been adequately analyzed. Our analysis of the twist-induced instability presents a treatment equivalent to that in Ref. [19] and is supplementary to the nonequilibrium ribbon model for inhomogeneous systems.

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