Dynamics of Chemical Excitation Waves Subjected to Subthreshold Electric Field in a Mathematical Model of the Belousov-Zhabotinsky Reaction

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Abstract We present a numerical study of the dynamics of spiral waves in a weak external electric field, using the Oregonator model of the Belousov-Zhabotinky (BZ) reaction. Both free and pinned spiral waves are studied in two types of electric fields: unidirectional (DC) and Circularly Polarised Electric Field (CPEF). Both free spirals and pinned spiral waves rotate faster in the DC field. The CPEF can help a free spiral to be spatially confined. A pinned spiral period can be controlled by varying the period of the CPEF. Both DC and CPEF can unpin the pinned spiral wave, but the minimum electric field required to unpin is much less with CPEF compared to DC. Thus, CPEF is more energy efficient to unpin a pinned spiral wave.

Keywords Excitable medium · Spiral wave · Belousov-Zhabotinsky reaction · Subthreshold stimulation · Unpinning · Critical threshold

1 Introduction

Excitable systems, in general, are non-equilibrium systems with a stable resting state. They can only be aroused to a transitory excited state after crossing a certain threshold. However, perturbations below the threshold go unnoticed since they cannot set off the system to an excited state. Following the excitation, the medium returns to their resting state after a certain time period called the refractory period, during which further perturbations cannot re-excite the system. Unlike the electromagnetic waves, which obey the superposition principle, excitation waves annihilate upon mutual

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S. Banerjee and A. Saha (eds.), *Nonlinear Dynamics and Applications*,
Springer Proceedings in Complexity,
https://doi.org/10.1007/978-3-030-99792-2_105

collision. Many excitable systems exist in nature, including the heart muscles [1, 2], chicken retina [3, 4], slime-mold aggregates [5], Xenopus oocytes [6, 7], and Belousov-Zhabotinsky (BZ) reaction [8, 9].

One of the characteristic features of a two-dimensional excitable medium is the fascinating patterns such as rotating spiral and target waves. However, in the case of systems like the heart muscle, the high-frequency rotating spiral waves are known to disrupt the natural sinus rhythm. Furthermore, rotating spirals get stabilized once they get pinned to an obstacle. The pinned spiral waves play a key role in the progression of dynamical disorders, including cardiac arrhythmia [10, 11], and epileptic convulsions [12]. Understanding the dynamics of the pinned spiral waves is crucial to develop efficient techniques to control them.

The dynamics of spiral waves and their interaction with the external perturbations can be easily studied in the Belusov-Zhabotinsky reaction. It is an oscillating system that produces patterns by oxidizing malonic acid in the presence of a metal catalyst such as ferroin. External forcing, such as periodic illumination [13] and electric field application [14], are commonly used to study spiral dynamics. The electric field is known to influence the transport of ionic species in chemical media [15]. As a result, the spiral core drifts by forming a parallel and perpendicular component to the direction of the applied field [16]. Li et al. developed a theory of spiral wave drift caused by weak ac and polarised electric fields. Using response function theory, they derive the spiral drift velocity and direction [17]. Circularly Polarised Electric Field (CPEF) with rotational symmetry has been utilized to regulate spiral drift [18]. Frequency synchronization occurs if the CPEF and spiral are having a comparable frequency [19]. The CPEF has been used in cardiac models to investigate the control of both 2D [20] and 3D [21] pinned excitation waves. Punacha et al. proposed a theory for WEH-induced unpinning and showed that spirals can always be unpinned below a threshold time period of CPEF [22]. Furthermore, a unidirectional field is used for the electrically forced release of pinned spiral waves in the BZ medium when the field strength surpasses a critical threshold (i.e., for supra-threshold fields) [23]. Previous studies, however, have not looked into how a subthreshold field, one that is below a critical threshold, interacts with free and pinned spirals in a BZ medium.

In this article, we investigate the dynamics of both free and pinned spirals in the BZ medium exposed to the subthreshold electric field. We compare the behavior of spiral waves with and without an obstacle. We find that the subthreshold electric field generates a shift in the spiral period. At greater field strengths, this effect becomes more pronounced. Compared to DC, CPEF has a lower critical threshold for unpinning, making it a more energy-efficient method to control spiral waves.

2 Methodology

We model the BZ reaction system using the two-variable Oregonator model [24, 25]. The activator, 'u', initiates the reaction, and the inhibitor, 'v', with its slow dynamics, returns the system to the resting state. Their combined effect will steer the entire dynamics. In BZ reaction, u and v corresponds to the chemical concentration of $HBrO_2$ and catalyst respectively. In the presence of an electric field, E, the dynamics of u, and v are given by the following equations.

$$\frac{\partial u}{\partial t} = \frac{1}{\epsilon}(u(1-u) - \frac{fv(u-q)}{u+q}) + D_u\nabla^2 u + M_u\mathbf{E}\cdot\nabla u \tag{1}$$

$$\frac{\partial v}{\partial t} = (u-v) + D_v\nabla^2 v + M_v\mathbf{E}\cdot\nabla v \tag{2}$$

Electric field (E) is implemented in above equations by using an advection term $\mathbf{E}\cdot\nabla u$ and $\mathbf{E}\cdot\nabla v$ respectively. The model parameters are $q = 0.002$, $f = 1.4$, with diffusion coefficients $D_u = 1.0$, $D_v = 0.6$ and ionic mobilities $M_u = 1.0$ and $M_v = -2.0$. The value of ϵ is 0.01 and is used to explicitly determine the system's excitability.

The entire 300×300 computation domain is discretized in space into grids of uniform size $dx = dy = 0.1$ space units (s.u). The temporal evolution is studied using the explicit forward Euler technique with a timestep, $dt = 0.0001$ time units (t.u). Space and time are both measured in dimensionless units. A five-point Laplacian operator gives the coupling between the grids. No flux boundary conditions are imposed on the domain boundary. We use the phase-field method to implement them on the obstacle boundary [26].

An anticlockwise rotating spiral (ACW), either free or pinned to an obstacle of radius, 'r' s.u, is created at the center of the domain. The diffusion coefficient D_u = 0.0001 is set inside the obstacle. After five sustained rotations of the spiral wave with a period (T_s) in the medium, we apply (i) unidirectional DC and (ii) rotating CPEF of strength E.

The DC field along the x-axis is modeled as

$$\mathbf{E}_{DC} = E\hat{i} \tag{3}$$

and we implement an anticlockwise rotating CPEF in the form

$$\mathbf{E}_{CPEF} = E\left(\cos\left(\frac{2\pi t}{T}\right)\hat{i} + \sin(\frac{2\pi t}{T})\hat{j}\right) \tag{4}$$

where T denotes the rotational period of the CPEF. Later, we vary the pacing ratio, i.e., $p = \frac{T_s}{T}$ from 0.5 to 2 in the steps of 0.25 by altering the rotational period of the field. We apply an electric field until the critical threshold for pinned spirals, which is the lowest field strength for unpinning.

3 Results and Discussion

Our numerical study involves the interaction of the electric field of subthreshold amplitude with the rotating spiral. We consider both free and pinned spiral waves in this study.

We start with a unidirectional DC electric field in the medium oriented along the positive x-axis. A free spiral traces out a large core with increasing field strength and moves towards the positive electrode, as shown in Fig. 1a. We define the angle formed by the drift direction with the negative x-axis (represented as OX) as 'Θ', whereas the linear distance traveled by the spiral tip in one spiral rotation is called 'λ'. We calculate λ as the distance between two adjacent petals, which can also be referred to as the petal width. With the strength of the advective field, both Θ and λ increases (see Fig. 1b, c). With increasing field strength, E from 0.2 to 0.8, Θ rises quickly, reaching saturation at around 90 degrees at high field strength. Therefore, the spiral drifts precisely perpendicular to the direction of strong advective fields. The direction of spiral drift also depends on its chirality [16]. On the other hand, λ varies slowly with field strength. As extremely high fields lead to wave break, we limited our study up to $E = 0.8$.

In addition to the drift parameters, we measure the rotational period of the spiral in the presence of the DC field. The normalised spiral period, T_N, is defined as $\frac{T_f}{T_s}$, where T_s and T_f are the spiral periods before and after the forcing, respectively. We observe that the forcing induces an increase in T_N. When the field strength reaches

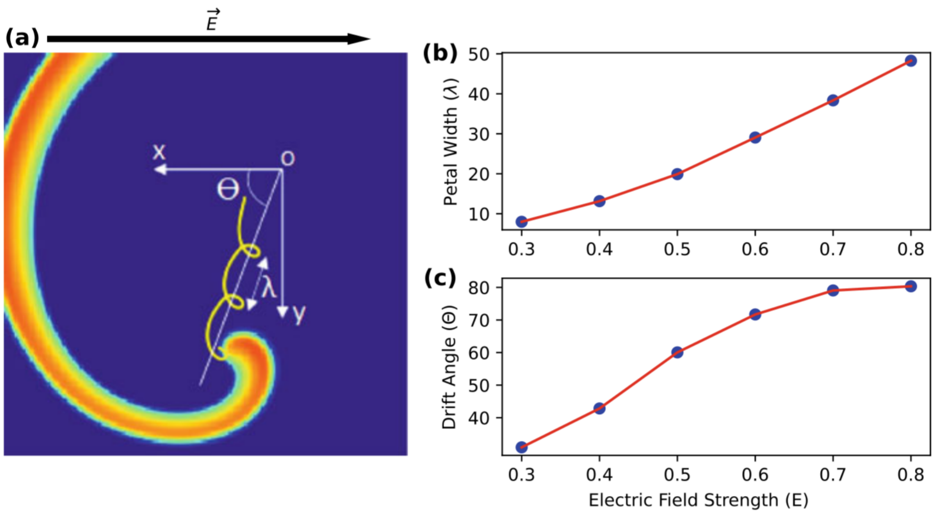

Fig. 1 Spiral drift in the presence of DC electric field. **a** An anticlockwise rotating free spiral drifts towards the positive direction of the field by forming an angle Θ and petal width, λ. The field, $\vec{E}$ is oriented in the positive x-direction, as indicated by the thick black arrow. **b**, **c** corresponds to the variation of λ and Θ with the field strength, respectively

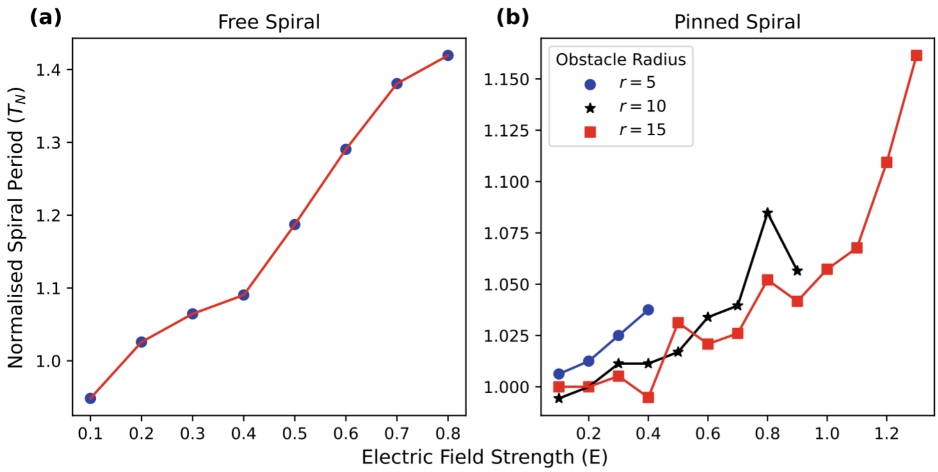

Fig. 2 Variation of spiral rotational period with the subthreshold field strength. a A free spiral's normalised time period (T_N), which increases with field strength. **b** T_N for a pinned spiral anchored to radius, r = 5, 10 and 15, respectively. The field strength (E) is varied till the wave was unpinned

E = 0.8, we see a 40% increase in the spiral period as in Fig. 2a. Hence, the field inhibits spiral rotation and slows it down.

To understand how stable pinned spirals interact with the applied field, we analyze spiral waves attached to obstacles with three different radii r = 5, 10, and 15. The spiral tip gets unpinned when the external forcing reaches a critical threshold [23]. We employ a field with a strength below the critical threshold to avoid unpinning. Like the free spiral, the pinned spiral attached to any obstacle of any size is slowed by the DC field. However, when compared to a free spiral, the increase in the rotational period is insignificant.

Unlike the DC field, CPEF is spatially uniform. In our simulations, we create an anticlockwise rotating CPEF with period T that has rotational symmetry with the spiral. The pacing ratio, $p = \frac{T}{T_s}$ indicates the extent of pacing. For each strength of the electric field, we vary p from 0.5 to 2 in the steps of 0.25. When subjected to CPEF, the spiral tip traces out meandering patterns if CPEF rotates too fast or too slow (see Fig. 3b). However, the motion of the free spiral tip could be spatially constrained for a range of p values closer to 1, as shown in Fig. 3c. In contrast to directed drift in the DC, the rotational symmetry of the CPEF causes the spiral tip to be confined to an area in the medium.

Surprisingly, the response of the pinned spiral to the electric field is strongly influenced by the pacing ratio, p. The spiral period increases with field amplitude for overdrive pacing ($p > 1$), meaning that the spiral slows down. The pacing ratio $p > 2$, on the other hand, does not affect the spiral dynamics (see Fig. 4). We infer that the spiral dynamics are unaffected by the exceedingly high pacing ratio. The spiral period is reduced, or the spiral advances faster when the field strength increases during underdrive pacing ($p < 1$). When the spiral period and the CPEF period are

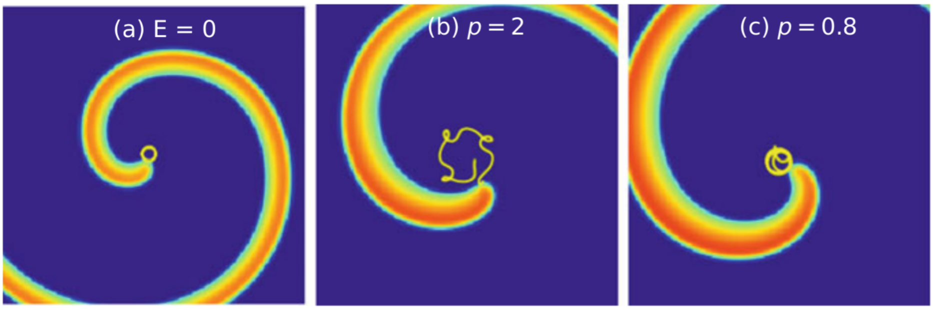

Fig. 3 The tip trajectory of the free spiral before and after applying CPEF. **a** A free spiral, in the absence of an electric field (i.e., E = 0), performs rigid rotation with a small core. From the same initial phase of the spiral (≈ 45°), CPEF with field strength, E =0.6, and pacing ratios of **b** $p = 2$ and **c** $p = 0.8$ is applied to the medium. Meandering occurs when $p = 2$, but $p = 0.8$ results in spatial confinement

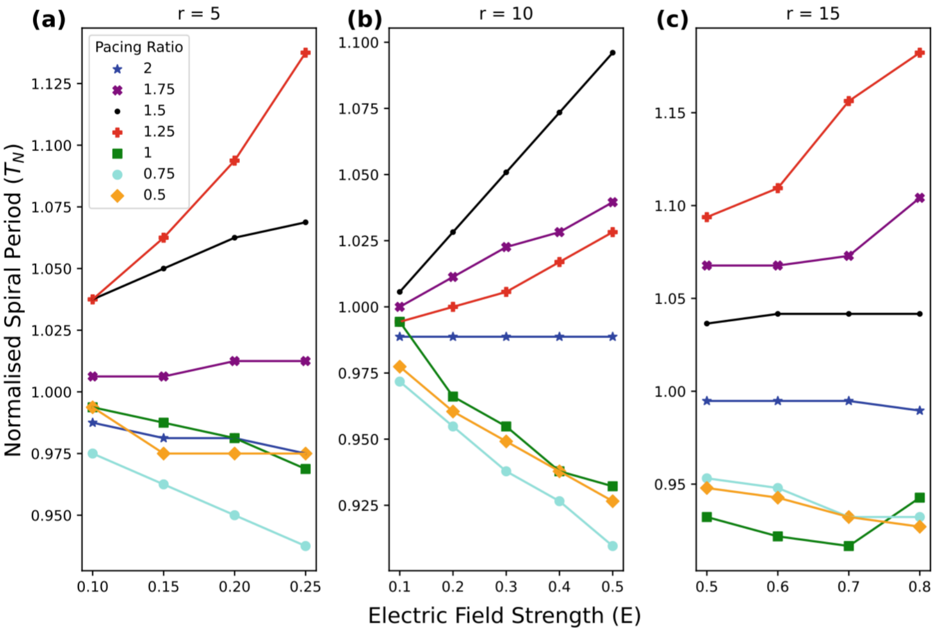

Fig. 4 Response of pinned spiral in the presence of CPEF with different strength and pacing ratio. **a–c** Shows the change in Normalised Spiral Period (T_N) as a function of field strength for pacing ratios p ranging from 0.5 to 2 for radii r = 5. **b** Is same as **a** for r = 10. **c** Is same as **a** for r = 15. T_N increases with the strength of the electric field for overdrive pacing and decreases for underdrive pacing

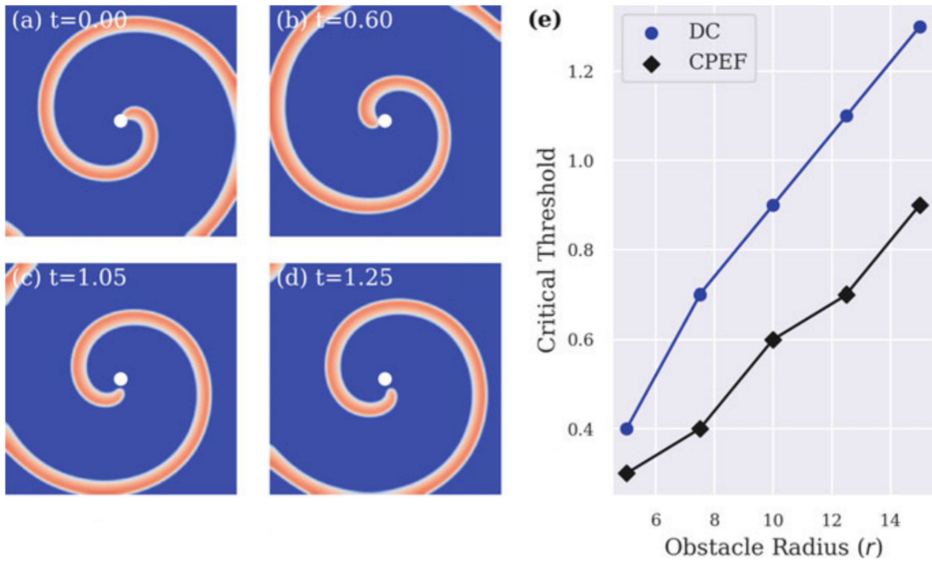

Fig. 5 Unpinning at a critical threshold. **a–d** Snapshots of DC electric field-driven unpinning from an obstacle of radius, $r = 7.5$ at the critical threshold of strength, $E = 0.7$. **e** For both DC (dots) and CPEF with overdrive pacing (diamond), the critical threshold for unpinning is linearly related to the obstacle size. The critical threshold for DC is higher than that of CPEF

both equal ($p \approx 1$), the electric field strength does not affect the T_N. Although the range of T_N varies, the trend mentioned above is followed for all obstacle sizes used in our simulation. Therefore, the spiral alters its rotational period as a response to the change in field frequency.

As the strength of the advective field increases, the pinned spiral's tip drifts away from the obstacle, a process known as unpinning. The critical threshold is the lowest field required to remove the spiral from the obstacle, which may also be thought of as the strength of the obstacle-spiral pinning interaction. In Fig. 5a–d, a DC electric field with a strength of $E = 0.7$ induces unpinning from an obstacle with a radius of r = 7.5 s.u. We investigate the critical thresholds for DC and CPEF for five obstacle sizes with radii ranging from 5 to 15. The pacing ratio is a crucial component in the case of CPEF. Underdrive pacing leads to unpinning only when the pacing ratio is very low. Moreover, unpinning at comparable frequencies ($p \approx 1$) is quite difficult. As a result, we estimate the critical threshold for overdrive pacing in our simulation.

As shown in Fig. 5e, the unpinning critical threshold is directly proportional to the obstacle radius in both DC and CPEF. Furthermore, unpinning may be influenced by the initial spiral phase at field initiation. Throughout this study, we have used the same initial phase ($\approx 45°$) of the spiral. In addition, the critical threshold for DC is higher than that for CPEF for a spiral fixed to any obstacle size. The low critical threshold is a benefit when comparing CPEF to DC. This result helps in the efficient selection of the best low-energy control method.

4 Conclusion

Our numerical work focuses on the interaction of a subthreshold amplitude electric field with a rotating spiral in a BZ medium. We used both unidirectional DC and rotating CPEF to investigate how the spiral dynamics are affected by the direction and frequency of the electric field. The unidirectional DC field slows both free and pinned spirals with increasing field strength. Despite the fact that an electric field increases the spiral period with field strength, the increase in the rotational period for a pinned spiral is negligible compared to that of a free spiral. With CPEF, however, the pacing ratio plays a crucial role in defining spiral dynamics. For a range of values of pacing ratio, p, a free spiral is spatially confined by CPEF. Furthermore, the period of a pinned spiral depends on the pacing ratio of the rotating field. Underdrive pacing causes the spiral period to decrease with field strength, while overdrive pacing causes it to increase. Pacing ratios that are greater than two (i.e., $p > 2$), on the other hand, have no effect. The critical electric field for unpinning by CPEF at overdrive pacing is much lower compared to that at the DC field.

We believe our work has implications for low energy control techniques used for spiral unpinning and control in cardiac dynamics. In particular, a lower critical threshold for CPEF compared to the DC field indicate that CPEF is more energy efficient for unpinning the pinned spiral waves.

5 Author Contributions

A.S and S.V.A conceived the idea and planned the simulations. S.P designed the numerical study as well as the computational framework. T.K.S supervised the project and provided constructive feedback. A.S performed numerical simulations, analyzed the data, and wrote the manuscript with contributions from all authors.

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