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Stabilization of collapsing scroll waves in systems with random heterogeneities

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In three-dimensional reaction-diffusion systems, excitation waves may form and rotate around a one-dimensional phase singularity called the filament. If the filament forms a closed curve, it will shrink over time and eventually collapse. However, filaments may pin to non-reactive objects present in the medium, reducing their rate of collapse or even allowing them to persist indefinitely. We use numerical simulations to study how different arrangements of non-reactive spheres affect the dynamics of circular filaments. As the filament contracts, it gets closer to and eventually touches and pins to objects in its path. This causes two possible behaviors. The filament can detach from the spheres in its path, slowing down the rate of contraction, or it can remain pinned to a collection of spheres. In general, more or larger spheres increase the chance that the filament remains pinned, but there are exceptions. It is possible for a small number of small spheres to support the filament and possible for the filament to pass through a large number of large spheres. Our work yields insights into the pinning of scroll waves in excitable tissue such as cardiac muscle, where scar tissue acts in a way similar to the non-reactive domains. *Published by AIP Publishing.*
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Excitable media, which exist in many chemical and biological systems, are capable of sustaining traveling waves. In two-dimensional systems such as the thin atrial tissue of the human heart, shallow chemical systems, and even bee hives, these waves may form spirals centered at phase singularities. In three-dimensional systems such as the thicker ventricles of the heart and deeper chemical systems, the three-dimensional analogues of spiral waves are called scroll waves and rotate around a curve called the filament. Scroll waves interact with non-reactive heterogeneities of various shapes, greatly changing the qualitative behavior of the wave. Inspired by the random nature of heterogeneities in natural systems, we simulate scroll waves in domains of randomly distributed non-reactive spheres and study how they affect the ability of the waves to persist over time.

I. INTRODUCTION

Excitation pulses–a much studied type of nonlinear wave–exist in a wide range of man-made and natural systems. Their main characteristics include a constant speed and amplitude as well as a trailing refractory zone that interdicts interference phenomena. In chemistry, prominent examples include concentration waves in autocatalytic reaction-diffusion media,[1] catalytic surface reactions,[2] corrosion processes,[3] and synthetic biochemical networks.[4] In biology, excitation waves often coordinate macroscopic phenomena such as the cell aggregation of social amoebae[5,6] or uterine contractions during labor.[7] In addition, they occur at the intracellular level–as exemplified by calcium waves in oocytes, where they prevent polyspermy[8]–or manifest themselves on very large lengthscales as in the cases of defensive behavior of giant honey bee colonies[9] or even epidemic outbreaks such as the bubonic plague.[10]

In most of these dissipative systems, excitation waves self-organize more complex spatial patterns among which rotating vortices have attracted the most attention. In two space-dimensions, the vortices typically take the shape of Archimedean spirals rotating around a central phase singularity.[11,12] The associated spiral tip moves along a small, circular orbit or follows more complicated trajectories such as epi- or hypotrochoids.[13] In three dimensions, wave rotation occurs around one-dimensional phase-singularities called filaments. The associated wave fields are known as scroll waves and can be thought of as continuous stacks of two-dimensional spirals. The filaments move with local speeds that are determined by the filament curvature[14] and some other, often less important factors.[15] Furthermore, the motion depends on the system-specific filament tension α causing loops to shrink ($\alpha > 0$) or expand ($\alpha < 0$).[16,17] For topological reasons, filaments can only terminate at internal or external system boundaries and must do so in pairs of opposite chirality.[18]

The effect of non-dynamic and impermeable heterogeneities on spiral tips and filaments is of short range extending less than one pattern wavelength but can generate complex and non-intuitive motion. Furthermore, filaments tend to self-wrap around thin heterogeneities, thus inducing large-scale changes in the wave field. Moreover, this local pinning can stabilize filament loops that would disappear in finite time due to their tension-induced shrinkage. Numerical studies have shown that impermeable heterogeneities may stop filament motion in the case of induced scroll wave drift.[19] In experiments with the autocatalytic Belousov-Zhabotinsky (BZ) reaction, this stabilization occurs for three or more small spheres and in some cases even for pairs.[20] Single spheres, however, do not stop the collapse but extend the life-time of the loop by 25%.[21] Similar experiments also revealed the stabilization by thin (complete and cut) tori and double tori.[22,23] The latter induces a topological mismatch between the simple filament loop and the pinning genus-2 surface.

The study of the effects of such inert or impermeable heterogeneities in the context of excitable systems is motivated in large parts by the intrinsically heterogeneous nature of all living systems. In biology, heterogeneities arise at different lengthscales from anatomical features, the cellular structure of tissues, and the compartmentalization of the intracellular space. A prominent example is the heart which conducts action potentials, a classic case of excitation waves, to orchestrate the pump action of this vital organ.[24,25] Above the level of individual cells, heterogeneities in the cardiac tissue include blood vessels, papillary muscle insertion points, and remodeled myocardium. The latter is scar tissue that forms after traumatic events such as infarction, and is characterized by a greatly reduced electric conductivity that can block action potentials. Furthermore, such regions can increase the rate of arrythmias and are likely to pin reentrant, vortex-like waves that are an important cause of tachycardia and fibrillation.[26,27] Since human ventricles are sufficiently thick, the corresponding wave patterns must be treated in a spatially three-dimensional setting, which clearly increases the complexity of the heterogeneity-induced dynamics significantly.[28]

Compared to the current understanding of spiral waves in homogeneous two-dimensional systems, little is known regarding the scroll wave dynamics in three-dimensional systems with strong heterogeneities. Earlier studies focused on single defect structures or dynamic heterogeneities in the form of noise[29] but to date no analyses of media with random static non-reactive non-diffusive heterogeneities have been reported. This article addresses this interesting case for the simplest example of randomly arranged spheres, considering the limiting case of complete wave blockage by the individual structures. Using a simple, two-variable model of excitable systems and parallel computing with a programmable graphics processing unit (GPU), we show that the collapse of scroll rings can be delayed or stopped by the random heterogeneities.

II. METHODS

Our simulations employ the Barkley model,[30] which is commonly used to describe excitable reaction-diffusion systems. The model is given by the following dimensionless equations

$$\frac{\partial u}{\partial t} = D_u \Delta u + \epsilon^{-1} u(1-u)\left[u - \frac{v+b}{a}\right], \tag{1}$$

$$\frac{\partial v}{\partial t} = D_v \Delta v + u - v, \tag{2}$$

where u and v are bounded by $0 \le u, v \le 1$. In the context of the BZ reaction, the variables u and v represent the concentrations of bromous acid and the oxidized form of ferroin.[23] The system parameters ϵ, a, and b are 0.02, 1.1, and 0.18, respectively. The diffusion coefficients are $D_u = D_v = 1$. This choice of parameters allows for scroll waves with positive filament tension that have no movement in the binormal z direction.[31] We integrate using the forward Euler method with a seven point finite difference scheme to discretize the Laplacian. Non-reactive non-diffusive spheres are randomly inserted into the domain sequentially before the initial conditions are set. If a sphere would overlap with an existing sphere, we randomly choose a new location until there is no overlap. These spheres are discretized by voxels of size $0.2 \times 0.2 \times 0.2$. The system boundary and the boundary with the inert objects obey no-flux (Neumann) boundary conditions. Simulations are performed on a $240 \times 240 \times 240$ grid with 0.2 spacing and a 0.005 time step.

We parallelize our solver by sectioning the domain into a $30 \times 30 \times 30$ grid of blocks. Each block is processed by a warp of the GPU and contains an $8 \times 8 \times 8$ grid of points. Each point is processed by a thread within a warp. Each thread can share information within its warp and each point on a block's boundary shares information with the warp for the adjacent block.

Each simulation is initiated with an expanding spherical wave with the following equations:

$$\begin{cases} u = 0.95 & 1 \le r \le 4, \\ u = 0 & \text{otherwise}, \end{cases} \tag{3}$$

$$\begin{cases} v = \dfrac{0.9(20-5r)}{15} & 1 \le r \le 4, \\ v = \dfrac{0.6}{6-5r} & 0 \le r < 1, \\ v = 0 & \text{otherwise}, \end{cases} \tag{4}$$

where r is distance from the center of the domain. At $t = 4$, we set the top half of the domain ($z \ge 24$) to $u = 0$ and $v = 0$ and the bottom half of the domain ($z < 24$) remains unchanged, which creates a scroll ring that is stationary in the binormal z direction. We define a point to be on the filament if $u = 0.5$ and $v = \frac{a}{2} - b$ and track it with the marching cube algorithm.[23,32] We assume the arc-length of the filament is proportional to the number of grid points that contain filament, thus $s(t) = \eta n$. Here, $s(t)$ is the arc length, n is the number of grid points that contain filament, and η is a constant determined by the initial condition where the filament is circular (thus the initial radius, R_0, is known) with the formula $\eta = 2\pi R_0/n$. The filament is constantly rotating, so we average the filament length over each period of rotation.

III. RESULTS

To better understand how scroll waves may interact with randomly distributed and sized heterogeneities, we investigate collapsing scroll rings in a domain with randomly distributed non-reactive spheres. In each simulation, we specify sphere size (each sphere in a single simulation has the same size) and the number of spheres. We do not allow spheres to overlap. Figure 1(a) (Multimedia view) displays a pinned scroll wave in such a domain. To facilitate visualization, only half of the scroll wave is shown. Figure 1(b) illustrates the scroll wave filament. The remaining panels depict the scroll wave with spheres removed (Fig. 1(c)) and the filament with only the spheres it is pinned to (Fig. 1(d)).

In a simulation with 60 spheres of radius 2.0, we observe a slowly collapsing scroll ring. Figure 2(a) shows the decline of the filament length over time. The filament length (blue) decreases slower than in the case where no spheres are present (orange). The filament is initially pinned to two spheres (Fig. 2(b), Multimedia view), but unpins and declines quickly. The filament length curve has occasional plateaus where pinning slows the collapse of the filament. For instance, a plateau occurs ahead of point C, due to the pinning to five spheres. At point C, the filament has just detached off the third leftmost sphere while it remains pinned to four other spheres (Fig. 2(c)). Eventually, the filament pins to the center-most sphere (Fig. 2(d)). The filament is now pinned to a set of five spheres, which is able to sustain the scroll wave for 50 time units until the filament detaches off all attached spheres and collapses. We conclude that the filament shrinks slowly while pinned to a set of spheres, but then shrinks rapidly as it transitions by detaching off a sphere and pinning to another. The effect pinning has on the filament length curve is harder to observe early in the simulation because the filament is constantly detaching from old spheres and attaching to new spheres and there is no clear transition of the filament leaving only one sphere and attaching to a new sphere.

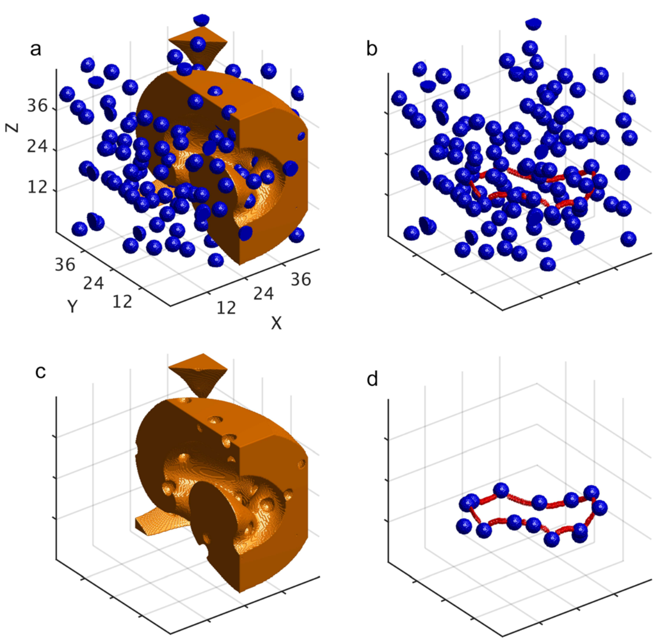

FIG. 1. A scroll wave pinned to spheres of radius 2.0 with 125 spheres in the domain. (a) Half of the wave profile. Orange represents $u > 0.3$. (b) The filament is red. (c) Half of the wave profile without spheres shown. (d) The filament with only pinned spheres. (Multimedia view) [URL: http://dx.doi.org/10.1063/1.4980076.1]

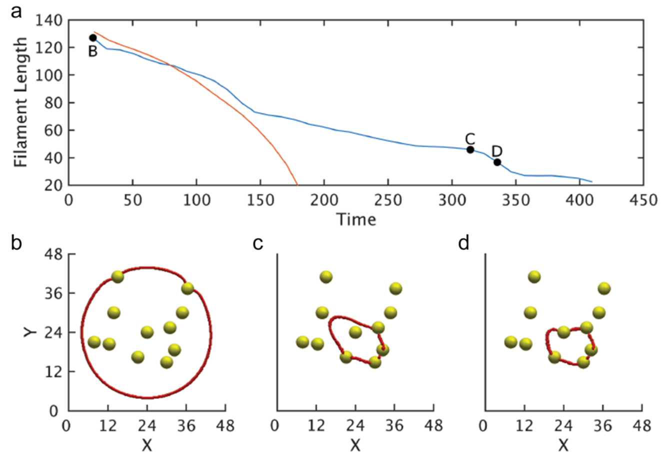

FIG. 2. A scroll ring collapsing in a domain with 60 spheres of radius 2.0. Of the 60 spheres, only the 11 that touch the filament at some point in time are shown. (a) The filament length as a function of time (blue). The orange curve shows the filament length of a scroll ring that has no interaction with heterogeneities. The labels correspond to the remaining figure panels. (b)–(d) A top view of the filament at $t = 9.0$, $t = 308.5$, and $t = 329.5$, respectively. (b) The scroll ring has just been initialized. (c) The filament has just detached off of a sphere. (d) The filament is now pinned to five spheres. (Multimedia view) [URL: http://dx.doi.org/10.1063/1.4980076.2]

In a simulation with more than twice the number of spheres (125 spheres) of the same radius, we observe a persistent scroll ring. Initially, the filament shrinks very rapidly. At $t = 275$, the filament starts to contract extremely slowly while it is still relatively large (Fig. 3(a)) and pinned to 12 spheres (Fig. 3(b), Multimedia view). The filament continues to gradually constrict for almost 200 time units until it detaches from the bottom red sphere (Fig. 3(b)) and quickly collapses due to its positive line tension. The shrinking dramatically abates when the filament pins to the middle red sphere in Fig. 3(c) at $t = 464$. While pinned to the red sphere, the filament length decreases very slowly (Fig. 3(a)) and eventually pins to the dark red sphere in Fig. 3(d) to become completely stationary. The filament is now fully pinned to 13 spheres and touches the leftmost green sphere as it rotates.

To explore minimum conditions for a persistent scroll ring, we begin to randomly remove spheres connected to the filament until the filament collapses. We wait until the scroll ring is stationary at $t = 1000$ to remove the first sphere and continue to remove one sphere every 400 time units (Fig. 3(a), red lines). In each case, the sphere to be removed next is colored dark red. The first and second spheres removed cause a spike in filament length followed by a stationary structure where the filament is pinned to the remaining spheres (Figs. 3(e) and 3(f)). These spikes are due to the filament taking up the space left behind when the sphere was removed. The leftmost sphere (red in Fig. 3(f)) is removed next. The leftmost sphere is chosen for removal since the filament was never truly pinned to it, and only touched it periodically as the filament rotated. Does such a heterogeneity affect whether the filament remains stationary? Removing the leftmost sphere does not cause a significant change in the filament length; it does, however, change the pinning arrangement. The filament switches from being pinned to the

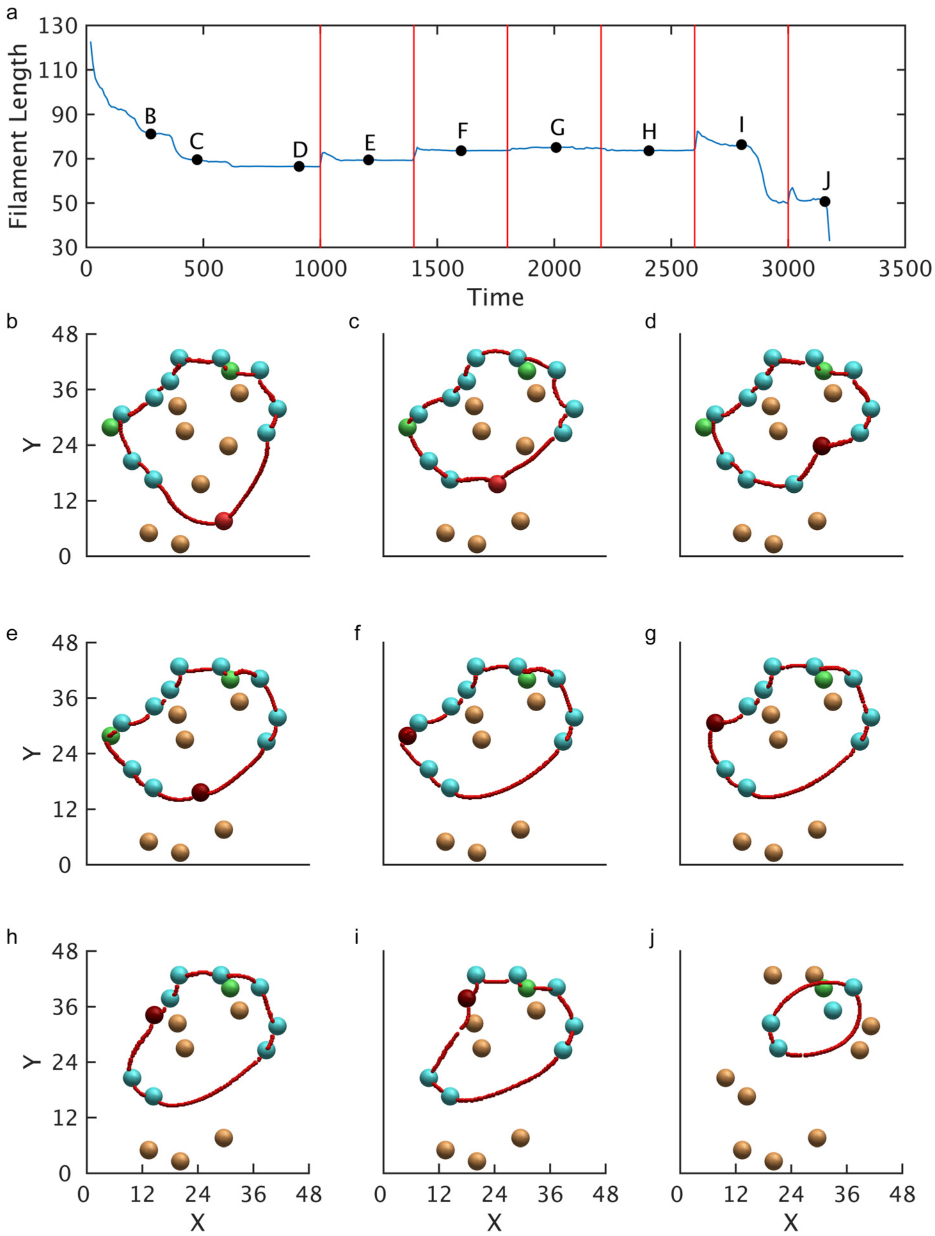

FIG. 3. A persistent scroll ring in a domain with 125 spheres of radius 2.0. Of the 125 spheres, only the 20 that touch the filament at some point in time are shown. (a) The filament length as a function of time. The red lines indicate the removal of a sphere. The labels correspond to the remaining figure panels. (b)–(d) A top view of the filament at $t = 274.5$, $t = 463.5$, and $t = 899.5$, respectively. The filament is contracting slowly in (b) and (c). The filament is stationary in (d). Figure 1(d) depicts (d) in three dimensions. (e)–(j) The same view with spheres removed at $t = 1200$, $t = 1600$, $t = 2000$, $t = 2400$, $t = 2800$, and $t = 3150$, respectively. In panels (b)–(j), the filament is pinned to the blue spheres, the filament periodically touches the green spheres, orange spheres have no contact with the filament, light red spheres are discussed in the text, and dark red spheres are soon to be removed. (Multimedia view) [URL: http://dx.doi.org/10.1063/1.4980076.3]

blue sphere closest to the dark red sphere in Fig. 3(f) to a state in which it only periodically touches the sphere (dark red in Fig. 3(g)), which suggests that a sphere touching, but not necessarily pinning, the filament can play a role in keeping the filament stationary. The now unpinned sphere is removed next, and again hardly affects the filament length (Fig. 3(h)). Removal of the fifth sphere causes another transient increase in filament length followed by a slowly contracting filament (Fig. 3(i)), which persists until the filament unpins from a sphere and quickly collapses to a new stationary state. Shortly thereafter, the sixth sphere is removed (Fig. 3(j)) and the filament ultimately vanishes. The filament is able to become permanently stationary when it pins to 13 spheres and it remains stationary even after 4 of these spheres are removed (Fig. 3(h)).

The first two examples illustrated that more heterogeneities improve the chances of obtaining a persistent scroll ring. How general is this result? To study this, we perform simulations in which the amount and size of spheres vary. The number of spheres ranges from 30 to 160 in increments of five, while the sphere radius ranges from 1.6 to 4.4 in increments of 0.2. For a given number of spheres, we set the sphere radius to 1.6 and run five simulations where each simulation has a different random arrangement of spheres. The number of simulations in which the scroll ring persists for 1000 time units is recorded. This procedure is repeated with increasing sphere radius until all five simulations yield persistent scroll waves or the sphere radius is 4.4. We stop increasing sphere size once we see five persistent simulations because we expect larger spheres to only facilitate scroll ring persistence. The results of these simulations are summarized in Fig. 4 where, for each non-yellow grid point, we track how many of the five simulations persist. We see that more spheres or larger spheres both lead to a higher number of persistent scroll waves. More spheres means there are more options for the filament to pin to, which raises the chance that the filament is attached to an arrangement of spheres that can sustain it. In addition, increasing sphere size causes

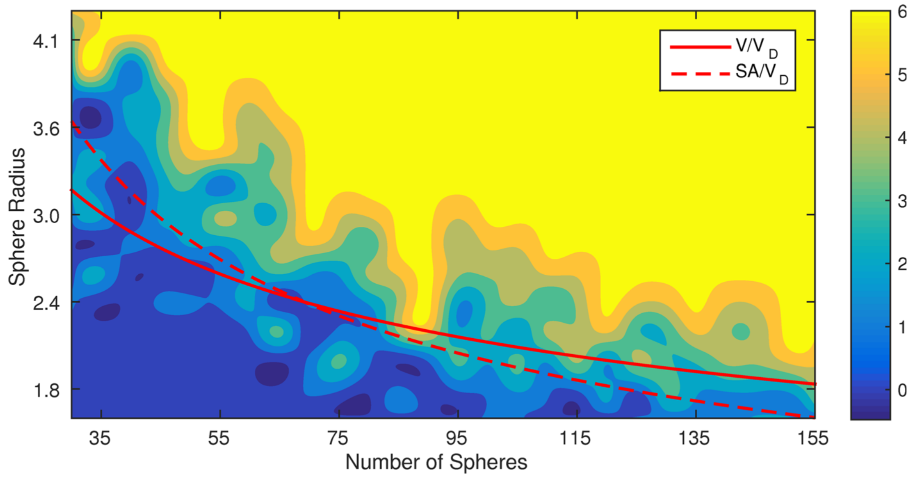

FIG. 4. For a fixed number of spheres and radius, five simulations are performed each with a different set of random sphere locations. We then show the number of simulations, out of five, for which scroll waves last for $t \geq 1000$. Orange represents five persistent scroll waves, while blue represents zero persistent scroll waves. The yellow regions (value of six) were not simulated. The color bar describes how many persistent scroll waves out of five occur at a particular color (with yellow as an exception).The solid red curve represents a constant total sphere volume (V) of 4000. Along the solid curve, 3.6% of the domain is taken up by spheres. The dashed red curve represents a constant total sphere surface area (SA) of 5000. Along the dashed curve, the ratio of total sphere surface area to volume of the domain (V_D) is 0.045.

the filament to detach from spheres more slowly, increasing the chance to pin to multiple spheres.

Figure 4 shows that more or larger spheres increase the likelihood of scroll wave persistence, but is this effect due to the total volume occupied by the spheres or the total surface area? Superimposed onto Fig. 4 is a solid curve of constant volume. Along the solid curve, the number of persistent scroll waves varies primarily from zero to three or four. A similarly placed dashed curve of constant surface area crosses points with a smaller range of persistence, primarily zero to two. This difference suggests the hypothesis that the total surface area is a better predictor for whether a scroll ring will persist.

We test this hypothesis by holding the total volume constant at 9310 while varying sphere radius and the number of spheres. At a given sphere radius, in increments of 0.2, we calculate the number of spheres that give total volume ≈9310 and run 15 simulations with random arrangements. Each simulation has a sphere radius no less than 1.6 and at least 30 spheres. We repeat this process for constant volumes of 4939 and 2208, and for constant surface areas of 6650, 4358, and 2548. Figure 5 summarizes these results. There is a large upward trend in Fig. 5(a) (slope = 1.7), indicating that even with constant volume, larger spheres facilitate scroll wave persistence. The upward trend is much less in Fig. 5(b) (slope = 0.53), which is the test for persistence with a constant surface area. The slope in Fig. 5(a) is significantly greater than the slope in Fig. 5(b), which suggests that the total surface area of the heterogeneities is a better indicator for the probability of persistence than total volume. Our conclusion is further confirmed in Table I, where we use the χ^2 test to determine if the probability of persistence for any

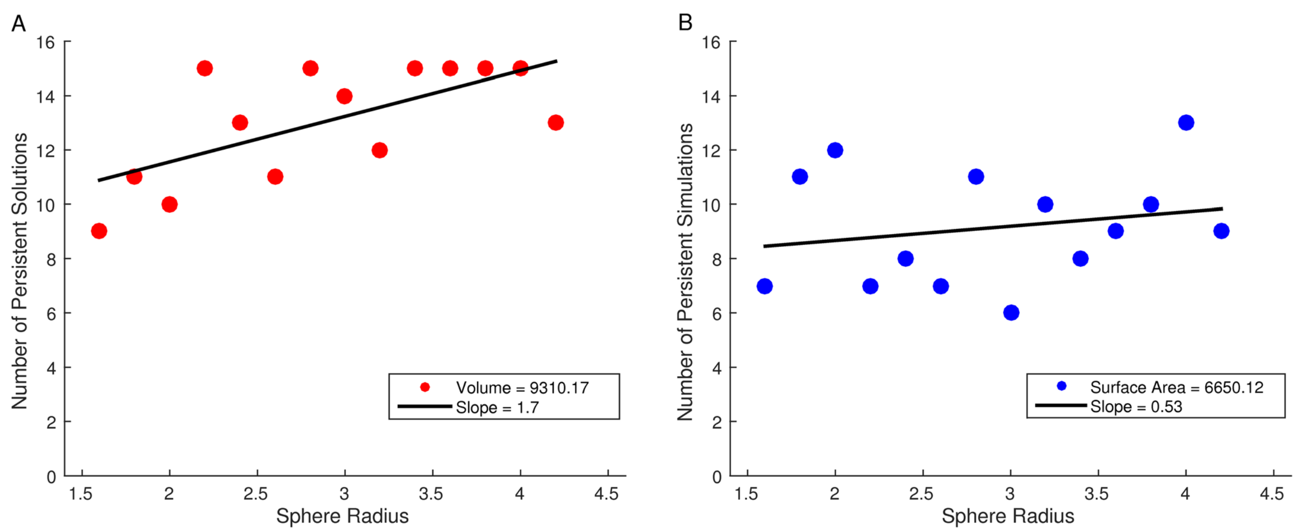

FIG. 5. Fifteen simulations are performed for each sphere radius, while the number of spheres is set to maintain a constant total volume or surface area. Each simulation has different random sphere locations. The number of simulations that persist up to $t = 1000$ is plotted versus the sphere radius. The best fit line is drawn through the points. (a) Total volume is held constant. (b) Total surface area is held constant.

TABLE I. The χ^2 test is used to determine if a binomial distribution with $n = 15$ and $\rho =$ sample mean could have created the results found for a given conserved value.

Constant value	Degrees of freedom	χ^2	p value (%)
Volume = 9310	13	24.9	2.40
Volume = 4939	9	400	0.00
Volume = 2208	5	7.10	21.3
Surface area = 6650	13	3.66	99.4
Surface area = 4358	9	5.77	76.3
Surface area = 2548	5	1.13	95.1

series of 15 simulations is given by the binomial distribution with $n = 15$ and ρ constant for each sphere radius. Here, the constant total surface area always has higher significance values than the constant total volume analog.

While the total surface area of all spheres affects the probability of pinning, whether a sphere arrangement leads to pinning or not ultimately depends on the position of the spheres. Multiple simulations with the same total surface area but different pinning situations make this evident. Because a free scroll ring's rate of collapse is proportional to curvature, so that larger scroll rings collapse more slowly,[14] we hypothesize that scroll waves with a larger filament have a greater chance to pin. We test our hypothesis by placing six spheres with radius $r = 2.0$ in a circular arrangement at $z = 24$ centered around the origin (Fig. 6(a), Multimedia view), which guarantees that the filament will interact with the spheres. We vary the radius of the circular arrangement (R) and examine scroll ring persistence. For $6.6 \leq R \leq 9.2$, the scroll ring eventually dies and for $R > 9.2$ or $R < 6.6$ the scroll ring persists indefinitely. The results in Fig. 6(b) match our expectations when $R \geq 7.0$. Here, we see that scroll rings last longer for larger values of R until they persist for more than $t = 1000$. Unexpectedly, we found that persistence also increased when the circle radius was decreased below seven, and for $R \leq 6.4$ scroll rings persisted past $t = 1000$. This trend does not match our original hypothesis and reveals that tight clusters of non-reactive objects can yield a persistent scroll ring. We studied at $5.6 \leq R \leq 12$ in similar numerical experiments with five or seven spheres. In the case of five spheres, scroll rings collapsed for every value of R. The opposite occurred in the case of seven spheres; scroll rings persisted for every value of R.

IV. CONCLUSIONS

We report that non-reactive spherical heterogeneities slow down, or in some cases prevent, scroll ring collapse. Once the filament attaches to a sphere, the collapse of the scroll ring slows down dramatically. Eventually, the filament detaches from the sphere and contracts quickly until it interacts with another sphere or vanishes. In many cases, the filament may stop shrinking entirely when pinned and become completely stationary except for periodic rotations. We found that the size and the number of non-reactive spheres in the domain impacts which of these two behaviors occurs. Our simulations with randomly distributed inert spheres demonstrate that having more or larger spheres in the domain increases the chance of the filament reaching a stationary state. In addition, the total surface area, compared to volume, of all spheres in the system is better at predicting whether the scroll ring filament will persist indefinitely.

We also found that the particular arrangement of non-reactive spheres has an important impact on whether the filament will persist. Figure 6 demonstrates this well, where spheres that are relatively close or far apart can sustain a stationary filament, but when the spheres are at intermediate distances the scroll wave filament collapses. It is unclear why intermediate distances are unfavorable to scroll wave persistence, and unclear why short distances are favorable for persistence.

Future studies should explore the impact random inert spheres have on scroll rings in qualitatively different reaction-diffusion systems. Filaments of scroll rings in systems without diffusion in the inhibitor variable, such as cardiac tissue, drift in the binormal z direction. It is unknown how this drift affects the filament's stationary states. Different choices of the parameters of the Barkley model can lead to unstable expanding scroll rings, which ultimately leads to spatiotemporal chaos known as Winfree turbulence. A recent study has shown that an inert cylinder can stabilize Winfree turbulence,[33] but to date it is unclear how randomly distributed heterogeneities would affect Winfree turbulence.

As we have mentioned in the introduction, most quantitative experiments on scroll wave pinning have been performed with the BZ reaction. It hence seems appropriate to briefly discuss the feasibility of BZ experiments on vortex pinning to randomly arranged, spherical objects. Such inert objects are readily available in the form of small glass or

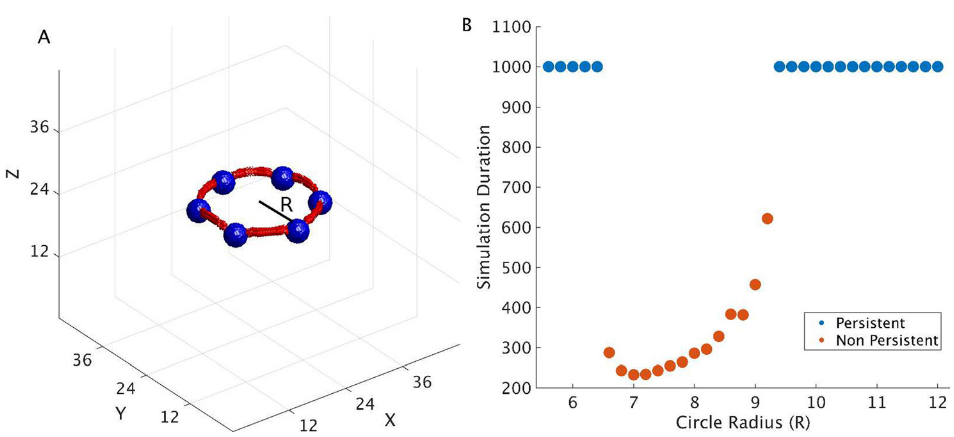

FIG. 6. (a) The filament of a scroll ring attached to six spheres of radius $r = 2.0$. The spheres are arranged in a circle with radius $R = 9.4$. (b) We perform a series of simulations where a scroll ring is attached to six spheres in a circular arrangement with radius varying from $5.6 \leq R \leq 12$. The scroll ring persists for $R < 6.6$ or $R > 9.2$ and has a minimum duration at $R = 7.0$. (Multimedia view) [URL: http://dx.doi.org/10.1063/1.4980076.4] [URL: http://dx.doi.org/10.1063/1.4980076.5] [URL: http://dx.doi.org/10.1063/1.4980076.6]

polymer beads but their placement will clearly require a gel system capable of holding the beads in place. To achieve a random placement, the system could be steadily build up in the vertical direction, while the beads would be introduced continuously at random horizontal locations. During this process, the experimentalists would also create the initial scroll ring following protocols described in Ref. 21 and elsewhere. Ideally, the beads would match the refractive index of the surrounding BZ system to allow for an unobscured optical measurement of the wave pattern and its filament; alternatively, magnetic resonance imaging could be employed.[34]

If these difficulties could be overcome, our computer simulations with the Barkley model make predictions that could be tested experimentally with the BZ reaction. The fundamental prediction is that scroll wave persistence is facilitated by increasing the number or size of spheres. Indeed, the probability of persistence appears to scale with the total surface area of the spheres. We note that the total volume of the spheres in our simulations is a small fraction (less than 5%) of the volume of the domain. Thus, a few small spheres can have a large impact on the scroll wave dynamics. A systematic experimental study of this phenomenon could validate these predictions and perhaps yield insights into specific sphere arrangements that optimize scroll wave stabilization.

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