Stability of knots in excitable media

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Through extensive numerical simulations we investigate the evolution of knotted and linked vortices in the FitzHugh-Nagumo model. On medium time scales, of the order of a hundred times the vortex rotation period, knots simultaneously translate and precess with very little change of shape. However, on long time scales, we find that knots evolve in a more complicated manner, with particular arcs expanding and contracting, producing substantial variations in the total length. The topology of a knot is preserved during the evolution, and after several thousand vortex rotation periods the knot appears to approach an asymptotic state. Furthermore, this asymptotic state is dependent upon the initial conditions and suggests that, even within a given topology, a host of metastable configurations exists, rather than a unique stable solution. We discuss a possible mechanism for the observed evolution, associated with the impact of higher-frequency wavefronts emanating from parts of the knot which are more twisted than the expanding arcs.

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There are a wide variety of naturally occurring excitable media which possess spiral wave vortices. Examples include chemical concentrations in the Belousov-Zhabotinsky reaction [1] and electrical depolarization waves in cardiac tissue [2]. The vortices in this last example are of particular significance, since they are believed to play a vital role in ventricular fibrillation and hence sudden cardiac death [3]. Both these systems, and many others, have a common mathematical description in terms of nonlinear partial differential equations of reaction-diffusion type. In the case of cardiac tissue, the simplest continuous mathematical model is the FitzHugh-Nagumo equation, and it is the investigation of dynamical three-dimensional solutions of this equation, which is the topic of this paper.

More than 20 years ago, it was conjectured that stable, or at least persistent, three-dimensional solutions (termed " organizing centres") might exist in excitable media in which two-dimensional vortices are embedded into three-dimensional space in such a way that they form knotted (or linked) vortex strings. The anatomy of these objects was clarified in terms of the topology of isoconcentration surfaces bordered by vortex strings [4]. The hope was that the nontrivial topology of a configuration, perhaps aided by a short-range repulsive force between vortex cores, or by an effect of phase twist along the vortex string, might provide a barrier to its decay [5]. However, others [6] argued against this optimism with the view that curvature, tension, and reconnection processes would ultimately lead to the collapse and extinction of all knots. A framework was proposed [7,8] for thinking about vortex string dynamics in the limiting case of slight curvature and twist, but attempts to verify it were successful only in the strict limit of no twist [9,10]. Ultimately, to address the fundamental issue of the existence of stable knots, one must turn to numerical methods. About a decade ago, a number of preliminary numerical investigations were performed [9,10], which suggested that certain knotted (and linked) configurations were stable, having a soliton-like behavior in which the knot moved through the medium as a rotating rigid body with a constant shape. However, due to computational constraints, such simulations were limited to time scales which never exceeded about one hundred vortex rotation periods (often substantially less) and used very symmetric initial conditions.

In this paper, we present the results of extensive numerical simulations of a duration well beyond a thousand times the vortex period, and using perturbed asymmetric initial conditions. We investigate several knots and links, and conclude that all appear to be metastable in the sense that small perturbations produce dramatic changes in the evolution over time scales of the order of thousands of vortex rotation periods. The evolution is quite exotic, and very far from the simple curvature and tension-induced collapse suggested previously. In all cases, the topology of the knot (or link) is preserved during the evolution, as we observe no reconnection events. Rather than a simple uniform contraction of the knot, which might be expected as a result of tension, we find that a particular arc of the knot both expands and contracts. After substantial variations in its total length, the knot eventually approaches a steady state. However, this state does not appear to be unique and suggests that, even within a given topology, a host of metastable configurations exists. We discuss a possible mechanism for the observed evolution, associated with the impact of higher-frequency wavefronts emanating from parts of the knot which are more twisted than the expanding arcs.

The FitzHugh-Nagumo equations are given by

$$\frac{\partial u}{\partial t}=\frac{(u-u^3/3-v)}{\epsilon}+\nabla^2 u, \quad \frac{\partial v}{\partial t}=\epsilon(u+\beta-\gamma v), \quad (1)$$

where $u(t,\mathbf{x})$ and $v(t,\mathbf{x})$ are both real fields with u the electric potential and v the recovery variable associated with membrane channel conductivity. We take the constants appearing in Eq. (1) to have the values $\epsilon=0.3$, $\beta=0.7$, and $\gamma=0.5$. This choice of constants is nongeneric and is motivated by our aim of trying to find stable knots. This set of values has a number of special properties which might be conducive to knot stability, such as the lack of meander of a

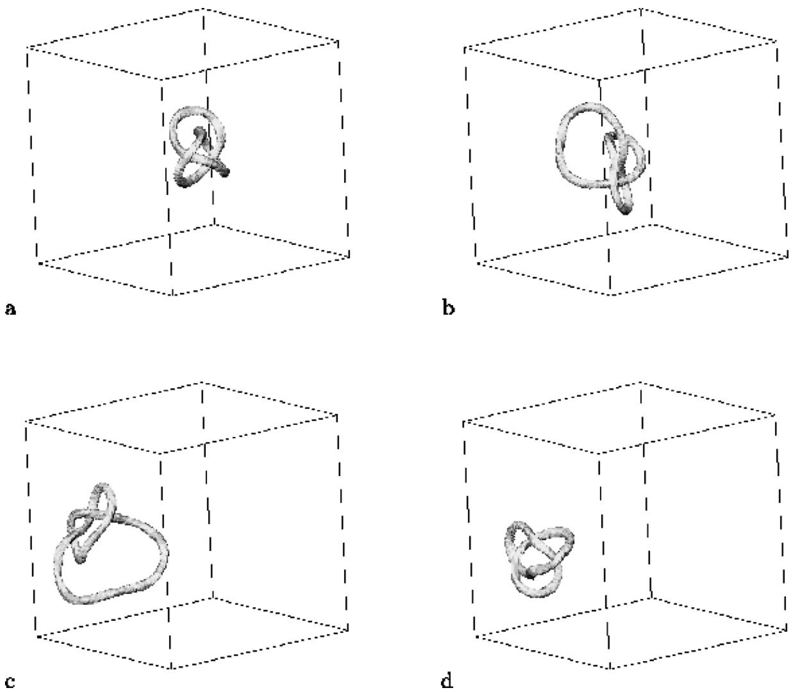

FIG. 1. The core of the trefoil knot at times $t=500$, 5000, 10 000, and 40 000.

two-dimensional vortex and the stability of an untwisted vortex ring in three dimensions. See Ref. [11] for a description of the properties of a two-dimensional vortex as a function of the parameters ϵ,β,γ.

In two-space dimensions, the FitzHugh-Nagumo equations with these parameter values have plane wave solutions which travel at a speed $c=1.9$ and rotating vortex solutions (often called spiral waves) with a period $T_0=11.2$. The vortex solution has u and v wavefronts in the form of an involute spiral with a wavelength $\lambda_0=cT_0=21.3$. Geometrically, this means that all lines which are perpendicular to the level curves of the field u, are tangent to a small circle of diameter λ_0/π. This circle represents the vortex core and is the region in space in which the gradients of the u and v fields differ substantially from being parallel. For later use, it is convenient to define the quantity

$$\Phi=|\nabla u\times\nabla v|, \tag{2}$$

which is highly localized at the vortex core.

We solve Eqs. (1) in three-space dimensions using an explicit finite difference scheme, which is accurate to second order in the spatial derivatives and to first order in the time derivative. Although this scheme appears very simplistic, it appears that the nature of these equations is such that more sophisticated or higher-order algorithms do not lead to substantial gains in efficiency or accuracy, although this can be achieved if one is willing to modify the FitzHugh-Nagumo equations to a form designed specifically for the applicability of a more efficient numerical approach [12]. For our simulations, we use a grid containing 201^3 points and a lattice spacing $\delta x=0.5$, so that our spatial coordinates are confined to the range $-50\leqslant x_i\leqslant 50$. The time step used is $\delta t=0.02$. In the x_1 and x_2 directions, we apply Neumann boundary conditions and in the x_3 direction, the boundary conditions are periodic. The selection of the x_3 direction as periodic is because we shall orient our knots so that they initially translate as rigid bodies moving in the x_3 direction, and we do not wish to impede their motion.

We create initial conditions which form knotted vortex strings by making use of complex curves as described in Ref. [13] and is similar to the approach used in Ref. [14] for the study of knotted topological solitons. Recall that a knot may be written as the intersection of a complex curve $\mathcal{C}$ with the unit 3-sphere S^3. Here, S^3 should be thought of as a compactified three-dimensional Euclidean space, with the explicit coordinates given by stereographic projection,

$$Z_0=\frac{2(x_1+ix_2)}{1+r^2},\quad Z_1=\frac{r^2-1+2ix_3}{1+r^2}, \tag{3}$$

where r is the Euclidean distance from the origin, and Z_0 and Z_1 are two complex coordinates satisfying $|Z_0|^2+|Z_1|^2=1$ and hence parametrize S^3. With this identification, the knot is the one-dimensional locus in space of the complex curve $\mathcal{C}$ with coordinates Z_0 and Z_1. As an example, to represent the $(m{:}n)$ torus knot, we take $\mathcal{C}=Z_1^m-Z_0^n$, where for later convenience we have identified $\mathcal{C}$ with its zero set. If $\mathcal{C}$ has p factors, then it describes an object with p components and hence this formalism can also be used to describe disconnected knots as well as links.

For a given knot (or link), we create initial conditions for the fields u and v from the associated curve $\mathcal{C}$ through the prescription

$$u=\Lambda_1\mathrm{Re}(\mathcal{C})+u_*,\quad v=\Lambda_2\mathrm{Im}(\mathcal{C})+v_*. \tag{4}$$

Here, Λ_1 and Λ_2 are two real constants (taken to be $\Lambda_1=2,\Lambda_2=1$) which are used to scale the initial conditions so that they cover the range of the excitation-recovery loop in (u,v) space associated with the ordinary differential equa-

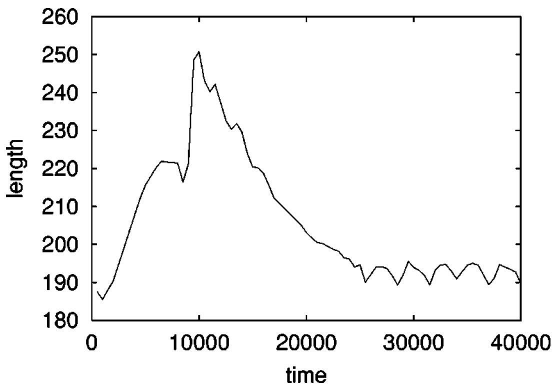

FIG. 2. The length of the trefoil knot as a function of time.

tion part of Eq. (1). The constants $u_*=v_*=-0.4$ are the values which can be roughly attributed to the vortex core.

The simplest nontrivial knot is the trefoil knot, given by the curve $\mathcal{C}=Z_1^2-Z_0^3$. We use this in the above prescription to obtain our initial conditions. In Fig. 1, we plot the isosurface $\Phi=0.01$, which indicates the core of the vortex string, at the times $t=500$, 5000, 10 000, and 40 000. Note that at time $t=0$ this isosurface vanishes, since the initial conditions do not produce the vortex string itself but only seed the field configuration which will form into a vortex string after a time scale of the order of ten vortex periods. In Fig. 1(a), the symmetric trefoil knot has clearly formed. In fact, the knot forms at a much earlier time, but it is slightly larger and quickly shrinks to this size. The knot moves in the x_3 direction (towards the back left-hand side of the box in the figure), with little change of shape, and at a speed of approximately $c/80$, where c denotes the wavefront speed given earlier. The knot also rotates around the x_3 axis with a period of around $160T_0$, where T_0 is the vortex period given above. Figure 1(b) reveals that the knot has drifted slightly away from the x_3 axis and one of the three lobes has expanded in comparison to the other two. Although the initial configuration has a cyclic C_3 symmetry, the cubic grid, and more importantly its boundary, breaks this symmetry and allows an asymmetric instability to develop. The larger lobe continues to expand, Fig. 1(c), and now the knot no longer simply translates in the x_3 direction, but rotates and follows a complicated path in space. Though still preserving the topology of a trefoil, the knot is now better viewed as a large expanding ring with a small knot tied in it. Eventually, the expansion of the arc stops and a contraction begins. By Fig. 1(d) the knot has regained its more symmetric form and has a similar length as before the expansion, but now it appears to be an asymptotic state. This can be seen by computing the length as a function of time, which is displayed in Fig. 2.

To understand a possible mechanism responsible for the expansion of one arc of the knot and the subsequent contraction to a steady state, we need to recall two facts. First, analytical and numerical work shows that a straight and uniformly twisted vortex line has a period which is slightly less than that of the two-dimensional vortex, or equivalently the untwisted vortex line [15,16]. Here, twist refers to the variation of the phase in the complex (u,v) plane as one moves along the vortex string. Second, it is known that for a system of two vortices in which the vortices have different periods (for example, as arises in a model with spatially varying parameters), the collision interface, which is the point at which the spiral wavefronts from the two vortices meet and annihilate, gradually moves towards the vortex with the larger period. In the absence of dispersion, the collision interface moves at a speed $\hat{c}=c|T_1-T_2|/(T_1+T_2)$ where T_1 and T_2 are the periods of the two vortices. Eventually, the collision interface reaches the core of the larger period vor-

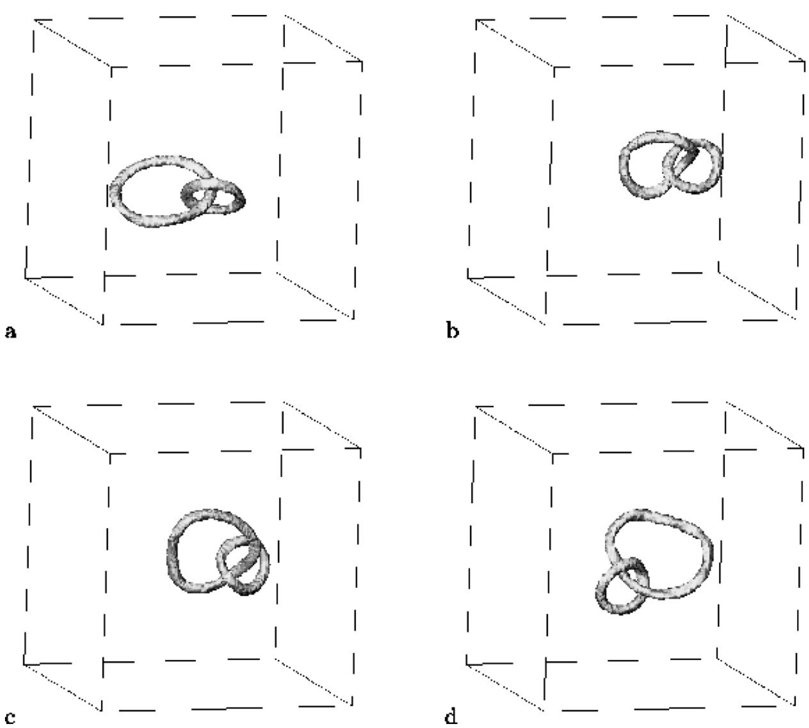

FIG. 3. The core of the perturbed linked rings at times $t=200$, 6200, 10 200, and 15 200.

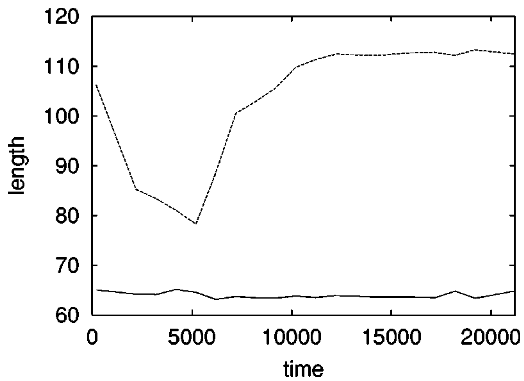

FIG. 4. The length of the small ring (bottom curve) and the large ring (top curve) as a function of time for the perturbed linked rings.

tex and it gets slapped away by the higher-frequency wavefronts emanating from the shorter period vortex [17,18]. Combining these two facts, we see that a reasonable explanation for the expanding arc is that the more knotted part has a greater local twist rate than at least some part of the large expanding ring, so its period is slightly less and this results in its higher-frequency wavefronts slapping away the ring and producing its expansion. This slapping mechanism is discussed in Ref. [19] in the context of stabilizing a knot against contraction. To check this hypothesis, we have examined the collision interface by taking a slice through the configuration in which the expanding arc and most parts of the knot pass almost perpendicularly through the selected plane. This reveals that the wavefront produced by the tightly knotted cores impacts almost on top of the core of the expanding arc, in agreement with our hypothesis for slapping induced expansion. The details will be presented elsewhere [20].

The simplest example, in which the above issues regarding stability can be investigated, is to study two rings linked once. Consider the complex curve $\mathcal{C}=Z_1^2-Z_0^2-\mu Z_0$, where μ is a real parameter. If $\mu=0$, then this curve is associated with two identical rings in which each contain one full twist and are linked once. This configuration has a C_2 symmetry corresponding to a rotation by 180° around the x_3 axis. The link formed from this initial condition moves along the x_3 axis as a rotating rigid structure and shows no sign of instability even up to $t=20\,000$. The reason this example differs from the trefoil knot in this respect is that a C_2 symmetry is clearly more compatible with the cubic lattice (and boundary) of the numerical grid than the C_3 symmetry of the trefoil knot. For this example, we therefore require an explicit perturbation to test the stability of this link. This is achieved by setting μ to be nonzero in the above curve, which distorts one of the rings, making it larger than the other and hence breaking the C_2 symmetry. The results of a numerical evolution with $\mu=0.5$ are displayed in Fig. 3, where we plot the vortex cores ($\Phi=0.01$ isosurface) at times $t=200$, 6200, 10 200, and 15 200. The larger of the two rings initially contracts, but this is followed by an expansion which yields an asymptotic state in which the larger ring has a length similar to that in the perturbed initial condition. In Fig. 4, we plot the lengths of the small ring (bottom curve) and the large ring (top curve) as a function of time. From this figure, it can be seen that the length of the small ring remains almost constant and an asymptotic state has been reached which is certainly very different from the unperturbed solution ($\mu=0$) in which both rings have an equal length. By examination of the collision interface, we again verify that the wavefronts from the small ring impact on the vortex core of the large ring. Moreover, an examination of the twist along each of the rings reveals that the small ring has a roughly constant positive twist along its length, but the large ring has a substantial variation in its twist rate, containing regions of *negative* twist even though the total twist along its length sums to one full turn in the positive direction. The fact that such a highly nontrivial distribution of twist occurs in an apparently asymptotic state is further evidence that a variety of metastable configurations exist in which the relative spatial distribution of the strings is in equilibrium under the action of several complicated forces in which the rate of twisting plays a vital role. To summarize, we have found a novel dynamical behavior of knotted vortex strings in the FitzHugh-Nagumo model with parameter values chosen to minimize any knot instabilities. It would be interesting to determine if our results are generic for the FitzHugh-Nagumo model with other parameter values and also for other excitable media. In fact, there is already some evidence for this in the initial expansion of a trefoil knot in a medium with equal diffusion of both reactants [21], but this example was regarded as an unexplained peculiarity at the time and simulations could not be performed for the length of time required to observe the full expansion and approach to an asymptotic state that we have described in this paper. It would certainly be worthwhile performing extensive numerical investigations, over very long time scales, on a variety of equations modeling different excitable media.

The construction of knotted vortex strings in laboratory experiments on excitable media would be of significant interest, though it is unlikely that the full evolution described in this paper could be studied in this setting since the typical lifetime of vortices in current experiments is limited to less than a hundred vortex periods.

Finally, the interaction and scattering of two initially well-separated knots are also worthy of investigation.

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