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Topological constraints and their breakdown in dynamical evolution

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Abstract

A variety of physical and biological systems exhibit dynamical behaviour that has some explicit or implicit topological features. Here, the term 'topological' is meant to convey the idea of structures, e.g. physical knots, links or braids, that have some measure of invariance under continuous deformation. Dynamical evolution is then subject to the topological constraints that express this invariance. The simplest problem arising in these systems is the determination of minimum-energy structures (and routes towards these structures) permitted by such constraints, and elucidation of mechanisms by which the constraints may be broken. In more complex nonequilibrium cases there can be recurring singularities associated with topological rearrangements driven by continuous injection of energy. In this brief overview, motivated by an upcoming program on 'Topological Dynamics in the Physical and Biological Sciences' at the Isaac Newton Institute for Mathematical Sciences, we present a summary of this class of dynamical systems and discuss examples of important open problems.

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(Some figures may appear in colour only in the online journal)

1. Introduction

It is a generic feature of unforced dynamical systems that they tend to relax towards an equilibrium configuration of minimum-energy subject to any constraints that may apply. Such constraints may have a topological character; to take an everyday example, in settling into an armchair one relaxes to a minimum-energy configuration subject not only to the comforting constraint of the armchair, but also to a multitude of internal constraints associated with



Figure 1. Minimum-energy configuration of a stiff wire in the form of a figure-of-eight knot; the two points of double contact are evident.

the morphology of the internal skeletal structure of the human frame and the interlinked cardiovascular system and other similarly complex vital networks. A more idealized simple system can be easily constructed from a stiff but elastic wire. If the wire has the form of a knot, for example the figure-of-eight knot (figure 1), it can be easily flattened to a plane and placed in a constraining envelope¹; when released from the envelope it will spring to a three-dimensional minimum-energy configuration, with elastic energy being dissipated in the process. This relaxation process is quite rapid, and is ultimately constrained by the topology of the knot: the wire cannot self-intersect, but in its new equilibrium state makes contact with itself at several locations (two 'double crossings' in the case of the figure-of-eight knot). In order to flatten the wire again, some force has to be applied, thus increasing the elastic energy from its minimum. The wire then finds a new equilibrium, subject now to the additional constraint of being confined to a plane.

These simple examples are but two of a large class of problems involving evolution under topological constraints which appear in a very diverse range of fields from Astrophysics and Fluid Mechanics to Molecular Biology. In recognition of the importance of this broad field, a six-month programme (July–December 2012) on the subject *Topological Dynamics in the Physical and Biological Sciences* will take place at the Isaac Newton Institute for Mathematical Sciences with the intention of promoting collaboration between applied mathematicians, physicists and biologists on a wide range of problems having common topological themes, such as mapping dynamical routes towards minimal-energy states compatible with constraints, and elucidating physical mechanisms whereby such constraints may be broken. Within this programme, a sequence of workshops will focus on four areas: (i) Topological Fluid Dynamics; (ii) Tangled Magnetic Fields in Astro- and Plasma Physics; (iii) Topological Aspects of DNA Function and Protein Folding; (iv) Quantized Flux in Knotted and Linked Systems. There will also be a period of focussed research on dynamical problems that involve the topology of surfaces. Our purpose here is not to provide a comprehensive review of these fields, which

have been the subject of various symposia over the last 25 years [3, 33, 43, 44, 53, 54, 57], but instead a brief overview highlighting the interrelationships among them. In section 2 we describe how the notion of 'Topological constraints and their breakdown' appears in each of these areas, and comment on some of the outstanding problems in each field. Section 3 presents a brief description of a case study from our own work which illustrates many of the key issues: a recent experimental investigation of soap film dynamics which reveals an intriguing topological transition in response to slow boundary deformation. The concluding section 4 poses several outstanding questions common to all the subfields.

2. Focus areas

2.1. Topological fluid dynamics

Topological ideas have played an essential role in fluid mechanics ever since Kelvin's 'Vortex theory of atoms' [62], which sought to describe the fundamental structure of matter in terms of knotted vortices in a hypothetical incompressible fluid medium (the ether). Kelvin's theory was short-lived, in part because the knotted vortex structures that he envisaged are almost invariably unstable, a fact that may now be recognized as one of the root causes of turbulence. The theory, unsuccessful though it was, nevertheless served to initiate the study of hydrodynamic instability and transition to turbulence; it also stimulated Tait's monumental study and classification of knots up to crossing number ten [60].

The simplest measure of linkage or knottedness of vortex lines is the 'helicity', the volume integral of the scalar product of vorticity and velocity, an invariant (subject to appropriate boundary conditions) of the Euler equations of ideal fluid flow [41]. Flows of simple structure (e.g. those with streamlines on a family of nested tori) may have a family of such helicity invariants. For complex flows with vortex lines that follow chaotic paths in space, there may be only a single helicity invariant, the volume of integration being the whole flow domain. The key problem for the Euler equations (and even more so for the Navier–Stokes equations at high Reynolds number) concerns regularity, and here helicity conservation is a relevant consideration: starting from smooth finite-energy initial conditions, does the vorticity field remain smooth for all time, or alternatively can it develop a finite-time singularity [18, 22]? If it does so, what is the topology of the vorticity field associated with the singularity? The answers to these questions will have an important bearing on our understanding of the mechanism of viscous dissipation of energy in turbulent flow.

Helicity plays another role in relation to the structure of turbulence. Much interest centres on the origin of 'coherent structures' in turbulent flows, often identified as regions of strong vorticity which are remarkably persistent in an otherwise chaotic environment [27]. In a region in which the helicity is maximal, velocity is either parallel or anti-parallel to vorticity; such a flow is locally 'Beltrami' (a particular steady solution of the Euler equations). In such a region, nonlinear transfer of energy to smaller scales is suppressed, so the structure can persist. Is this the underlying cause of coherent structures? Much direct numerical simulation (DNS) of turbulence [71] is aimed at answering this question; and again it is the topology of the vorticity field, through the helicity for example, on which attention needs to be focussed. A good example of the structure of the vorticity field in turbulence as revealed by DNS is shown in figure 2.

2.2. Tangled magnetic fields in astro- and plasma physics

Magnetic fields in stars and in the interstellar medium are believed to be the result of 'dynamo action', i.e they arise spontaneously and are maintained against ohmic decay by a self-inductive



Figure 2. Intense vorticity iso-surfaces in a DNS of homogeneous turbulence (reprinted from [71], with permission); this simulation was carried out in a periodic box with 40963 grid points, and at a turbulent Reynolds number $Re_{\lambda} = 732$; this Reynolds number is $O(Re^{1/2})$, where $Re = u_0L/\nu$. This figure shows a 'zoomed-in' high vorticity region of size $(7482 \times 1496)l_{\nu}$, where l_{ν} is the 'inner' Kolmogorov scale. Vorticity fluctuations down to this scale are reasonably well resolved.

process: flow across the magnetic field induces current, which, by Ampère's law, generates the self-same magnetic field. Helicity of the inducing velocity field is known to be a powerful agent in this self-inducing process, essentially an instability whereby a magnetic field can grow exponentially from an infinitesimal level until the Lorentz force reacts back upon the flow, establishing some kind of statistical equilibrium. This effect of helicity is known as the 'alpha effect', after the seminal paper of Steenbeck, Krause and Radler [58]. Not surprisingly, the field that is generated is also helical in character, its magnetic helicity being defined as the volume integral of the scalar product of the magnetic field and its vector potential, a gauge-independent measure of the degree of linkage of the magnetic lines of force, also known to be an invariant of the equations of ideal magnetohydrodynamics [69].

Dynamo theory has been given an enormous boost by the relatively recent experimental verification of turbulent dynamo action in the Cadarache laboratory (France). This experiment [45] involves a turbulent flow of liquid sodium driven by counter-rotating co-axial propellers in a large cylindrical container. Centrifugal and Ekman-suction effects conspire to generate a mean flow with nonzero helicity; there is little doubt that the turbulent fluctuations have a similar 'chiral' property, and that an associated alpha-effect is responsible for the magnetic field that is spontaneously generated. Here is a remarkable situation in which theory, intensively developed during the 1970s, anticipated experimental confirmation by some 30 years!

Magnetic helicity plays a contrasting role in the complementary context of magnetic relaxation. The topology of interlinked magnetic flux tubes is conserved in a perfectly conducting fluid (the magnetic lines of force are frozen in the fluid). The Lorentz force associated with such a field generally drives a flow which dissipates energy (to heat) if the fluid is even slightly viscous. Thus energy decreases subject to the constraint of conserved magnetic topology. This process inevitably continues until a minimum-energy magnetostatic equilibrium is established [42]. Such equilibria are stable within the perfectly conducting-fluid scenario. However, in general they contain tangential field discontinuities (i.e. current



Figure 3. Filament destabilization observed by TRACE in Active Region 9957 of the sun on 27 May 2002. The filament started to rise shortly before 18.00 UT; the X-ray flux (recorded by the GOES satellite) rose in step, reaching a maximum around 18:10 UT, just as the twisting filament reached a maximum elevation of ~80 000 km. The magnetic field subsequently remained steady, while the plasma within cooled and flowed back down to the solar surface along the distorted magnetic flux tubes. Reprinted with permission from [25]. Copyright 2007 Springer.

sheets—cf the tangential discontinuities where the bendy wire of figure 1 makes self-contact). These current sheets are the seat of so-called resistive instabilities that are diffusive in origin, and that permit reconnection of field lines with associated change of field topology [49]. Such processes of relaxation to topologically complex magnetostatic equilibria, the inevitable formation of current sheets, and the explosive reconnection events that can ensue [25], are of central importance for the understanding of solar activity [5, 38, 50], the eruption of flares, coronal heating, etc. They are equally important for the better understanding of processes in thermonuclear fusion devices such as the tokamak of ITER [26], which call for magnetic confinement systems that are stable enough to ensure the sustainable generation of fusion energy. Applying these ideas to the looped and twisted magnetic field lines arcing away from the solar surface (figure 3) we recognize that the anchoring regions of the loop ends move slowly compared with the internal relaxation dynamics of the loop. The loop dynamics is thus subject to slow deformation at the boundary, and may rapidly equilibrate to such changes or jump discontinuously. This feature is common to a number of dynamical problems.

2.3. Topological aspects of DNA function and protein folding

Soon after the discovery of the structure of DNA it was recognized that geometrical and topological features associated with the double-helical arrangement would influence its function. For example, Levinthal and Crane [36] noted that the process of DNA replication, which entails unwinding the molecule into two separate strands joining the double helix at a Y-shaped junction, could proceed in an energetically more favourable way if each of the lengthening arms and the shrinking double helix rotated about their respective axes, rather than the entire structure rotating rigidly about the double helix alone. Later work by Călugăreanu [14], White [67] and Fuller [23] established the interrelated concepts of link, twist and writhe of space curves and their application to structures such as closed loops of DNA [9].



Figure 4. Electron micrograph of a knotted loop of DNA. Reprinted with permission from [66]. Copyright 1985 The American Association for the Advancement of Science.

During the processes of replication, transcription or recombination, DNA molecules may become supercoiled, knotted or catenated. These processes are dynamic and are modulated by the activity of enzymes of two types: 'recombinases' (genetic recombination enzymes) which break double-stranded DNA at specific locations and rearrange and reconnect the ends; and 'topoisomerases' (enzymes that act on the topology of DNA) which permit strand passages by mechanisms that also involve breaking and reconnecting the DNA phosphate backbone. The transient DNA breaks induced by topoisomerases are promising targets for cytotoxic, antibacterial, and anti-tumour drugs. Recent structural and biochemical studies have elucidated mechanisms associated with each of these enzyme types.

The fact that biological processes can lead to knotted DNA molecules like that shown in figure 4 has led to extensive studies of the distribution of naturally occurring knots. This in turn led to the discovery that the migration speeds of these knotted molecules have a simple relationship to their topological properties; their electrophoretic mobility scales directly with the average crossing number of the knot [17, 56, 65]. In contrast to more macroscopic systems described in earlier sections, the three-dimensional conformation of knotted DNA molecules is very much a problem in statistical physics, as the molecules themselves are typically much longer than the persistence length (the length on which thermal energy $k_{\rm B}T$ can bend the molecule). When DNA is tightly packed, as in chromosomes, its equilibrium dimensions are strongly influenced by thermal fluctuations, whose constraint by the impenetrability of the molecular backbone produces a loss of entropy and a fluctuation-induced swelling pressure [40]. One of the important questions is how DNA topoisomerases can preferentially act in the direction decreasing the level of catenation and knotting below the levels that would result from random passages. A model for this [10] postulates that the local curved geometry of DNA–DNA juxtapositions could provide the discrimination needed by the topoisomerases. This has been confirmed in simulations [13] and by the crystal structure of topoisomerase bound with DNA [19].

It is now known that, like DNA strands, proteins also can exhibit knotted structure. The number of proteins known to form knots is growing, as is understanding concerning the folding

process and the potential advantages of knotted structure [59, 64]. It is in the context of DNA that the concept of the 'ideal' or 'tight knot' has been developed [29]. As the name would suggest, a tight knot is the geometrical form that a knot in a rope of circular cross-section will adopt if pulled tight, the ends being joined in the minimum length manner. We may think of the tight-knot configuration as maximizing rope volume for prescribed length, or alternatively as minimizing length for prescribed volume. From the latter point of view, the problem is close to that of a relaxing knotted magnetic flux tube in an incompressible fluid, reduction of length being caused by the Maxwell tension in the tube. The minimum length is then in effect a measure of minimum energy. The difference however is that the cross-section of the flux tube need not remain circular; moreover the magnetic field may be twisted around the axis of the tube, a complication not normally considered in the tight-knot context. Many intriguing mathematical problems are raised by such considerations.

Topological considerations are not only associated with molecules, but can also arise at the cellular scale. For example, certain mutant strains of bacteria fail to separate on cell division, giving rise to exponentially growing linear structures which buckle and supercoil as they grow. This can give rise to a hierarchy of shape transformations in which there is a delicate interplay between growth time scales and competing modes of instability [68]. In this more macroscopic context there are also fascinating applied mathematical aspects of the mechanics of elastic knots [2]. Finally we mention the provocative recent study [52] that investigated the statistics of spontaneously formed knots in strings that are mechanically agitated. It was found that the probability of forming a given knot bore a simple relationship to measures of the knot complexity, thus raising fundamental questions in nonequilibrium filament dynamics.

2.4. Quantized flux in tightly knotted and linked systems

Quantized flux is for the most part studied in relation to the quantized vortex lines in the flow of liquid Helium II, and other low-temperature systems [4]. The process of vortex reconnection, which is well-studied in classical fluids [32], is in these quantum systems thought to be a crucial feature of superfluid turbulence. These line-like objects are phase defects in the complex superfluid order parameter, and reconnections occur when two quantized vortices approach, cross, and exchange tails; their singular nature produces highly non-Gaussian velocity statistics [48]. An important technical development [6, 7] which allowed for the first time the direct visualization of reconnection events, is the introduction of micron-sized frozen hydrogen tracer particles into the superfluid, some of which get trapped in vortex cores. Imaging of these tracers with a laser sheet reveals reconnection events such as those in figure 5. Analysis of many events of this type shows that the separation of the vortices with time *t* varies approximately as $t^{1/2}$, consistent with basic scaling arguments.

A quite different manifestation of the tight-knot scenario described in an earlier section is found in the extreme context of the 'quark- gluon' plasma, the hypothesized state of matter in the universe just microseconds after the Big Bang. Experiments in the relativistic heavy ion collider (Brookhaven National Laboratory) involving collision of gold nuclei produce a quark-gluon plasma that, remarkably, behaves like a liquid of very low viscosity [46]. Gluons are the quantum chromodynamic (QCD) analog of photons, and chromoelectric (magnetic) fields are the analog of our familiar electric (magnetic) fields. Chromoelectric flux tubes connect quarks allowing the transmission of force between them. As the quark-gluon plasma cools after a collision it hadronizes and turns into free baryon, meson and other states including glueballs. Particle physics experiments are far simpler—a typical event may be proton + proton \rightarrow handful of particles. Hence the individual events are much easier to analyze. It has been conjectured that 'glueballs' (solitonic solutions of the QCD equations) are



Figure 5. Quantized vorticies exist in the superfluid state of liquid Helium below the lambda transition at 2.17 K. Using microscopic tracer particles of frozen hydrogen, three time series illustrate reconnection events. Images are separated by about 100 ms each. Figure courtesy of G P Bewley *et al* [7].

knotted QCD tubes [10, 11]; these are manifest as vacuum excitations with an energy spectrum which is in principle measurable. Buniy and Kephart have found a correlation between the low-energy levels measured in these experiments, and the ground-state energies of knots of low crossing number; the two appear to be linearly related up to knots of crossing number nine (as far as measurements are available). All of the states they identify with glueballs have been discovered in particle physics experiments over the last \sim 30 years. The suggestion that these fundamental excitations in matter in its most primitive form are knotted QCD flux tubes is quite compelling. Kelvin would have been gratified to see this re-emergence of his basic idea, albeit at a more fundamental physical level. At this level, the QCD tubes are quantized with universal cross-sectional radius on the quantum scale determined by the QCD force field, so relaxation to a minimum-energy state conserves cross-section rather than volume. Nevertheless, the concept of knotted flux tubes in a minimum-energy (stable) configuration is just what Kelvin was seeking to substantiate! More generally, one can ask about the deeper possible connections between physical knots and quantum knots, between topological and quantum entanglement [30, 37].

3. A case study

While the four areas discussed in section 2 contain many fascinating dynamical phenomena involving topological constraints, they also present serious experimental challenges in the visualization and/or control of the underlying processes. This motivates the search for simple laboratory realizations in which the dynamics occurs on demand and where possible topological rearrangements can be visualized and studied reproducibly. One such example which has recently been addressed involves interconversions of minimal surfaces spanning deformable wire frames [24].

Ever since the work of Euler [21] and Lagrange [34] on functional extremization the problem of finding area-minimizing surfaces spanning prescribed contours has been recognized as a rich and challenging avenue for mathematical research. The most significant rigorous results are the solution of 'Plateau's problem', namely, the existence proofs by Radó [51] and



Figure 6. Topological transition of a soap film Möbius strip [24]. As its frame is gradually distorted, a critical point is reached at which the one-sided film (a) transforms rapidly to a two-sided solution (b). Scale bar in (a) is 2 cm.

Douglas [20] of minimal surfaces spanning a given contour. Because soap films spanning wire frames provide such a simple realization of these surfaces much can be learned from experimentation with them. For instance, the possibility that there may be more than one minimal surface that can span a given contour, and that small deformations of a frame can trigger transformations between minimal surfaces, was emphasized in 1940 by Courant [16]. One of his most intriguing examples is the competition between the one-sided Möbius strip and a two-sided film. This can be visualized with a doubly looped wire frame; when it is removed from the soap solution, it often possesses a second disc-shaped surface that can be destroyed to leave the Möbius strip (figure 6(a)). Smoothly untwisting the loops renders that minimal surface unstable, with a rapid transition to the two-sided film (figure 6(b)).

The instability of the Möbius strip soap film as its frame is deformed is reminiscent of the loss of stability of the catenary that spans two parallel circular wires as they are pulled apart. Experiments show that the collapse of a catenary preserves the axisymmetry of the initial condition and produces a pinching singularity on axis, away from the boundary [55]. Extensive theoretical studies [35] of inviscid collapse dynamics have shown excellent agreement with detailed observations on the interface shape and dynamics in the neighbourhood of the singularity. Related work [63] on submerged air bubble pinchoff has shown the possibility of broken axisymmetry in a system which is axisymmetric in the far field, but with singularities still occurring away from boundaries.

Surprisingly, despite the many decades since Courant highlighted the instability of the Möbius strip soap film, there was no systematic study of this archetypal problem in change of topology, so the basic question of what dynamical process brings a one-sided surface to a two-sided one remained unanswered, along with the specific questions: Is the singularity in the bulk or at the boundary? What is the local geometry at the singularity? What is the time evolution of the film near the singularity? While some of these questions have been addressed for the simpler case of a network of soap film junctions [28], as found in soap froths, and one other case of an interconversion between minimal surfaces has been considered, the helicoid-catenoid transition [8], the study of this kind of dynamical interconversion of minimal surfaces is inchoate, even if the rigorous study of minimal surfaces themselves is extraordinary well-developed [15, 47].

A systematic study [24] of the Möbius strip-to-disc transition has given answers to the questions raised above. First, through the introduction of fluorescent dye into the film and systematic refinement of the experimental protocol it is possible to obtain and visualize highly reproducible collapse dynamics. High-speed imaging reveals that the transition always occurs at the boundary of the film (figure 7), never in the 'bulk', so the process is indeed fundamentally different from the collapse of a catenary. The throat diameter *D* exhibits an intriguing crossover



Figure 7. Collapse of the Möbius strip 'throat' [24]. Frames from a high-speed movie at 5.4 ms intervals show formation of a singularity at the frame. The dynamics of the collapse is quantified by the throat diameter D(t) indicated in (*a*).



Figure 8. Schematic illustration of linking of Plateau border (red) and wire frame (gray) for (*a*) the Möbius strip topology and (*b*) the two-sided solution. (*c*) Caustic visible from highly curved surface after the collapse of the Möbius strip surface [24].

in power-law behavior as it collapses to the wire, asymptotically displaying the well-known 2/3 exponent associate with a balance of surface tension and inertia [31], but showing a distinct early time scaling that may derive from viscous dissipation in the coating film on the wire.

Second, close examination revealed that not only does the orientability of the film change at the transition, but so too does a second topological quantity. To see this, we imagine constructing two closed contours, the centreline of the wire frame and the centreline of the Plateau border, where the soap film meets the wire. If we dip a circular frame into the soap solution the minimal surface spanning the frame is a flat disc. It is clear that for this two-sided film the two contours are simply concentric circles and are of course unlinked. Surprisingly, this is not the case for the Möbius strip film spanning the double-loop: the two contours are actually doubly linked. These contrasting situations are illustrated in figure 8(a) and (b) with the help of ruled surfaces that span a series of parameterized contours [39]. Thus, the Möbius strip-to-disc transition involves *reconnection* of the Plateau border, a phenomenon conceptually similar to vortex reconnection. After the transition the border wraps tightly around the frame, producing a region of high Gaussian curvature that is visible through a light caustic (figure 8(c)).

Since the linking number of the Plateau border and the wire frame is a quantity defined at the boundary, it is perhaps not surprising that the singularity associated with reconnection is driven to occur at the frame. But it is not at all obvious whether this fact alone is enough to ensure that the *only* singularity that occurs will be at the boundary; nevertheless, this is what is observed. Stepping back from this particular problem we are led to ask about the generality of these results on interconversions of minimal surfaces driven by boundary deformation. Are there general principles by which the types of singularities (and their locations) can be deduced



Figure 9. A soap film with the topology of a section of a Klein bottle.

from the topology of the minimal surface? Can one derive equations of motion that encapsulate these transitions?

To put these questions in perspective we conclude this section by illustrating an unusual minimal surface (figure 9) spanning a frame whose shape was suggested in Almgren's well-known work on minimal surfaces [1]. There are several distinct films that can span this frame; the one shown is actually a section of a Klein bottle. Since a Klein bottle can be viewed is two Möbius strips sewn together, it is not surprising that this surface has zero linkage of its Plateau border with the frame. Nevertheless, upon slow boundary deformation it exhibits two singularities associated with Plateau border reconnections with opposite twist changes. This highlights the subtleties of the connection between topology changes and singularity structure.

4. Conclusions

We have seen a number of examples in the physical and biological sciences in which dynamical evolution is induced by slow variations in boundary conditions and can lead to a singular change of topology. In these problems there may be more than one topological quantity associated with the system that can undergo a discontinuous change during the evolution. For example, the soap films described above can be characterized by their sidedness and their linking number with the frame. However, it is not necessary that both quantities change under boundary deformations. As shown in figures 6–8, the Möbius strip changes *both* quantities when it collapses, whereas the 'Klein bottle section' in figure 9 changes sidedness *without* altering the linking number. Another aspect of the importance of understanding the role of topological quantities during dynamical evolution is found in the study of magnetic relaxation, where Taylor's hypothesis of the conservation of magnetic helicity [61] is not always sufficient to explain the final state of the system because of the existence of other equally important topological invariants [70].

These are but two examples that illustrate a common set of problems: the lack of a systematic way of understanding (i) which topological invariants break down during dynamical evolution, (ii) how they jump to new values and (iii) where the associated singularity occurs, particularly in bounded domains. A full understanding of these issues in the context of a system for which both the experiments are highly controllable and the mathematical description is tractable may open the way to a much more generally applicable theory.

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