Topological invariants in magnetohydrodynamics and DNA supercoiling

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Abstract. We discuss the structure of topological invariants in two different media. The first example relates to the problem of reconnection in magnetohydrodynamics and the second one to the supercoiling of DNA. Despite the apparently different systems, the behavior of magnetic spread lines and supercoiling process in DNA display some common features based on the existence of topological invariants of Hopf's type.

1. Introduction

The Gauss linking coefficient (1833), determining the necessary condition of *unlinkability* of two closed curves, was the first example of topological invariants of an ensemble of linked curves. Despite relatively simple form of Gauss formula, a lot of topological depths hidden in it. It became clear only in the XXth century. In parallel, and mainly independently from mathematicians, similar constructions (helicity) were discovered by specialists in magneto and hydrodynamics. But only in the second part of the XXth century it has become clear how the relation between topology and certain appropriate areas of physics and even molecular biology can benefit from topological methods known to mathematicians.

In this paper we restrict ourselves to study topological invariants in two apparently different media. We consider the behavior of magnetic spread lines in the process of reconnection and DNA supercoiling. We prove the existence of Hopf's type topological invariants and give their explicit formulae in both cases.

2. Magnetic Hydrodynamics

2.1. Introduction

In perfectly conducting moving plasma, the magnetic and electric fields, $\vec{H}$ and $\vec{E}$, respectively, obey the following relationship: $c\ \vec{E} + \left(\vec{v} \times \vec{H}\right) = 0$ [1, 2], where $\vec{v}$ is the velocity field of its macroscopic motions[1]. The so called freezing-in theorem is fulfilled in this case. It states, in particular, that the topological structure of the magnetic field lines is conserved, and only smooth deformations are possible. This leads also to the conservation of linking numbers. To draw such a conclusion one should assume, of course, that the vector fields $\vec{E}$, $\vec{H}$, and $\vec{v}$ are smooth enough.

[1] It should be reminded that $\nabla \cdot \vec{H} \equiv 0$ as for any magnetic field.

When the electric conductivity is finite, then the equation for $\vec{H}$ in the frame of (isotropic) magnetic hydrodynamics (MHD) takes the form:

$$\frac{\partial \vec{H}}{\partial t} = \nabla \times \left(\vec{v} \times \vec{H}\right) - \nabla \times \nu \left(\nabla \times \vec{H}\right) . \tag{1}$$

where $\nu > 0$ is the so called *magnetic viscosity*. Generally, Eq. (1) shows that no invariant, characterizing the structure of set of magnetic field lines exist in this case. Indeed, at $\vec{v} = 0$, for example, the magnetic field dissipate at $t \to \infty$. It means that only a mode of $\vec{H}(\vec{x})$ with lowest damping rate survives for sufficiently long times, whose topological structure does not depend on the topology of the set of magnetic field lines at $t = 0$.

For this reason, the topic of this paper looks, at first glance, quite trivial: any topological invariant is conserved at $\nu = 0$ (perfectly conducting plasma), and there are no topological invariants at all for $\nu > 0$. The question becomes less trivial if we ask ourselves about the rates of disruption of invariants at very low magnetic viscosities $\nu > 0$.

Consider configuration of plasma and magnetic field of characteristic size L. Let the time evolution of this configuration be described by Eq. (1) and by the remaining MHD equations [1, 2] determining in particular $\vec{v}(\vec{x}, t)$. In this case, there are two typical time scales: the diffusion time scale $\tau_d = L^2/\nu$ and the hydrodynamic time scale $\tau_H = L/c_A$, where $c_A = \sqrt{H^2/4\pi\rho}$ is the Alfven velocity, and ρ is the plasma density. The dimensionless parameter, the magnetic Reynolds number $\mathrm{Re}_m = \tau_d/\tau_H$, becomes very large when $\nu \to 0$. In this case, changing of the magnetic field topological structure may take place at time intervals that are much shorter that τ_d. Indeed, it is possible that the nature of MHD motions is such that there occurs a spontaneous sharp decrease in the spatial scales of $\vec{v}$ and $\vec{H}$ at times $\tau \sim \tau_H$. Examples of such kind are encountered in various problems: in turbulence [3], during formation of shock waves [3], and current sheets [4, 5]. Therefore, the role of the second term in (1) becomes important at times $\tau \sim \tau_H$. In this case, the topological structure of the magnetic field lines is not completely destroyed, as it happens when $\tau \sim \tau_d$. Accordingly, the question of the existence of topological invariants that are conserved in time periods $\tau \ll \tau_d$ is entirely well-posed and quite important.

Taylor [6] was the first author who addressed this question with a similar formulation. His result can be formulated as follows. If in a system there is a very small-scale MHD turbulence resulting in a situation in which $\left\langle \vec{j}^2 \right\rangle \gg \left\langle \vec{j} \right\rangle^2$ (here $\langle \ldots \rangle$ denotes spatial averaging), and if rapid topological changes are also possible, then, the following invariant is conserved:

$$h = \int\limits_{\Omega} \vec{A} \cdot \vec{H}\, dV . \tag{2}$$

Here $\vec{A}$ is the vector potential of the field $\vec{H}$ ($\vec{H} = \nabla \times \vec{A}$) and Ω is the whole domain of the system, at the boundary of which $\vec{H}_n|_{\partial\Omega} = 0$. This invariant admits an interpretation in terms of the total link of the magnetic field lines [7, 8]. Following Arnold, we shall call it the asymptotic Hopf invariant. For simply connected domains, which are the only domains that will be considered in the present paper, relation (2) is gauge invariant. For multi-connected domains, this is not so, which calls for minor technical complications [including limitations on the form of $\vec{A}$]. All the results, with minor specifications, remain valid in the general case.

Taylor's result can be reformulated in another equivalent form. The rapid reconstruction of the topology of the field lines at $\tau \ll \tau_d$ can modify the link of the individual field lines as a result of small-scale turbulence, but preserves the overall link. Kadomtsev [9] formulated the analogous result for magnetic-field configurations that vary during large-scale reconnections of the field lines.

In our paper [10], a formal definition of of the large-scale reconnection process was presented in terms of cuts and splices. It allowed us to impart precise meaning to the principal assertion

concerning the conservation of the sole topological invariant – the asymptotic Hopf invariant – in the problem of rapid reconnection in simply connected domains. In multi-connected domains (such as tokamaks) the total magnetic fluxes are also conserved. This definition gives specific form to Kadomtsev's idea, eliminating an uncertainty in the introduction of the reconnection concept.

In our publication [11], these results were further developed. For a magnetic field $\vec{H}$, approximated by a system magnetic flux tubes with internal winding, a set of topological invariants was explicitly defined. The invariants are conserved on smooth large-scale flows $\vec{v}\,(\vec{x},t)$. This definition generalizes ideas of topological invariants of higher order [14]. Introducing the process of reconnection, as discussed above, we obtain a way of changing the internal winding of each magnetic flux tube as well as of such mutual linking of different flux tubes. This consideration allows us to take a fresh approach to conservation of the only topological invariant during the process of reconnection, that is, the asymptotic Hopf invariant.

These results were applied recently to investigation of magnetic field structure in solar corona [12].

2.2. Definitions

Here we introduce definitions of the concepts considered in the previous section.

Firstly, let us consider the linking coefficient of the link l consisting of a finite number of oriented closed curves l_j $(j = 1, 2, \ldots)$ in sphere S^3 [13]. The linking coefficient of the first order $k_1\,(l_1, l_2)$ is well defined for every pair of nonintersecting curves. The linking coefficient $k_1\,(l_1, l_2)$ is equal to the algebraic sum of intersections numbers of the curve l_1 with the surface Z spanned on l_2, with the orientation induced by the orientation of l_2.

The linking coefficient of order p is defined for $p + 1$ closed lines. The definition uses the so called Milnor coefficients [14]. A more convenient definitions using differential forms is presented in the book [13] and will be used below. We give the construction of coefficient k_p in the simplest nontrivial case $p = 2$, when $k_1\,(l_i, l_j) = 0$ (where $i,\, j = 1,\, 2,\, 3$). The generalization to an arbitrary p (under condition $k_i = 0$ at $i < p$) and comparison with other link invariants $l = \{l_i\}$ along with the proofs were also presented in the book [13].

Let $B_i \subset S^3$ be the boundary of some tubular neighborhood of the closed l_i. Suppose that B_i does not intersect any l_j. Then[2]

$$\int\limits_{B_1} u_1 \wedge u_2 = -\int\limits_{B_2} u_2 \wedge u_1 = k_1\,(l_1, l_2)\ , \tag{3}$$

where u_i are one-forms dual (by Alexander) to l_i. Equations similar to Eq. (3) can be defined directly on the whole S^3 with the help of closed two-forms v_i defined on $S^3 \backslash l_i$, so that $\int_{Z_i} v_i = \mathrm{Ind}\,(Z_i, l_i)$, where Z_i is a two-dimensional cycle in $S^3 \backslash l_i$, and $\mathrm{Ind}\,(Z, l)$ is the index of intersection of l with Z. The three-forms $u_1 \wedge v_2$ and $v_1 \wedge u_2$ are defined now on the whole S^3 and

$$\int\limits_{S^3} u_1 \wedge v_2 = -\int\limits_{S^3} v_1 \wedge u_2 = k_1(l_1, l_2)\,. \tag{4}$$

We shall call the first order linking coefficient $\bar{k}_1$ for the link $l = (l_1, \ldots, l_n)$ the value

$$\bar{k}_1\,(l) = \max_{1 \le i < j \le n} |k_1\,(l_i, l_j)|\ . \tag{5}$$

One can show that, if $k_1\,(l_1, l_2) = 0$, the following condition is true. There exist such one-form u_{12} on $S^3 \backslash\,(l_1 \cup l_2)$ and such two-forms v_{12} and v'_{12} on S^3, that $d\,u_{12} = u_1 \wedge u_2$, $d\,v_{12} = -v_1 \wedge u_2$

[2] We omit some topological details connected with the definition of forms on the manifolds of the type of $S^3 \backslash l_j$ [13].

and $d\,v'_{12} = u_1 \wedge v_2$. Let us suppose that $\bar{k}_1(l) = 0$ for $l = (l_1, l_2, l_3)$. Then the following differential forms

$$\begin{aligned} \tilde{u}_{123} &= u_{12} \wedge u_3 + u_1 \wedge u_{23}\,, \\ \tilde{v}_{123} &= -v_{12} \wedge u_3 + v_1 \wedge u_{23}\,, \\ \tilde{v}'_{123} &= u_{12} \wedge v_3 + u_1 \wedge v_{23} \end{aligned}$$

are closed and $\tilde{v}_{123}$ and $\tilde{v}'_{123}$ may be determined on the whole S^3. Here u_{ij} and v_{ij} are defined similarly to u_{12} and v_{12}. As it was shown in Ref. [13], all the following integrals

$$\int\limits_{B_1} \tilde{u}_{123} = -\int\limits_{B_3} \tilde{u}_{123} = \int\limits_{S^3} \tilde{v}_{123} = \int\limits_{S^3} \tilde{v}'_{123}$$

are integers. This integer is called the linking coefficient of degree 2: $k_2(l_1, l_2, l_3)$.

Let us now consider some class of magnetic fields denoted as D and satisfying the conditions quoted below. A magnetic field of this class does not vanish only into a finite number N of magnetic flux tubes $T_i = D_2 \times S^1$ $(i = 1, \ldots, N)$. The flux tube T_i carries magnetic induction flux Φ_i. Different magnetic fields of the class D may have different $\{T_i\}$, $\{\Phi_i\}$ and N. Let us also consider cross-sections of any magnetic flux tube T_i. The field lines flow entails a diffeomorphism of these cross-sections. We assume that the "polar" coordinate system can be introduced so that a diffeomorphism, mentioned above, transforms coordinate lines of the coordinate system into each other. This means that the field lines in T_i belong to magnetic surfaces which are two-dimensional tori embedded one in other while the winding number does not depend on the magnetic surface belonging to the tube T_i. Thus the class D is defined.

One may assume that an arbitrary magnetic field is in some sense well approximated by fields of the class D. We consider below only fields of the class D.

Let us introduce closed field lines $l(T_i)$ belonging T_i and corresponding to the poles of the coordinate systems mentioned above. The curves $l(T_i)$ may be knotted. Let us consider a field line $\gamma \subset T_i \backslash l(T_i)$ and a surface $Z(T_i)$ spanned on $l(T_i)$. Then the winding number φ_i is defined as an average number of intersections of γ with $Z(T_i)$ per a revolution along $l(T_i)$.

Now define the flux tubes linking number:

$$\hat{k}_1(T_i, T_j) = \begin{cases} \varphi_i & \text{for} \quad i = j \\ k_1(l(T_i), l(T_j)) & \text{for} \quad i \neq j \end{cases}, \tag{6}$$

and

$$\hat{k}_p(T_{i_0}, \ldots, T_{i_p}) = k_p(l(T_{i_0}), \ldots, l(T_{i_p})) \tag{7}$$

for $p \geq 2$. The latter definition implies that all first order linking coefficients are vanish. See above.

Let us introduce also

$$h_{p,\sigma}\left\{\vec{H}\right\} = \sum_{i_0, \ldots, i_p} \left[\prod_{m=0}^{p} \Phi_{i_m}\right] \hat{k}_p(T_{i_0}, \ldots, T_{i_p}) \left[\operatorname{sgn} \hat{k}_p(T_{i_0}, \ldots, T_{i_p})\right]^{\sigma}, \tag{8}$$

where the "parity" $\sigma \in (0, 1)$.

These quantities, defined on the class D, depend neither on the way of partition of the field $\vec{H}$ on the flux tubes nor on their ordering. Different ways of these partitions are possible if some winding numbers φ_i are rational.

The freezing-in theorem [1, 2] leads to conservation (at $\nu \equiv 0$) of topological structure of magnetic field lines as well as magnetic fluxes Φ_i of each magnetic flux tubes T_i. It means

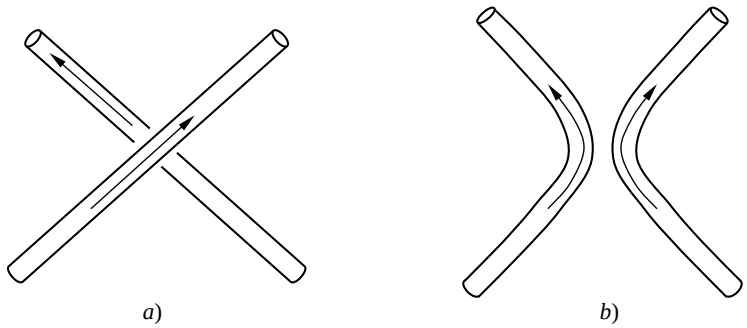

Figure 1. Shown is 'process' of reconnection: a) before the reconnection; b) after the reconnection.

conservation of all $h_{p,\sigma}\left\{\vec{H}\right\}$, if the field evolves in time according to Eq. (1), when $\nu \equiv 0$, and the field $\vec{v}$ is smooth enough.

Using [8], it is easy to understand that

$$h_{1,0}\left\{\vec{H}\right\} = h\,. \tag{9}$$

Of course, the conservation of h at $\nu = 0$ is well known. Other conservation laws are apparently new.

Now we introduce the concept of reconnection on the class $D_1 \subset D$. The class D_1 is determined be the condition:

$$\Phi_i = \Phi_j \qquad \text{for any} \;\; i \;\; \text{and} \;\; j\,.$$

Below, we imply by the reconnection in a restricted sense, a transformation of $\vec{H}$ such that $D_1 \to D_1$. This transformation implies a cut and a glue of two neighboring flux tubes (see Fig. 1), so that no other flux tubes are carried through the formed gap in the process of the instant reconnection. The cut-and-glue procedure should obey the following conditions:

(i) A map arising from gluing together the cut end-walls is smooth.

(ii) If two parts of cut field lines are glued together, then two remaining parts of the lines are glued together also.

(iii) The condition $\nabla \cdot \vec{H} = 0$ is conserved.

(iv) Magnetic surfaces are glued together with magnetic surfaces. It means that this gluing process follows the definition of the class D.

Here, by the reconnection in broad sense, we imply the reconnection in the restricted sense combined with an evolution according to Eq. (1) with the smooth velocity field $\vec{v}$ and $\nu = 0$. The more detailed analysis of the concept of MHD reconnection are carried out in our paper [10], where we have presented a phenomenological basis of such definition. It should be point out that the definition of reconnection (for a wider class of magnetic fields) presented in Ref. [10] required more restrictive conditions than the conditions 1-4. However the present less restrictive conditions are sufficient for our goals.

Let us note, that the reconnection's transformation determined above, is reversible, i.e. in the sense the reconversion is also a reconnection transformation.

2.3. Statements

The topological structure of the set of magnetic field lines is changed by a reconnection. It is easy to see that if two magnetic flux tubes T_1 and T_2 are reconnected in a resulting flux tube T': $(T_1, T_2) \longrightarrow T'$, then

$$\hat{k}_1(T', T') = \hat{k}_1(T_1, T_1) + \hat{k}_1(T_2, T_2) + 2\hat{k}_1(T_1, T_2) , \quad (10)$$

$$\hat{k}_1(T_3, T') = \hat{k}_1(T_3, T_1) + \hat{k}_1(T_3, T_2) . \quad (11)$$

As far as we know, these formulae were first introduced in Ref. [11].

The coefficient 2 in Eq. (10) can be explained qualitatively in the following way. Any field line γ' belonging T' consists of two parts γ_1 and γ_2. The part γ_1 belonged initially (priory the reconnection) T_1, whereas γ_2 belonged initially T_2. The line $l(T')$ can also be considered as composition of $l(T_1)$ and $l(T_2)$. Hence the surface $Z(T')$ spanned on $l(T')$ can be considered as composition of two surfaces $Z(T_1)$ and $Z(T_2)$, spanned on $l(T_1)$ and $l(T_2)$, correspondingly. The average number of intersections of γ_1 with $Z(T')$ is equal to $\hat{k}_1(T_1, T_1) + \hat{k}_1(T_1, T_2)$. The first term of this sum comes from intersections with $Z(T_1)$, whereas the second one comes from intersections with $Z(T_2)$. The number of intersections of the path γ_2 with $Z(T')$ is equal analogously to $\hat{k}_1(T_2, T_2) + \hat{k}_1(T_1, T_2)$. As a result we obtain Eq. (10).

The conservation of h [see Eq. (9)] during the reconnection is a consequence of Eqs. (10) and (11), and the definition (7). I.e. the topological structure of a magnetic field under the reconnection process is not destroyed completely.

Let us show that in general case there are no additional to h integrals of motion conserved under the reconnection's process.

Let us consider, for example, the special case $h = 0$. Due to a finite number of reconnections we are able to transform the set of flux tubes $\{T_i\}$ with the flux Φ_0 in each flux tube into one unknotted tube T with the same Φ_0. Since h is conserved, so T has the winding number $\varphi = 0$. Thus all field lines are unlinked. Then all magnetic fields belonging to D_1 with given Φ_0 can be transformed into each other. The extension to the case $h \neq 0$ is quite evident. This means the absence of quantities determined only by $\vec{H}$ other than h and conserved by the reconnections.

3. Supercoiling in DNA

Topological methods were successfully applied to the description of the DNA supercoiling. The DNA described by the Calŭgareanŭ formula (CF) [15][3] :

$$Lk = Tw + Wr ,$$

where Lk is the Gauss linking coefficient and Tw is the twist and Wr is the writhing number correspondingly. For the readers convenience we add the definitions of these quantities, see details in the book [13] and the references cited there.

Let γ be a closed smooth curve embedded in R^3 and v a normal vector on γ. We choose a vector $v(t)$ with length small enough, that $v(t)$ intersects γ only in one point. The v terminals sweep a curve γ_v which inherits the orientation of γ. The vector v sweeps a band embedded in R^3. The Lk will be the the Gauss linking coefficient of γ and γ_v. We define the twist of v as:

$$Tw = \frac{1}{2\pi} \int_\gamma v^\perp \cdot dv ,$$

[3] The paper [16] includes an interesting history of the creation of the CF formula, its future fate and the relation with the notion of Helicity.

where $v^{\perp}$ is the normal vector to γ. The twist is a continuous quantity. Now we define another continuous quantity the writhing number Wr. Wr only depends on γ. Let us consider the Gauss map for $\gamma \times \gamma$, i.e.

$$\phi : \gamma \times \gamma \to S^2\,, \quad \phi(x,y) = \frac{y-x}{|y-x|}\,,$$

pairs $(x,y) \in \gamma$. Let dS be the area element on S^2. Then $\phi_\star(dS)$ is induced by ϕ.

The writhing number Wr is the integral

$$Wr = \frac{1}{4\pi}\int_{\gamma\times\gamma} \phi_\star(dS)\,.$$

Usually, the (CF) formula applies for a continuous ribbon but in the realistic process removal supercoils takes place exclusively by cutting edges of the DNA ribbon, twisting and sewing the ribbon. We call this "discrete" ribbon as a ladder, following the paper [17]. Thus the (CF) should be modified as:

$$(Lk - q) = \widetilde{Tw} + \widetilde{Wr}\,.$$

Here q is the number of cutting-sewing events and $\widetilde{Tw}$ and $\widetilde{Wr}$ are modified parameters of the (CF). Since we deal with with the ensemble of cuts and sews the final formula after averaging over all states looks like

$$\langle Lk - q\rangle = \left\langle \widetilde{Tw}\right\rangle + \left\langle \widetilde{Wr}\right\rangle\,.$$

This explains the applicability of topological methods to study scDNA relaxation caused by enzymatic activity of topoisomeras. We would like to show, following a brief remark in [17] that intrinsic hydrodynamics behavior of a the free-rotating DNA is closely related to the hydrodynamics behavior of uniaxial nematic liquid crystal [18].

The order parameter of an uniaxial nematic has the form

$$A_{ik} = A_0\left(n_i n_k - \frac{1}{3}\delta_{ik}\right)\,,$$

where $\vec{n} = (n_1, n_2, n_3)$ is the unit vector, and δ_{ik} is the Kronecker delta function. The order parameter is invariant under the reflection $\vec{n} \to -\vec{n}$.

Topological characteristics of the DNA are related to hydrodynamics equations by the formula

$$\frac{\partial \vec{n}}{\partial t} = \{H, \vec{n}\}\,,$$

where H is the Hamiltonian of the energy density: $H = \int E\, dr^3$. E depends of the states of the system and $\{H, \vec{n}\}$ denotes the Poisson bracket. On the other hand, director $\vec{n}$ in the case of appropriate boundary conditions relates to the Gauss coefficient Lk:

$$Lk(\gamma, \gamma_v) = \int (\vec{n}, \nabla, \vec{n})\, dV\,.$$

Here dV is the volume element of a ball embracing the band (γ, γ_v).

4. Conclusion

Let us formulate two main results of this paper.

(i) We determined the set of topological invariants in terms of of magnetic flux tubes and proved the conservation of asymptotic Hopf's invariant under reconnection.

(ii) We generalized Calŭgareanŭ formula for the DNA ladder and relate DNA kinetic to the equation similar to the hydrodynamics equation of nematic liquid crystal. It makes possible the development the theory of dynamic of the supercoiling DNA parallel to nematodynamics and its comparison with experiment (see[17]).

In connection with our paper we would like to formulate some unsolved problems.

(i) The Calŭgareanŭ formula derived in conjecture that a band formed a trivial knot. What is a generalization of the formula in case of non-trivial band knotting?

(ii) Does a generalization of the CH formula exist when γ and γ_v have a trivial Gauss coefficient but non- trivial high order coefficient?

Similar question is interesting in the case of several linking curves. In this case the role of band is played by a Seifert surface. This result would be interesting for applications in interacting chains of DNA. However, at present there are no experimental confirmations of existence of such structures.

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