Proc. Nat. Acad. Sci. USA
Vol. 68, No. 4, pp. 815–819, April 1971

The Writhing Number of a Space Curve

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Communicated by Max Delbrück, February 8, 1971

ABSTRACT **A geometric invariant of a space curve, the writhing number, is defined and studied. For the central curve of a twisted cord the writhing number measures the extent to which coiling of the central curve has relieved local twisting of the cord. This study originated in response to questions that arise in the study of supercoiled double-stranded DNA rings.**

1. INTRODUCTION

It is a common observation that when a cord is twisted it tends to form loops or coils. This effect has been cited in physics to explain the instability of twisted magnetic fields [1] and in molecular biology to explain the twisting of circular duplex DNA molecules into "superhelices" [2–6]. J. Vinograd asked the author whether a quantitative analysis of the effect is possible. Such an analysis is initiated here in terms of a quantity we call the writhing number of a closed space curve. This same quantity appears in the work of Călugăreanu [7] and Pohl [8] on closed space curves as a form of Gauss integral. Because our interest here is in space curves that are the central curves of elastic rods we use the term *writhing number*, after the definition of *writhe* as a transitive verb: to twist into coils or folds [9].

The mathematical properties of the writhing number are described in sections 2 and 3; section 3 is not required to understand the other sections. Section 4 shows how the writhing number enters into the analysis of the elastic properties of a twisted and closed thin rod; it is shown quantitatively how the elastic energy due to local twisting of the rod may be reduced if the central curve of the rod forms coils that increase its writhing number. Finally, section 5 discusses the suitability of the twisted and closed thin rod as a model for the elastic properties of a double-stranded DNA ring.

2. THE WRITHING NUMBER OF A SMOOTH SIMPLE CLOSED CURVE

By a *curve* X is meant a three-dimensional vector $X(t)$ depending continuously on a parameter t, $a \leq t \leq b$. The curve X is *smooth* if the function $X(t)$ is of class C^∞ and if $X'(t) \neq 0$ for all t. If a curve is smooth one may use its arclength s as a parameter and define its unit tangent $T = X'(s)$. X is *closed* if $X(a) = X(b)$ and, when X is specified to be smooth, if the derivatives of all orders of X agree at a and b. X is *simple* if it has no self-intersections, i.e., $X(t_1) = X(t_2)$ only when $t_1 = t_2$, unless the curve is closed, when the exception $X(a) = X(b)$ is allowed.

By a *strip* (X,U) is meant a smooth curve X together with a smoothly varying unit vector $U(t)$ perpendicular to X at each point [10]. The strip (X,U) is called simple and closed if X is simple and closed and if U and all its derivatives agree at a and b. For any simple closed strip the curves $X + \epsilon U$ given parametrically by $X(t) + \epsilon U(t)$ are, for all sufficiently small positive ϵ, simple closed curves disjoint from X. There are now two ways to describe the number of times the curve $X + \epsilon U$ winds about X:

(*a*) Since X and $X + \epsilon U$ are disjoint closed curves, their linking number $Lk(X,X + \epsilon U)$ is defined [11]. For sufficiently small ϵ the linking number is independent of ϵ, hence for such ϵ we may call $Lk(X,X + \epsilon U)$ the linking number of the strip (X,U). The linking number of (X,U) is an integer independent of the direction of travel along X and does not change if (X,U) is deformed smoothly through simple closed strips.

(*b*) The vectors T, U and $V = T \times U$ define a moving frame (T,U,V) along X. Let Ω denote the angular velocity vector describing the rate of rotation of the frame with respect to arclength s, so that $T' = \Omega \times T$, $U' = \Omega \times U$ and $V' = \Omega \times V$. Let ω_1, ω_2 and ω_3 be the components of Ω referred to the moving frame, i.e., $\Omega = \omega_1 T + \omega_2 U + \omega_3 V$. Then ω_1 represents the angular rate at which U revolves about X. Following Love [12] we call ω_1 the *twist* of the strip at each point of the curve. Define the *total twist* of the strip (X,U) to be the integral of ω_1 with respect to arclength over the curve and, in order to obtain a quantity comparable to the linking number, define the *total twist number* $Tw(X,U)$ to be the total twist divided by 2π: $Tw(X,U) = {}^1/_{2\pi}\oint \omega_1 ds$. The total twist number need not be an integer.

If the curve X is a simple plane curve then the linking number $Lk(X,X + \epsilon U)$ and the total twist number $Tw(X,U)$ are equal. For a space curve this equality does not in general hold. However, it can be verified that

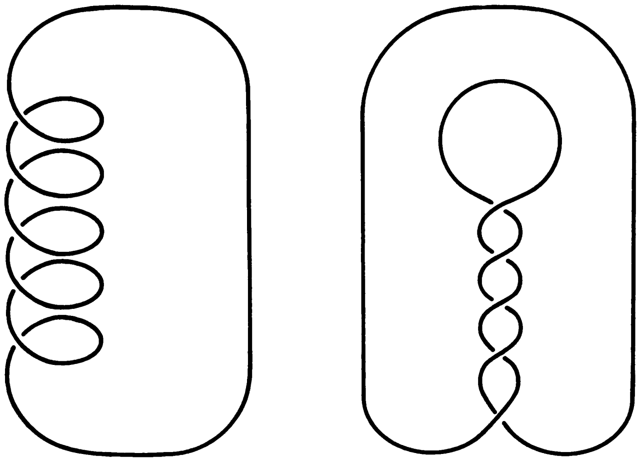

FIG. 1. Two configurations observed in the central curve of a twisted cord: the coil C at the left and the twisted loop or reentrant helix R at the right, each completed to a closed curve. For the sense of winding shown, the writhing numbers of the two curves are negative.

If C is wound as a helix with pitch angle α on a cylinder of radius r, a calculation ignoring the twist along the curve joining the ends of the helix gives $\mathrm{Wr}(\mathrm{C}) \sim \mathrm{N}(\text{signum } \alpha - \sin \alpha)$ where N is the (not necessarily whole) number of turns. A similar calculation for R gives $\mathrm{Wr}(\mathrm{R}) \sim -\mathrm{N} \sin \alpha$. For either curve, the part that is helically wound has length $\ell_h = 2\pi r \mathrm{N} \sec\alpha$ and curvature $\kappa = r^{-1} \cos^2\alpha$.

for any two strips (X,U) and (X,U^*) based on the same space curve X the equation $Lk(X,X + \epsilon U) - Tw(X,U) = Lk(X,X + \epsilon U^*) - Tw(X,U^*)$ holds. The difference $Lk(X,X + \epsilon U) - Tw(X,U)$ is thus a geometric invariant of the space curve X itself, which we call the *writhing number* $Wr(X)$. The starting point of our analysis is the defining relation for the writhing number:

$$Wr(X) = Lk(X,X + \epsilon U) - Tw(X,U). \qquad (1)$$

The writhing number is invariant under rigid motions and dilatations; it is independent of the direction of travel along X; reflection across a plane changes the signs of Wr, Lk and Tw.

To compute the writhing number of a smooth simple closed curve X from the defining relation (1) it suffices to compute the linking number and the total twist for any strip based on X. If the curvature of X never vanishes, so that the principal normal P is everywhere defined, then the twist of the strip (X,P) is the torsion τ of the curve X [7, 8, 10]. This method is used to obtain the writhing numbers of the curves in Fig. 1; here one uses the standard formula $\tau = r^{-1} \cos \alpha \sin \alpha$ for the torsion of a helix wound with pitch angle α on a cylinder of radius r. In some cases, however, other choices of U may be more convenient. For example, if X lies on the unit sphere one may select $U = X$; for this choice $Lk(X,X + \epsilon U) = 0$ and $\omega_1 = U' \cdot V = T \cdot (T \times U) = 0$, giving the result that the writhing number of any smooth simple closed curve located on a sphere is zero. More generally, if U is taken normal to a surface containing X, ω_1 is the *geodesic torsion* τ_g of the curve in the surface. A useful formula for geodesic torsion is $\tau_g = {}^1/_2(\kappa_1 - \kappa_2)\sin 2\theta$, where κ_1 and κ_2 are the principal curvatures of the surface and θ is the angle made by the curve and the line of curvature for which κ_1 is the normal curvature.

3. THE DIRECTIONAL WRITHING NUMBER

A smooth simple closed space curve X and a fixed unit vector $\boldsymbol{\sigma}$ are said to be *in general position* if the tangents to X are never parallel to $\boldsymbol{\sigma}$. In this case the curves $X + \epsilon\boldsymbol{\sigma}$ are disjoint from X for all sufficiently small $\epsilon > 0$, hence for such ϵ we may define the *directional writhing number* of X in the direction $\boldsymbol{\sigma}$ by $Wr(X,\boldsymbol{\sigma}) = Lk(X,X + \epsilon\boldsymbol{\sigma})$. The directional writhing number is an integer which is unchanged if the direction of travel along X is reversed or if $\boldsymbol{\sigma}$ is replaced by $-\boldsymbol{\sigma}$. The notion of directional writhing number essentially appears in refs. 2–6, where its dependence on direction is not recognized, so that it is not distinguished from the writhing number. The symbols τ, α and β in reference 5 correspond to Wr, Lk and Tw, respectively.

If X and $\boldsymbol{\sigma}$ are in general position then orthogonal projection of X onto a plane with normal $\boldsymbol{\sigma}$ defines a smooth closed plane curve X_σ for which undercrossings and overcrossings can be distinguished at each self-intersection. Suppose now that X_σ has only a finite number of self-intersections, each of which is the projection of exactly two points of X, and suppose further that the unit tangent T_0 to X_σ for the overcrossing (if we say that $\boldsymbol{\sigma}$ points upward) is not parallel to the unit tangent T_u for the undercrossing at each self-intersection (if these conditions do not hold they can be obtained by a perturbation of X). Now assign to the j-th self-intersection of X_σ the number $\mu_j = +1$ if $(T_0,T_u,\boldsymbol{\sigma})$ form a right-handed triple or $\mu_j = -1$ if $(T_0,T_u,\boldsymbol{\sigma})$ form a left-handed triple. Then the directional writhing number is equal to the sum of the μ_j's [11, 13]:

$$Wr(X,\boldsymbol{\sigma}) = \sum \mu_j. \qquad (2)$$

Given the appropriate plane representation of X, formula (2) enables one to compute $Wr(X,\boldsymbol{\sigma})$ by inspection (see Fig. 2; in Fig. 1 both directional writhing numbers are equal to -5).

The writhing number of a space curve X is equal to the average of all its directional writhing numbers, the average being taken with respect to area on the unit sphere (*, †):

* This result is obtained by averaging Eq. (1) for the strips $(X, |\boldsymbol{\sigma} \times T|^{-1}\boldsymbol{\sigma} \times T)$ over all directions $\boldsymbol{\sigma}$ in general position with X (the exceptional directions lie on the set of measure zero consisting of the curves $\pm T(s)$ traced by the tangents to X).

† Since formula (2) makes sense for simple space curves that are not closed, formulas (2) and (3) together can be used to extend the notion of writhing number to such curves.

$$Wr(X) = \frac{1}{4\pi}\iint Wr(X,\sigma)dS. \qquad (3)$$

This integral-geometric formula for the writhing number makes it possible to compute $Wr(X)$ to any desired accuracy by averaging $Wr(X,\sigma)$ over a finite sample of directions σ, the sample being chosen either at random or according to a systematic scheme (see Fig. 2).

The writhing number of a space curve X that nearly lies in a plane is approximated by $Wr(X,\sigma)$, where σ is perpendicular to the plane. A precise statement of this type is the inequality

$$|Wr(X) - Wr(X,\sigma)| \leqq \frac{1}{2\pi}\left(1 - \left(\frac{\ell_p}{\ell}\right)^2\right)^{1/2} \left(\ell_p \oint \kappa_p{}^2 ds_p\right)^{1/2} \qquad (4)$$

where ℓ is the length of X and κ_p, ℓ_p, and ds_p denote the curvature, length, and element of arclength of the plane projection of X.‡ Note that all the quantities in (4) except $Wr(X)$ and ℓ are determined by the plane representation of X. Since the lengths of DNA rings are known, inequality (4) enables one to compute upper and lower limits for the writhing number of a DNA ring from an electron micrograph of it.

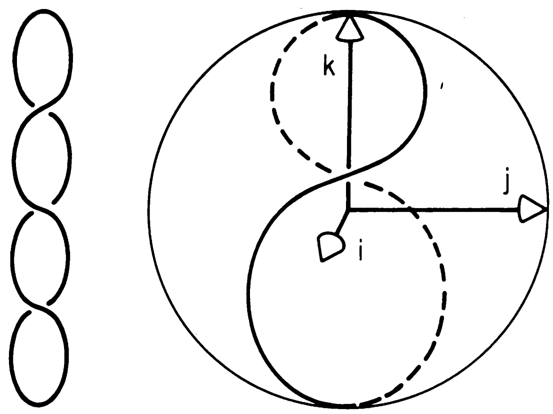

FIG. 2. At the left, a plane representation of a space curve X. The values of μ assigned to the three self-intersections are, reading down, −1, +1, and +1. Hence, for σ normal to the page Wr(X, σ) = +1. At the right is a curve S lying on a sphere. We know from section 2 that Wr(S) = 0. In this example the writhing number turns out to be the average of the directional writhing numbers in the directions of the **i**, **j**, **k** axes, since Wr(S, **i**) = −1, Wr(S, **j**) = 0, and Wr(S, **k**) = +1.

4. THE ELASTIC ENERGY OF A TWISTED AND CLOSED THIN ROD

According to the discussion in Love, the deformed position of a thin rod of circular cross section defines a strip (X,U), where X is the curve described by the centers of the cross sections and U is tangent to a surface containing X which, before deformation, was a plane containing the axis of the rod. The elastic energy of its deformed position is given in the ordinary approximate theory by the integral $E = {}^1/_2 \int_0^\ell (A\kappa^2 + C\omega_1{}^2)dx$, where ℓ is the length of X, A is the coefficient of flexural rigidity of the rod, κ is the curvature of X, C is the coefficient of torsional rigidity of the rod and ω_1 is the twist of (X,U) [12, 14]. Unless the above energy expression is specified, the following discussion will apply to a more general relation between stress and strain, whereby ${}^1/_2(A\kappa^2 + C\omega_1{}^2)$ is replaced by an unspecified smooth function $\varphi(\kappa,\omega_1)$ of κ and ω_1.

Now suppose that the rod is twisted and its ends butted together in such a way that lines parallel to the axis of the undeformed rod go into closed curves. (X,U) is then a simple closed strip. When X has zero writhing number $Lk(X,X + \epsilon U)$ is the total twist number of the rod; for a general closed space curve X the total twist number of the rod is equal to $Lk(X,X + \epsilon U) - Wr(X)$. Once the ends of the rod have been joined, deformations of the rod cannot change the linking number Lk.

In what follows we shall be interested in the positions of elastic equilibrium of the rod, i.e. those whose elastic energy is a relative minimum, corresponding to various values of Lk. For large values of Lk this problem makes sense only if we take into account the thickness of the rod. Otherwise a twisted loop as in Fig. 1, if allowed to twine on a cylinder of arbitrarily small radius, can raise the writhing number of the central curve to any value whatever while keeping the end loops large and the pitch angle nearly vertical in such a way that the curvature remains bounded. The consequence of this is that any linking number imposed on the rod can be "unwound" so that the twist vanishes and the elastic energy remains bounded. To avoid this "paradox" we introduce the thickness of the rod by specifying that the central curve X of a "rod of diameter d" must satisfy the following constraint: any segment joining two distinct points of X and perpendicular to X at each end must have length at least d. The minimum values of deformation energy may not be attained by rods corresponding to smooth strips (the overlap constraint may require discontinuities in the curvature), hence we must regard these equilibrium rods as limits of minimizing sequences of rods corresponding to smooth strips.

For rods of molecular size the twist ω_1 is not an observable quantity, whereas the shape represented by X can be seen with the electron microscope (if X is nearly flat) or studied indirectly via its effect on sedimentation rates (Upholt, W. B., H. B. Gray, Jr., and

‡ Results of this type are obtained by regarding X as a curve in the surface generated by the perpendiculars to the plane projection of X and taking U normal to this surface to compute $Wr(X)$. One finds $Lk(X,X + \epsilon U) = Wr(X,\sigma)$ and the twist, using the formula given for τ_0, to be $\kappa_p(\sin\theta)(ds_p/ds)$, where θ is the angle $T(s)$ makes with the plane. By applying the inequalities of Schwartz and Hölder to the expression for $Tw(X,U)$, one obtains the inequality (4). This inequality was suggested to the author by D. W. Boyd.

J. Vinograd, to be published). For this reason it is expedient to take the problem of finding the equilibrium configurations of the rod in two steps: first, to eliminate the variable ω_1 by adjusting ω_1, for given X and Lk, to give a minimum value $E(X,Lk)$ of E; second, to find those shapes X that minimize $E(X,Lk)$. To find the minimizing ω_1 is a calculus of variations problem with a side condition specifying the total twist number, leading to the equation $\partial/\partial\omega_1\{\varphi(\kappa,\omega_1)\} =$ constant. For each value of the constant this equation determines ω_1 (implicitly and, hence, possibly not uniquely) as a function of κ; the constant must then be adjusted to make the total twist number equal to $Lk - Wr$.

If the above procedure is applied to the integrand $\varphi = {}^1/_2(A\kappa^2 + C\omega_1{}^2)$ the minimizing ω_1 is found to have the constant value $2\pi\ell^{-1}(Lk - Wr)$, giving $E(X,Lk) = {}^1/_2A\ell\bar{\kappa}^2 + 2\pi^2C\ell^{-1}(Lk - Wr)^2$, where $\bar{\kappa}$ is the root-mean-square value of κ. This expression for $E(X,Lk)$ shows that in equilibrium X will assume a position that comprises between reducing its curvature and matching Wr to Lk by writhing, the point of compromise depending on the ratio A/C of the elastic coefficients. The relation between Wr, Lk, and this ratio can be analyzed in the following way. Let $g(Wr)$ denote the infimum of the values of $(1/8\pi^2)\ell^2\bar{\kappa}^2$ for curves X of length ℓ and given writhing number Wr which satisfy the overlap constraint imposed on the central curve of a rod of diameter d. Then the (absolutely) least value of $E(X,Lk)$ must have the form

$$4\pi^2\ell^{-1}A\ g(Wr) + 2\pi^2\ell^{-1}C(Lk - Wr)^2.$$

If this expression attains its minimum for a value of Wr where the derivative $g'(Wr)$ exists, then the following relation between Wr, Lk, and A/C must hold for a rod in a least-energy position of elastic equilibrium:

$$Lk - Wr = (A/C)g'(Wr). \tag{5}$$

The function g is determined by the ratio d/ℓ of the diameter to the length of the rod. Eq. (5) shows that the ratio A/C of the elastic coefficients can be found if one knows Lk, Wr, and d/ℓ for a single twisted and closed rod in a least energy position of elastic equilibrium, provided $g'(Wr)$ exists and is not zero.

5. SPECULATIONS ON THE ELASTIC PROPERTIES OF DOUBLE-STRANDED DNA MOLECULES

Is the thin rod of circular cross section an appropriate model for the elastic properties of a double-stranded DNA molecule? If one looks at its fine structure, the molecule is not axially symmetric, but if its twist rate in the unstrained state is sufficiently large compared to the variations of its central curve that are encountered then we may regard the molecule as elastically isotropic in all directions perpendicular to the central curve. However, the relation between stress and strain may well be such that the deformation energy per unit length is expressible in the form $\varphi(\kappa,\omega_1) = {}^1/_2(A\kappa^2 + C\omega_1{}^2)$ only for very small deformations. For if one sign of the twist ω_1 tightens the double helix, the other sign loosens it, hence there is no reason to expect the symmetry $\varphi(\kappa,\omega_1) = \varphi(\kappa,-\omega_1)$. For the same reason the stiffness, measured by the rate of change of φ with respect to κ, may depend on ω_1. If φ is expanded in powers of ω_1, ω_2, and ω_3 (see section 2) then the relation $\kappa^2 = \omega_2{}^2 + \omega_3{}^2$ [10, 12] and the assumption of elastic isotropy for directions perpendicular to the central curve (so that φ depends only on ω_1 and κ) imply that the quadratic part of the expansion must have the conventional form ${}^1/_2A\kappa^2 + {}^1/_2C\omega_1{}^2$. But this second-order approximation to φ may be insufficient unless both κ and ω_1 are small. If the molecule is a closed ring of length ℓ then the average value of κ cannot be less than $2\pi/\ell$ [15].

For a linear polymer Landau and Lifschitz [16] have derived a relation between its coefficient of flexural rigidity A, the absolute temperature T, and the mean square of the distance between its ends. The double-stranded DNA rings studied by Vinograd and others bring in the twist and the deformation-invariant parameter Lk. Electron micrographs of these molecules for various values of Lk suggest that for large Lk their shape is less influenced by random forces. Thus for $Lk = 0$ they look more like random closed curves than circles, while for large Lk one sees clearly recognizable twisted loops which, for still larger Lk, change into branched forms (paper submitted to *J. Mol. Biol.* by Upholt, Gray, and Vinograd). Calculations of the deformation energy $E(X,Lk)$ for twisted closed rods, using $\varphi = {}^1/_2(A\kappa^2 + C\omega_1{}^2)$, suggest an equilibrium shape similar to the twisted loop over a range of values of Lk. The breakdown of the twisted loop into a branched form is not fully understood as yet, but one can show that for sufficiently large Lk the twisted loop can no longer represent a configuration of (absolutely) least energy. The reason for this is that the thickness of the rod limits the possible writhing numbers the twisted loop form can attain. Other shapes such as the coil of Fig. 1, while having more curvature for small writhing numbers, can attain larger writhing numbers for a given length and diameter and so reach lower energy levels for large linking numbers by reducing the twist. These considerations suggest that the closed thin rod, with no account taken of statistical forces, may be an appropriate model for closed double-stranded DNA rings for large linking numbers. Such a model may help to determine for DNA the energy of deformation per unit length, both as a function of curvature and of twist.

1. Dungey, J. W., *Cosmic Electrodynamics* (Cambridge University Press, London and New York, 1958).
2. Vinograd, J., J. Lebowitz, R. Radloff, R. Watson. and P. Laipis, *Proc. Nat. Acad. Sci. USA*, **53**, 1104 (1965).
3. Vinograd, J., and J. Lebowitz, *J. Gen. Physiol.*, **49**, 103 (1966).

4. Glaubiger, D., and J. E. Hearst, *Biopolymers*, **5**, 691 (1967).
5. Bauer, W., and J. Vinograd, *J. Mol. Biol.*, **33**, 141 (1968).
6. Vinograd, J., J. Lebowitz, and R. Watson, *J. Mol. Biol.*, **33**, 173 (1968).
7. Călugăreanu, G., *Czechoslovak Math. J.*, **11**, 588 (1961).
8. Pohl, W. F., *J. Math. Mech.*, **17**, 975 (1968).
9. Webster's Third New International Dictionary.
10. W. Blaschke, *Einführung in die Differentialgeometrie* (Springer-Verlag, Berlin, Göttingen and Heidelberg, 1950).
11. F. Brock Fuller, in *Mathematical Problems in the Biological Sciences, Proceedings of Symposia in Applied Mathematics*, ed. R. E. Bellman (American Mathematical Society, Providence, 1962), Vol. 14.
12. A. E. H. Love, *A Treatise on the Mathematical Theory of Elasticity*, 4th Ed. (Dover, New York, 1944).
13. W. Blaschke, *Vorlesungen über Integralgeometrie* (VEB Deutscher Verlag der Wissenschaften, Berlin, 1955).
14. Landau, L. D., and E. M. Lifshitz, *Theory of Elasticity* (Pergamon Press, London, Paris, and Frankfurt, 1959).
15. W. Fenchel, *Bull. Amer. Math. Soc.*, **57**, 44 (1951).
16. Landau, L. D., and E. M. Lifschitz, *Statistical Physics*, 2nd. ed. (Pergamon Press, Oxford and New York, 1969).