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GEOMETRY AND EQUILIBRIA OF PARALLEL BUNDLES OF ELASTIC RODS

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Summary. *Geometrical conditions of existence of curved bundles of hexagonally packed rods are presented. Closure of the bundle results in a group of automorphisms of the cross-sectional lattice. The elastic energy accounts for bending and torsion of the rods. Equilibria of the bundle correspond to solutions of a variational problem formulated for the axis of the bundle. The Euler-Lagrange equations are obtained in terms of curvature and torsion and the problem is reduced to the quadrature. The Ilyukhin-type equations describe the shape of the bundle in special cylindrical coordinates. The results are of universal nature and are applicable to various fibrous structures, including DNA and nanotubes.*

1 INTRODUCTION

It is known that the densest packing of infinite straight cylinders is hexagonal when all their axes are parallel. It evidently corresponds to hexagonal packing of discs in a plane. Geometrically, it means that all pairs of neighbouring axes are located at constant distance to each other. If the rods are not straight, it is still possible to arrange them in parallel bundles so that the neighbouring strands keep being in continuous contact to each other. The parallel bundle is twistless since an arbitrary small twist of one strand around another immediately destroys the perfect hexagonal packing.

Complicated spatial structures arise when the rods are in contact with themselves as in closed or cycled bundles. The closedness condition imposes a severe constraint on the whole structure. Indeed, take an orthogonal cross-section of the bundle. Then, what plays a role is the mapping of the 2D hexagonal lattice in the cross-section onto itself. The automorphisms that preserve both the distances and the connectivity, form a discrete infinite group. Its study results in characterization of all possible closed hexagonally packed bundles: the writhing number of each axis that realizes the mapping should equal $n/6$, where n is integer. One consequence of the automorphism group structure is that it is impossible to form a closed hexagonally packed bundle with a single filament: frustration is inevitable.

Clarification of the geometry is accompanied by consideration of mechanical properties. Assuming that the strands may be characterized as thin uniform isotropic elastic rods, we compute the elastic energy of the bundle. A continuum limit case of circular cross-section of the bundle is studied in more detail. We show that the equilibria of the bundle may be described as extremal solutions to a variational problem for the axial curve in space. The functional is represented as a linear combination of three integrals: the first is the length, the second is the total torsion and the last a function of the squared curvature. This formulation makes it possible to apply the procedure for derivation of the Euler-Lagrange equations in terms of curvature and torsion [1]. The problem reduces to the quadrature because the functional involves only integral torsion and torsion is not coupled with curvature. With knowledge of curvature and torsion the spatial shape of the bundle may be readily computed by integration of the Ilyukhin-type equations in the specially chosen cylindrical coordinates which are widely used in the statics of rods.

2 GEOMETRY

Let a rod in the parallel bundle have the axis $\mathbf{r}(s)$, s being the arclength. The vector $\mathbf{m}$ connects the closest points on $\mathbf{r}(s)$ and on an axis of another rod in the bundle. Then the main equation that describes the arrangement of rods in the hexagonally packed bundle reads

$$\frac{d\mathbf{m}}{ds} = -\varkappa(\mathbf{m}\cdot\mathbf{N})\mathbf{T},$$

where $\mathbf{T}$ and $\mathbf{N}$ are, resp., the tangent and the principal normal to $\mathbf{r}(s)$ and $\varkappa$ the curvature of this curve.

If the bundle is closed, then 2D hexagonal cross-sectional lattice maps onto itself. The automorphisms that preserve both the distances and the connectivity, form a discrete infinite group with finite generator. This allows us to characterize all possible closed hexagonally packed bundles: the writhing number of each axis that realizes the mapping should equal $n/6$, where n is integer.

3 MECHANICS OF EQUILIBRIA

Assume that the cross-section Ψ of the bundle is a circle of radius R. The elastic energy of each strand is computed as the bending and torsion energy of the thin isotropic uniform elastic rod of circular cross-section. All the rods in the bundle have identical mechanical properties and the same thickness.

The centreline of a parallel bundle of circular cross-section made up with isotropic uniform thin elastic rods in equilibrium is an extremal for a linear combination of three integrals

$$\mathcal{F} = \lambda_1 \mathcal{L} + \lambda_2 \mathcal{T} + \lambda_3 \mathcal{K}, \tag{1}$$

where $\mathcal{L} = \int ds$ is the length of the axis, $\mathcal{T} = \int \tau \, ds$ is the total torsion and $\mathcal{K} = \int f(\varkappa^2) \, ds$ with $f(\varkappa^2) = 1 - \sqrt{1 - R^2\varkappa^2(s)}$ (cf. the single rod case with $f(\varkappa^2) = \varkappa^2(s)$ [2]).

Conversely, for any closed extremal $\mathbf{r}(s)$ of the functional (1) with writhe $\mathcal{W}r(\mathbf{r}) = n/6$, $n \in \mathbb{Z}$, and with the curvature $\varkappa(s) \leq R^{-1}$ for some positive R, there exists a parallel bundle in equilibrium with axis $\mathbf{r}$ and with circular cross-section of radius R made up with thin elastic rods. The winding number p is determined by the fractional part of the writhe. The distribution of twist rates ω_{1m} of the rods satisfies the conditions

$$\frac{c \iint_\Psi \omega_{1m} d\sigma}{\pi b} = \frac{\lambda_2}{\lambda_3} \quad \text{and} \quad p\omega_{1m}\mathcal{L} = p \int_0^{\mathcal{L}} \tau \, ds + 2\pi j_m, \quad j_m \in \mathbb{Z},$$

where b and c are the bending and torsional rigidity densities.

The Euler-Lagrange equations for (1) may be obtained by adapting equations (77), (78) [1], which are valid for more general functional $\int \phi(\varkappa, \tau) \, ds$, to our case with $\phi(\varkappa, \tau) = \lambda_3 f(\varkappa^2) + \lambda_2 \tau + \lambda_1$:

$$\lambda_3\{8\varkappa^3\varkappa_s^2 f''' + 4\varkappa(\varkappa\varkappa_{ss} + 3\varkappa_s^2) f'' + 2[\varkappa_{ss} + \varkappa(\varkappa^2 - \tau^2)] f' - \varkappa f\} + \lambda_2\varkappa\tau - \lambda_1\varkappa = 0, \tag{2}$$

$$\lambda_3[8\varkappa^2\varkappa_s\tau f'' + 2(2\varkappa_s\tau + \varkappa\tau_s) f'] - \lambda_2\varkappa_s = 0, \tag{3}$$

where the prime $'$ denotes the derivative with respect to the squared curvature $u \equiv \varkappa^2$: $f' = \frac{df(u)}{du}$. We can reduce the order of the above system by using two first integrals of (2), (3).

In case of the thin rod, it is known that there exist special cylindrical coordinates $\{\rho, \theta, z\}$ in which the centreline is expressed in an especially convenient way. This remains valid in the general case [1]. We direct the z-axis along the constant force vector $\mathbf{F} \neq \mathbf{0}$ and the polar angle θ is measured from the axis $\mathbf{M} \times \mathbf{F}$. The radial distance is given by

$$\rho^2 = \frac{4\lambda_3^2\varkappa^2(f')^2 + \lambda_2^2 - M_z^2}{F^2}, \tag{4}$$

where M_z is the constant z-component of the moment $\mathbf{M}$. To find the other coordinates one needs to integrate

$$\frac{dz}{ds} = \frac{1}{F}[\lambda_3(2\varkappa^2 f' - f) - \lambda_1], \tag{5}$$

$$\frac{d\theta}{ds} = -\frac{1}{\rho^2}\left(M_z \frac{dz}{ds} + \lambda_2\right). \tag{6}$$

Equations (4), (5), (6) generalize Ilyukhin's equations for the thin elastic rod to the parallel bundles.

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