ON THE PERFECT HEXAGONAL PACKING OF TUBES

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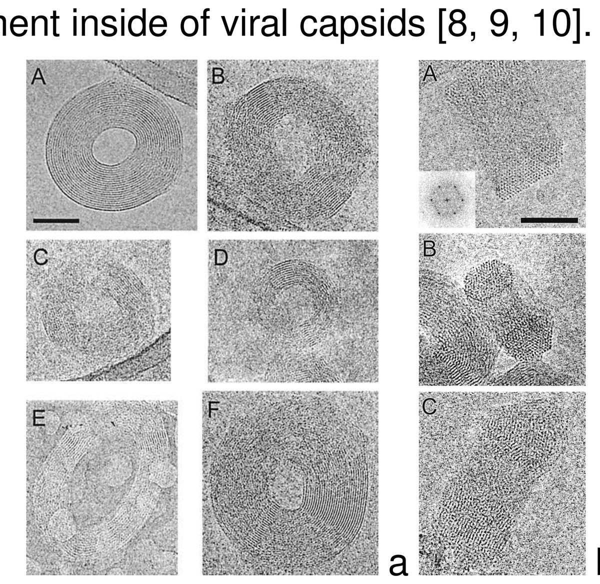
Abstract. In most cases the hexagonal packing of fibrous structures extremizes the energy of interaction between strands. If the strands are not straight, then it is still possible to form a perfect hexatic bundle. Conditions under which the perfect hexagonal packing of curved tubular structures may exist are formulated. Of particular interest are closed bundles like DNA toroids or spools. The closure or return constraints of the bundle result in an allowable group of automorphisms of the cross-sectional hexagonal lattice. The structure of this group is explored. Examples of an open helical-like and closed toroidal-like bundles are presented. A possible implication on a condensation of DNA in toroids and its packing inside a viral capsid is briefly discussed [1].

Introduction

It is known that the densest packing of infinite straight cylinders is hexagonal when all their axes are parallel [2]. It evidently corresponds to hexagonal packing of disks in a plane. The hexagonal packing of tubular objects occurs in numerous instances at nano to macro scale. Among examples there are nanotubes [3], high density columnar hexatic liquid crystalline DNA mesophases [4] and others. In most cases, this packing extremizes the interaction energy between filaments. Geometrically, it means that all pairs of neighbouring axes are located at constant distance to each other.

In some instances, the filaments are not straight. Then, the natural question arises of whether it is still possible to reach the same maximal density of packing. If yes, then the second question can be formulated as: what is the set of configurations of infinite (or closed) tubes that have the maximal density? By a tube (or a tubular neighbourhood) here we understand the set of all points in space whose distance from the smooth axial curve does not exceed the constant thickness radius. We can set the scale by fixing this radius to 1. Moreover we will assume that *the global curvature* of the axes is less or equal to 1. Thus, the tubes cannot overlap, but they are perfectly flexible. It will be shown in the following that the densest packing class includes curvilinear axes, which should be *relatively parallel*. This implies that an arbitrary small twist of one axis around another immediately destroys the hexagonal packing.

A complicated structure arises when the tubes are in contact with *themselves*. An important example is a condensation of DNA in toroids [5, 6, 7] or a DNA arrangement inside of viral capsids [8, 9, 10].



a b

These pictures are taken from [7]. They show cryoelectron micrographs of DNA toroids with the plane of the toroid (column a) approximately coplanar with the microscope image plane (top-view) and (column b) orthogonal to the microscope image plane (edge-view). Hexagonal packing of DNA is clearly seen on the right figure (A).

Unconstrained tube packing

We start with consideration of a perfect tube of some length with axis $\mathbf{r}_0(s)$, s being the arclength parametrization. Let the tube be in a continuous contact with the maximal allowed number of other tubes of the same thickness. This number equals 6 [11], thus it may be said that the tubes are hexagonally packed. Denote the axes of the neighbouring tubes by $\mathbf{r}_j(s)$, $j = 1,\ldots,6$. We can choose the same parametrization for all the tubes such that for every s the points $\mathbf{r}_j(s)$, $j = 1,\ldots,6$ are the closest to the central axis $\mathbf{r}_0(s)$ and they lie in the vertices of a regular triangular lattice.

The vector field $\mathbf{m}_{j0}(s) \equiv \mathbf{r}_j(s) - \mathbf{r}_0(s)$ is relatively parallel [12]. It implies that there is no twist of vectors $\mathbf{m}_{j0}(s)$ about the central axis. We can add more layers of the tubes in the same manner as first six tubes. Proceeding this way will allow us to build a bundle of parallel tubes that fill up some domain in space. The hexagonal packing provides the maximal density in this domain.

Let us now obtain an equation that governs the position of the neighbouring tube for a given central axis. We omit the index j for clarity. Since $\|\mathbf{m}\| = const(=2)$, we can write

$$\frac{d\mathbf{m}}{ds} = \omega \times \mathbf{m}, \qquad (1)$$

and the vector ω may be represented as $\omega = \omega_1\mathbf{m} + \omega_2\mathbf{T}\times\mathbf{m}$ [11], where we denote by $\mathbf{T} = \frac{d\mathbf{r}}{ds}$ the tangent to the central axis.

By definition, the vector $\mathbf{m}$ connects the closest points on two curves, which implies $\mathbf{m}\cdot\mathbf{T} = 0$. Differentiating this equation and further substitute eq. (1) for $\frac{d\mathbf{m}}{ds}$, we come to $\omega_2\mathbf{m}^2 = \mathbf{m}\cdot\frac{d\mathbf{T}}{ds}$, or, with the help of the Serret-Frenet equations, $\omega_2\mathbf{m}^2 = \kappa\mathbf{m}\cdot\mathbf{N}$. where $\mathbf{N}$ is the principal normal to $\mathbf{r}(s)$ and κ the curvature of this curve. Finally, the equation for the orientation vector $\mathbf{m}$ can be given the form

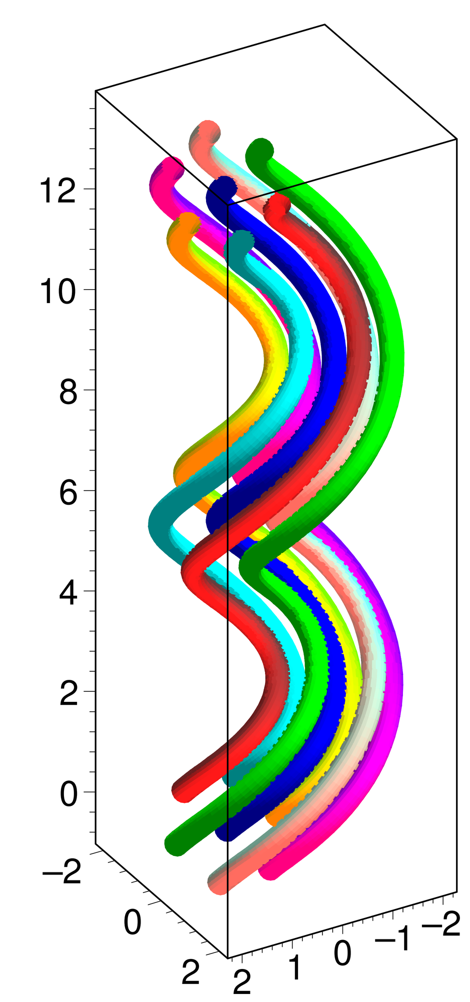
$$\frac{d\mathbf{m}}{ds} = -\kappa(\mathbf{m}\cdot\mathbf{N})\mathbf{T}. \qquad (2)$$

This is the main equation that describes the arrangement of tubes in the hexagonally packed bundle.

Remark. In the continuum limit, the elastic Frank-Oseen energy density

$$e = \frac{1}{2}K_1[\nabla\cdot\mathbf{T}]^2 + \frac{1}{2}K_2[\mathbf{T}\cdot(\nabla\times\mathbf{T})]^2 + \frac{1}{2}K_3[\mathbf{T}\times(\nabla\times\mathbf{T})]^2$$

reduces to the term $\frac{1}{2}K_3\kappa^2$, with K_3 being the bending rigidity.



EXAMPLE: a regular helical curve: $\mathbf{r}(s) = (\cos as, \sin as, \sqrt{1-a^2}s)$, $0 \le a \le 1$. Equation (2) transforms to the system

$$\frac{d\xi}{ds} = a\eta, \quad \frac{d\eta}{ds} = a(a^2-1)\xi,$$
$$\frac{dm_z}{ds} = a^2\sqrt{1-a^2}\xi, \qquad (3)$$

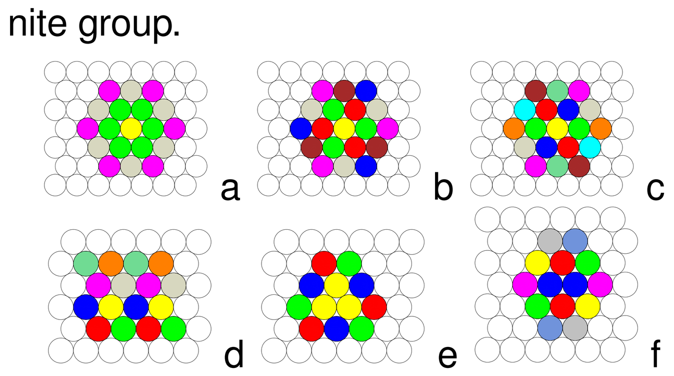
and the first two components of the vector $\mathbf{m} = (m_x, m_y, m_z)$ are expressed as $m_x = \xi\cos as - \eta\sin as$, $m_y = \xi\sin as + \eta\cos as$. The explicit solution of eq. (3) is easy to find:

$$\xi = c_1\cos\tau s + c_2\sin\tau s,$$
$$\eta = \sqrt{1-a^2}(c_2\cos\tau s - c_1\sin\tau s),$$
$$m_z = a(c_1\sin\tau s - c_2\cos\tau s),$$

where $\tau = a\sqrt{1-a^2}$ is the torsion and $\mathbf{m}^2 = c_1^2 + c_2^2$. The figure shows a bundle of six tubes arranged at constant distance from the central tube (shown in blue) and from the neighbours. At every section which is orthogonal to their axes the crossing points form the hexagonal lattice. The tubes are shown thinner to ease representation.

Cycled bundles

In this work, particular attention is given to *closed* bundles of hexagonally packed tubes. The closedness condition imposes a strict constraint on the whole structure. Indeed, take an orthogonal cross-section of the bundle. Then, we study 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.

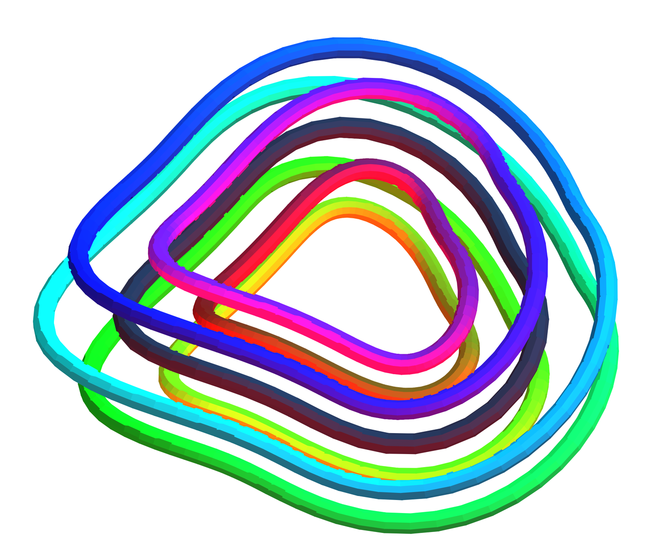


a b c d e f

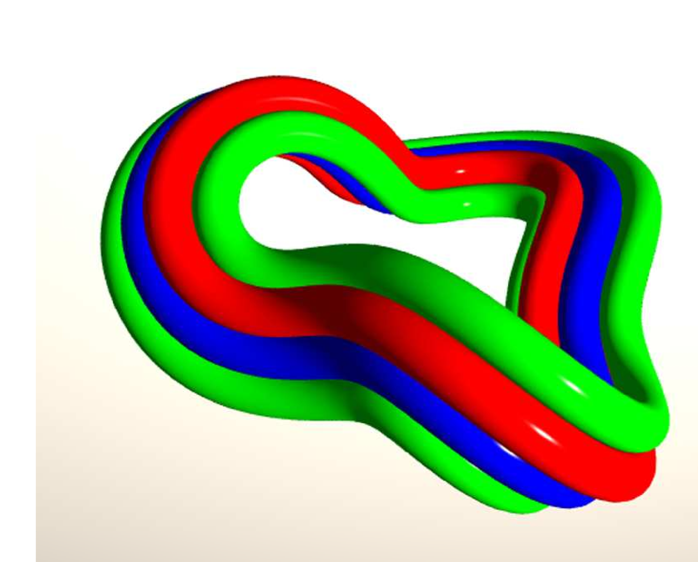
The automorphism group of the lattice is finitely generated by the following set of transformations:

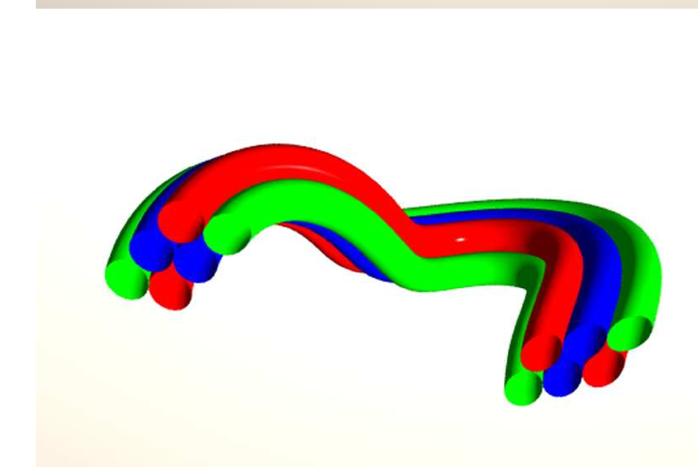
1. an identity map,
2. translations along the lattice vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ (fig. d),
3. a rotation through $\frac{1}{3}\pi$ around the origin (figs. a,b,c),
4. a rotation through $\frac{2}{3}\pi$ around $\frac{1}{3}(\mathbf{e}_1+\mathbf{e}_2)$ (fig. e),
5. a rotation through π around $\frac{1}{2}\mathbf{e}_1$ (fig. f).

This allows us to characterize all possible closed hexagonally packed bundles: *the writhing number* [13] of each axis that realizes the mapping should equal $n/6$, where n is integer. Here are the examples:



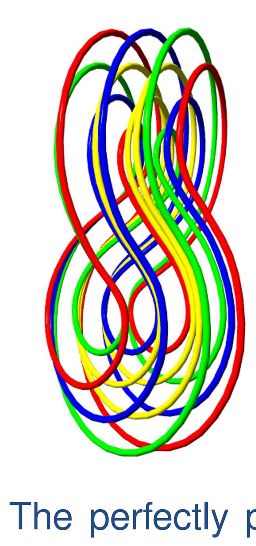
The perfectly packed bundle made up of two closed tubes (cf. case (a)). The core (dark) makes one turn and the second tube winds six times. The colour variation codes the arclength. The tubes are shown thinner to ease representation.

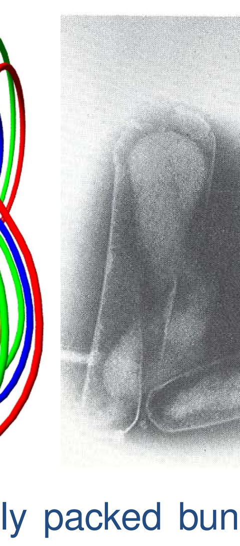




The perfectly packed bundle that corresponds to case (f).

Under certain conditions, the DNA toroids may deform taking on a warped shape [14]. Generally, this deformation affects the interstrand distances and the interaction energy between strands. This effect may influence the twist-bend instability of the DNA condensates [15]. A perfectly packed structure may have its overall shape that closely resembles the warped DNA toroids.





Left. The perfectly packed bundle made up of four closed tubes (cf. case (e)). The tubes are shown thinner to ease representation. *Right.* The DNA bundle looks like twisted skein of yarn (an electron micrograph from [14]).

Concluding remarks

It is shown that curvilinear tubular filaments may be packed in the most compact way in some spatial domain. Such a packing extremizes the interaction energy between neighbouring filaments and it is only possible if the bundle is twist-free.

An equation is derived that governs the relative positions of the tubes in the hexagonal bundle.

Particular attention is given to cycled arrangements of the tubes. The corresponding automorphisms of the hexagonal lattice in the cross-section are classified.

The cycled structures are only possible if *the writhe* of the central axis is $n/6$, n an integer. The automorphism group structure forbids a cycled hexagonally packed bundle made up with a single filament: frustration is inevitable (cf. [16]).

The results are of a universal nature and are applicable to various fibrous structures, in particular, to a condensation of DNA in toroids as well as to its packing inside the viral capsids.

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