Eur. Phys. J. E **4**, 445–449 (2001)

THE EUROPEAN PHYSICAL JOURNAL E
EDP Sciences

Helical close packings of ideal ropes

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Received 2 November 2000

Abstract. Closely packed conformations of helices formed on an ideal rope are considered. The pitch *vs.* radius relations which define a closely packed helix are determined. The relations stem from the turn-to-turn distance and curvature-limiting conditions. Plots of the relations are shown to cross each other. The physical sense of the crossing point is discussed.

PACS. 87.16.Ac Subcellular structure and processes: Theory and modelling; computer simulation

1 Introduction

The phenomenon of coiling is observed in various biological and physical systems such as the tendrils of climbing plants [1], one-dimensional filaments of bacteria [2] or cylindrical stacks of phospholipid membranes interacting with an amphiphilic polymer [3]. In some cases the phenomenon occurs in conditions in which the helical structures created by coiling become closely packed. A single, closely packed helix is one of them. In a different context helix formation was studied in Monte Carlo simulations by Maritan *et al.* [4]. Below we present a simple analytical argument leading to the determination of the parameters of the optimal closely packed helix.

Take a piece of a rope of diameter D and try to arrange it into a right-handed helix, see Figure 1, described parametrically by the set of equations:

$$\begin{aligned} x &= -r\sin(\xi)\,, \\ y &= r\cos(\xi)\,, \\ z &= \frac{P}{2\pi}\xi\,. \end{aligned} \tag{1}$$

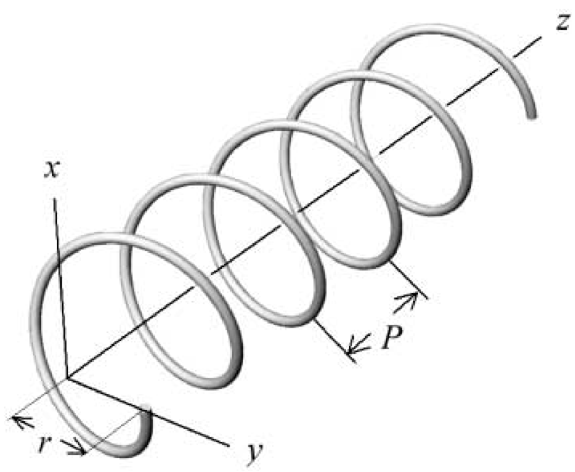

Fig. 1. The radius and pitch of a helix defined by equation (1).

The helix is well defined if its radius r and pitch P are specified. As is easy to check experimentally, when the helix is formed on a real rope, not all values of r and P are accessible. Being material, the rope cannot be arranged into shapes, which violate its self-impenetrability. If, for instance, one chooses to form a helix with $r = 2D$, its pitch cannot be made smaller than about $1.003D$. This is the value at which the consecutive turns of the helix become closely packed. For a smaller pitch, overlaps would occur, see Figure 2.

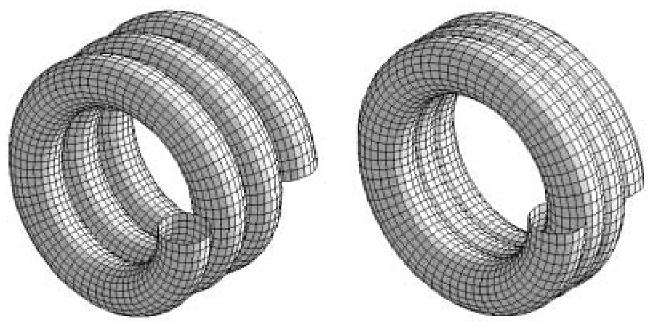

Fig. 2. When, at a given radius, the pitch of the rope helix is too small overlaps appear; $r = 2$, $P = 1.003$ on the left and $P = 0.5$ on the right.

A general question arises: what are the limits for the radius and pitch values of a helix formed with a rope of

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the diameter D? The question was posed some time ago in discussions connected with the problem of ideal knots [5]. The calculations we present here were directly stimulated by a recent paper by Maritan *et al.* who performed Monte Carlo simulations on a rope confined within a box. As indicated by the authors, the pitch-to-radius ratio of the optimal helix they discovered matches very well the value of the ratio found in the α-helix discovered by nature in the evolution processes. Possible implications of their results were discussed by Stasiak and Maddocks [6].

The symbolic algebra and numerical techniques we present below are analogous to those we applied when considering the problem of the close packings of two ropes twisted together [7].

2 Ideal rope

The considerations presented below are valid for the so-called ideal ropes, *i.e.* ropes which, from a physical point of view, are completely flexible, but at the same time perfectly hard. Assume that the axis of such a rope is shaped into a smooth curve C. At any point on the curve, a tangent vector $\mathbf{t}$ is defined. The rope is ideal if each of its cross-sections, perpendicular to the tangent vector $\mathbf{t}$, makes a circle of diameter D, and none of the circles overlaps with any other.

Let the ideal rope be shaped into a closely packed helix H of a radius $r \gg D$. To understand better what we mean by the "closely packed helix", we may imagine that the rope is wound as tightly as possible onto a cylinder of diameter $(2r - D)$, see Figure 3.

In such conditions the consecutive turns of the helix remain at the smallest possible distance equal to D. The points, at which the closely packed rope stays in touch with itself, are located on a helix H' of radius $r' < r$ (the pitch of H' remains the same as that of H). Now, let us remove the inner cylinder and try to make r smaller and smaller, keeping all the time the helix closely packed. As r goes down, the pitch P goes up. Below we determine the relation $P_{\mathrm{CP1}}(r)$ which in the minimum turn-to-turn distance conditions binds r and P. Experiments prove that at a certain value of r, the path determined by the $P_{\mathrm{CP1}}(r)$ relation is abandoned and the consecutive stage of the squeezing process is governed by a different limiting condition, which is that the local curvature κ of the helix cannot be larger than $2/D$. This new condition binds P and r in a different manner. We shall also find its shape $P_{\mathrm{CP2}}(r)$. At the point at which both relations cross, the closely packed helix has a special, optimal shape discussed by Maritan *et al.* [4].

3 The closely packed helix limited by its doubly critical self-distance

Consider the ideal rope shaped into a helix H whose consecutive turns touch each other. For a given r, what should the pitch P of the helix be, to keep its turns closely packed? We shall answer the question.

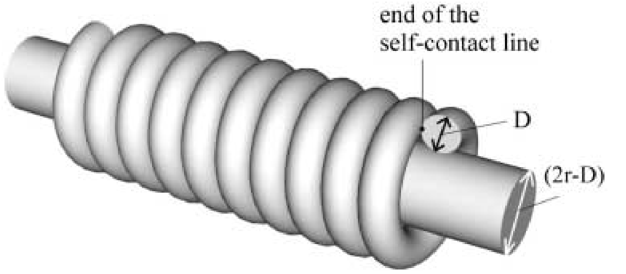

Fig. 3. Rope a diameter D wound as tightly as possible on a cylinder of diameter $(2r - D)$.

Consecutive turns of the helix touch each other if the minimum of the distance from any point P_1 of the helix to the points located at the beginning of the next turn is equal to D. Let P_2 be the point at which this minimum distance is reached. Let $\mathbf{t}_1$ and $\mathbf{t}_2$ be the vectors tangent of H at P_1 and P_2, respectively. Obviously, in such a situation, the $\overrightarrow{P_1P_2}$ vector is perpendicular both to $\mathbf{t}_1$ and $\mathbf{t}_2$. $\overrightarrow{P_1P_2}$ belongs both to the plane Σ_1 located at P_1 and perpendicular to $\mathbf{t}_1$ and to the plane Σ_2 located at P_2 and perpendicular to $\mathbf{t}_2$. Thus, $\overrightarrow{P_1P_2}$ belongs to the line along which $\Sigma_1$and Σ_2 cross. Let P_1 located at (x_1, y_1, z_1) be given; let it be the point of H defined by $\xi_1 = 0$:

$$
\begin{aligned}
x_1 &= 0\,, \\
y_1 &= r\,, \\
z_1 &= 0\,.
\end{aligned} \tag{2}
$$

The components of the tangent vector $\mathbf{t}_1$ located at P_1 are equal to

$$
\begin{aligned}
t_{1x} &= -r\,, \\
t_{1y} &= 0\,, \\
t_{1z} &= \frac{P}{2\pi}\,.
\end{aligned} \tag{3}
$$

Consequently, the Σ_1 plane going through P_1 and perpendicular to $\mathbf{t}_1$ is defined by the equation

$$
rx - \frac{P}{2\pi}z = 0\,. \tag{4}
$$

Let

$$
\begin{aligned}
x_2 &= -r\sin(\xi)\,, \\
y_2 &= r\cos(\xi)\,, \\
z_2 &= \frac{P}{2\pi}\xi
\end{aligned} \tag{5}
$$

be the coordinates of the point P_2 located in the vicinity of the next turn, *i.e.* at the ξ values close to 2π. The point must belong to the Σ_1 plane. Consequently, its coordinates given by equation (5) must fulfil equation (4), which gives

$$
r^2\sin(\xi) + \frac{P^2}{4\pi^2}\xi = 0\,. \tag{6}
$$

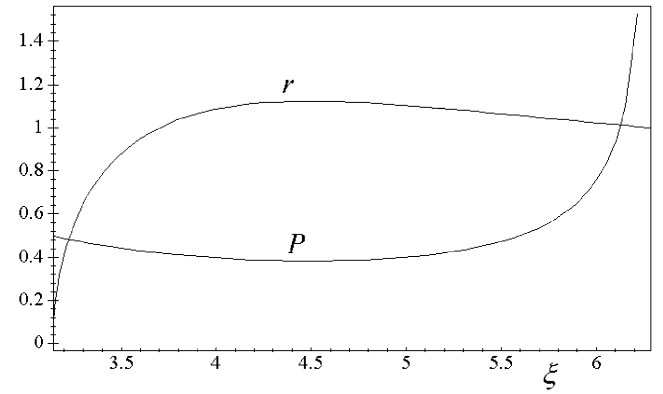

Fig. 4. Shapes of the $P(\xi)$ and $r(\xi)$ functions given by equation (7); $D = 1$.

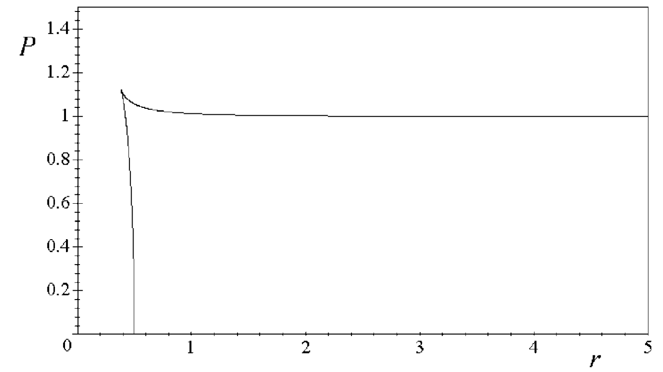

Fig. 5. The $P_{\mathrm{CP1}}(r)$ relation described parametrically by the $P(\xi)$ and $r(\xi)$ functions shown in Figure 3.

The square of the distance between P_1 and P_2 should be equal to D^2, which results in equation

$$2r^2 - 2r^2\cos(\xi) + \left(\frac{P}{2\pi}\right)^2 \xi^2 = D^2 . \tag{7}$$

Solving equations (6) and (7) for r and P gives a set of formulas:

$$P = 2\pi D\sqrt{\frac{\sin(\xi)}{2\xi\left[\cos(\xi)-1\right]+\xi^2\sin(\xi)}}\,,$$
$$r = D\sqrt{\frac{\xi}{2\xi\left[1-\cos(\xi)\right]+\xi^2\sin(\xi)}}\,, \tag{8}$$

which in a parametric manner describe the relation $P_{\mathrm{CP1}}(r)$ between P and r. The relation must be fulfilled by helices whose consecutive turns are closely packed. (Notice that here ξ becomes a free parameter which serves to describe the shape of the $P_{\mathrm{CP1}}(r)$ relation.) The shapes of $P(\xi)$ and $r(\xi)$ functions are shown in Figure 4, where we present them in the potentially interesting interval of $\pi \in (\pi, 2\pi)$.

The shape of the $P_{\mathrm{CP1}}(r)$ relation obtained using the parametric plot is shown in Figure 5.

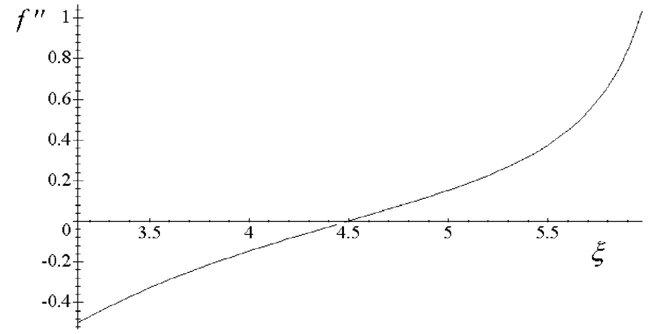

Fig. 6. The second derivative of the square distance function.

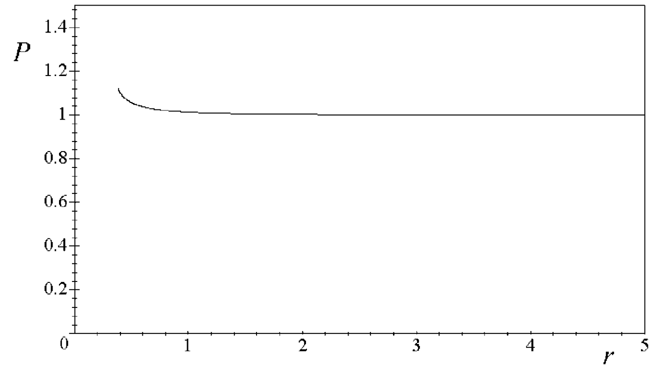

Fig. 7. The dependence of the pitch P on the radius r found in closely packed helices; $D = 1$.

As seen in the figure, the $P_{\mathrm{CP1}}(r)$ relation contains two branches. To find which of them presents the physically sensible solution, we look for the range of ξ over which the function of the square distance

$$f(\xi+\Delta\xi) = 2r^2 - 2r^2\cos(\xi+\Delta\xi) + \left(\frac{P}{2\pi}\right)^2(\xi+\Delta\xi)^2 \tag{9}$$

displays a minimum *vs.* $\Delta\xi$, with P and r in the relation described by equation (8). (When the minimum exists, the turn-to-turn distance we are calculating becomes identical with the doubly critical self-distance introduced by J.K. Simon [8]:

$$\mathrm{dcsd}(h) = \min_{x\neq y}\{|h(x)-h(y)| : h'(x)\perp(h(x)-h(y)),\; h'(y)\perp(h(x)-h(y))\}\,,$$

where h is the helix parameterised by arc-length x, $h(x)$ and $h(y)$ are points located on the helix, $(h(x) - h(y))$ is the vector which joins the points and $h'(x)$ and $h'(y)$ are the tangent vectors at $h(x)$ and $h(y)$, respectively.) To reach the aim, we substitute equation (8) into equation (9), expand it into a Taylor series truncated at the $(\Delta\xi)^2$ term and differentiate it twice with respect to $\Delta\xi$. The second derivative obtained in this way equals

$$\frac{\mathrm{d}^2 f}{\mathrm{d}(\Delta\xi)^2} = \frac{2\xi\cos(\xi) - 2\sin(\xi)}{\xi\left[\xi\sin(\xi) + 2\cos(\xi) - 2\right]}\,. \tag{10}$$

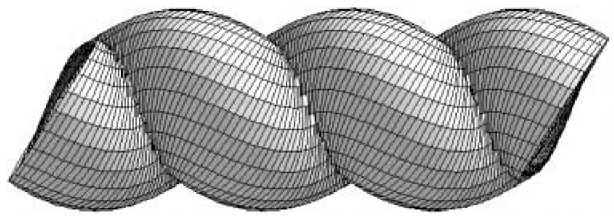

Fig. 8. If the local curvature of the helix is too large the impenetrability of the ideal rope is also violated. For the helix presented in the figure $r = 0.1$ and $P = 1$, thus its local curvature is $k = 2.83$.

In Figure 6 we present the relation within the range of interest $(\pi, 2\pi)$.

The second derivative is positive in the interval $(4.49341, 2\pi)$. Replotting the $P_{\mathrm{CP1}}(r)$ relation only within this range reveals which of its branches presents the required solution, see Figure 7.

The result we obtained remains in agreement with intuition: a closely packed helix, whose radius is squeezed, increases its pitch. As seen in the figure, $r = 0.5$ seems to limit the squeezing process. Is this really the case?

4 Closely packed helix limited by its curvature

There exists another mechanism, which limits the set of possible (r, P) values of the helices formed on an ideal rope. It stems from the fact that the ideal rope of diameter D cannot have a local curvature larger than $2/D$. The following heuristic reasoning indicates the source of the limitation. Let $h(x)$ be a helix of curvature κ parameterised by an arc-length. Let $h'(x)$ be the field of its tangent vectors. Imagine that a disk of diameter D, centred on $h(x)$ and perpendicular to $h'(x)$ is swept along the helix. The circular border of the moving disk determines within the space the surface of the ideal rope. Consider the traces $d(x_1)$ and $d(x_2)$ of the disk in two consecutive positions $h(x_1)$ and $h(x_2)$ separated by an infinitesimal arc dx. Because of the non-zero curvature of the helix along which the disk was swept, disks $d(x_1)$ and $d(x_2)$ are not parallel to each other —they are inclined by an angle κdx. When $\kappa > 2/D$ the disks overlap. Consequently, the surface of the rope determined by the edges of the swept disk becomes non-smooth. Figure 8 illustrates the situation.

Let us consider the analytical consequences of this inequality. The curvature of a helix defined by equation (1) equals

$$\kappa = \frac{r}{r^2 + \frac{P^2}{4\pi^2}} \,. \tag{11}$$

It is easy to show that equation $\kappa = 2/D$ is fulfilled if

$$P_{\mathrm{CP2}} = \pi\sqrt{2rD - 4r^2} \,. \tag{12}$$

Figure 9 presents relation (12) together with relation (8) discussed above. One can see that their plots cross. As a result, some parts of the $P_{\mathrm{CP1}}(r)$ and $P_{\mathrm{CP2}}(r)$ solutions become inaccessible.

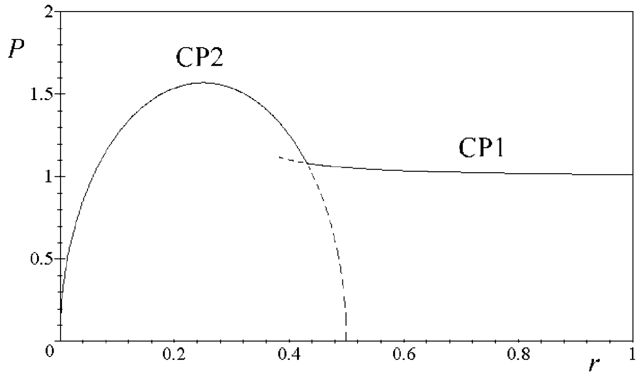

Fig. 9. $P_{\mathrm{CP1}}(r)$and $P_{\mathrm{CP2}}(r)$ solutions plotted together. The mutually inaccessible parts of the solutions are marked with a dashed line; $D = 1$.

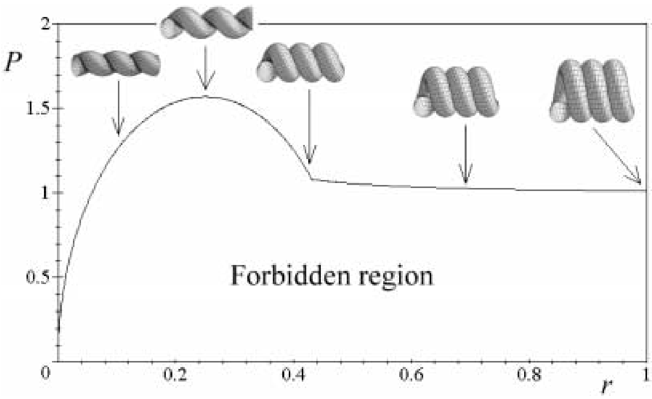

Fig. 10. Plot of the relation between the radius and the pitch of the closely packed helices together with their images at a few representative points of the plot; $D = 1$.

Numerically determined coordinates of the crossing point are as follows:

$$r_0 = 0.431092 \,, \qquad P_0 = 1.08292 \,. \tag{13}$$

The mutually accessible parts of the $P_{\mathrm{CP1}}(r)$ and $P_{\mathrm{CP2}}(r)$ solutions define, within the (r, P) plane, a borderline $P_{\mathrm{CP}}(r)$ below which one cannot go; helices found in this forbidden region are impossible to build with a perfect rope. Figure 10 presents the borderline $P_{\mathrm{CP}}(r)$ together with the images of the closely packed helices located at a few representative points.

The helix seen in the cusp point at which the CP1 and CP2 solutions meet, is the optimal helix discussed in [4].

5 Physical properties of the optimal helix

Monte Carlo simulations performed by Maritan *et al.* were aimed at finding those shapes of the rope, for which the radius of gyration becomes minimized. The radius of gyration is a geometric property of a curve. It is defined as the root-mean-square distance of a set of points (obtained by a discretisation of the curve) from its centre of mass.

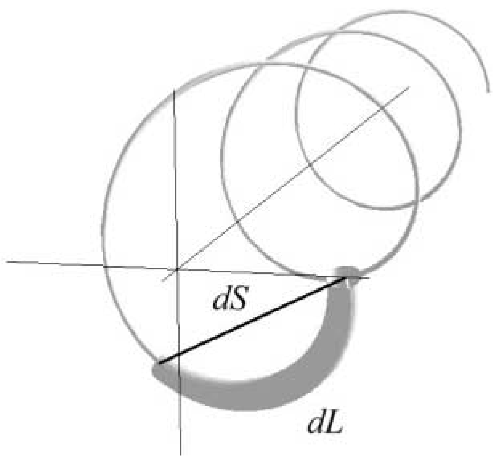

Fig. 11. The relation between dL and dS.

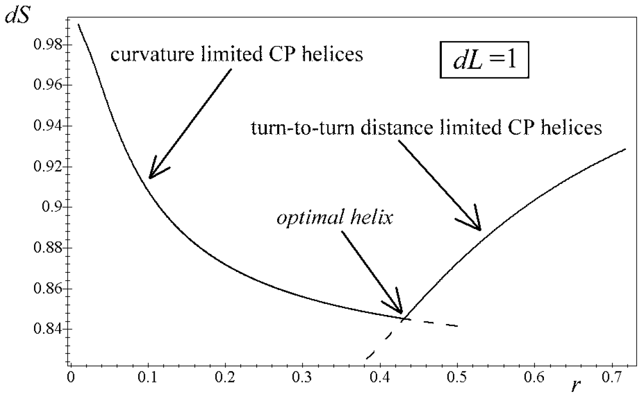

Fig. 12. dS *vs.* r for closely packed helices.

Does the optimal helix minimize some physical properties of the curve?

Let us imagine that equal masses, $m = 1$, are distributed along an ideal rope at equal distances dL. The rope is then shaped into a closely packed helix. What is the energy of the gravitational interaction between the masses? Obviously, the energy depends on the Euclidean distance dS between them, see Figure 11. The distance dS is always smaller than dL and its value depends on the parameters of the helix into which the rope is shaped. As shown above, the values of the parameters are limited by the turn-to-turn distance (the doubly critical self-distance) and the curvature of the helix.

The calculations we performed show that, for a given dL, dS reaches its minimum within the optimal helix, see Figure 12.

Consequently, the energy of gravitational interactions reaches its minimum as well. One can certainly find a few other cases, in which the optimal helix of Maritan *et al.* also proves to be optimal.

6 Discussion

We have shown that, looking for closely packed helices formed on the ideal rope, one has to consider two cases: helices limited by the turn-to-turn distance and helices limited by the local curvature.

As indicated by Maritan *et al.* [4], the two cases can be brought into one: helices limited by the global curvature, a notion introduced by O. Gonzalez and J. Maddocks [9]. The radius of the global curvature at a given point P of a space curve C is defined as the radius of the smallest circle which goes through the chosen point and any other two points P_1, P_2 belonging to C and different from P. Putting a limit on the global curvature of a helix, one limits both the local curvature and the closest distance between its consecutive turns. As a result, the union of accessible parts of the above-presented partial solutions $P_{\mathrm{CP1}}(r)$and $P_{\mathrm{CP2}}(r)$ can be seen as a single solution $P_{\mathrm{CP}}(r)$. The solution shown in Figure 10 answers the problem formulated as follows: what is the relation between the pitch P and the radius r of helices whose global curvature equals $2/D$? Asking simpler, synthetic questions helps to find simpler, synthetic answers.

There exists another, equivalent formulation of the problem. Instead of the global curvature, one can use the notion of the injectivity radius [10]. The injectivity radius of a smooth curve K is the maximum radius of the disks which, centered on each point of K and perpendicular to its tangent, remain disjoint. In terms of the injectivity radius the closely packed helices can be seen as the helices whose injectivity radius is equal to the predetermined radius of the used tube.

This work was supported by KBN under Project 5PO3B01220. PP thanks Andrzej Stasiak and Giovanni Dietler for helpful discussions. He also thanks Herbette Foundation, Institute of Experimental Physics at UNIL and the Mathematics Department at EPFL for financial support.

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10. See, *e.g.*, E. Rawdon in *Ideal Knots*, edited by A. Stasiak, V. Katritch, L.H. Kauffman (World Scientific, Singapore, 1998) p. 143.