The topology of physical filaments

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ABSTRACT:

Filamentous material may exhibit structure dependent material properties and function that depends on their entanglement. Even though intuitively entanglement is often understood in terms of knotting or linking, many of the filamentous systems in the natural world are not mathematical knots or links. In this talk we will introduce a novel framework in knot theory that can characterize the complexity of open curves in 3-space in general. In particular, it will be shown how the Jones polynomial, a traditional topological invariant in knot theory, is a special case of a general Jones polynomial that applies to both open and closed curves in 3-space. Similarly, Vassiliev measures will be generalized to characterize the knotting of open and closed curves. When applied to open curves, these are continuous functions of the curve coordinates instead of topological invariants. We will apply our methods to proteins and show that these enable us to create a new framework for understanding protein folding, which is validated by experimental data. Next we will show that the topological entanglement captured by mathematical methods indeed captures polymer entanglement effects in polymer melts and solutions. We will demonstrate this by using topology to predict a critical lengthscale in entangled polymers, the entanglement length, which is in agreement with experimental estimates. These methods open a new mathematical direction in knot theory that can help us understand polymer and biopolymer function and material properties in many contexts with the goal of their prediction and design.

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