

Writhe Geometry at Finite Temperatures

The geometry of DNA molecules has been extensively studied using the properties of smooth curves and ribbons as idealizations of the properties of stiff chiral molecules. At finite temperatures this description breaks down due to the absence of a Frenet frame. Angular correlations can still be calculated using a frame defined from parallel transport, leading to a description for the writhe of a polymer which is very close to that of a Berry phase.

If we constrain an molecule so that its ends are maintained parallel but with the system otherwise free to fluctuate, then angular rotation, ϕ , between the two ends of the molecule can be decomposed into two components, $\phi = 2\pi(\mathcal{T}w + \mathcal{W}r)^{1,2}$; Twist, $\mathcal{T}w$, describes the internal torsional degrees of freedom of the molecule while writhe, $\mathcal{W}r$, quantifies the tortuosity of the polymer in space. $\mathcal{W}r$ is often calculated from the formula $2\pi\mathcal{W}r + \int \tau ds = \Delta \bmod(2\pi)$, where τ is the geometric torsion of the polymer calculated using the Frenet frame and s the curvilinear distance along the molecule. The term Δ , present when the molecule is open, is the angle between the principle normals of the chain at the two ends.

We now consider how these remarks can be generalized to finite temperatures. The writhing of the polymer is determined by a bending energy, controlled by κ the bending modulus. At non-zero temperatures the distribution of orientations of a stiff polymer is governed by a Fokker-Planck equation³ so that the tangent to the molecule, $\mathbf{t}(s)$, diffuses as a function of the internal coordinate s on a sphere, \mathcal{S}_2 , with diffusion coefficient $k_B T/\kappa$. Thus the shape of a thermalized stiff molecule is the integral of a realization of a Brownian trajectory. However the Frenet frame and τ are only defined for \mathcal{C}^3 curves⁴: For a thermalized stiff molecule both τ and its integral are divergent and can not be used to calculate the angle of rotation between two ends of a molecule; the usual link between writhe and the torsion is lost at non-zero temperatures.

Rather than choosing the Frenet frame we can instead *define* a frame based on the tangent $\mathbf{t}(s)$ and an arbitrary initial vector $\mathbf{n}(0)$, perpendicular to $\mathbf{t}(0)$,

and thus part of the tangent space of \mathcal{S}_2 . As we move along the chain we let $\mathbf{n}(s)$ evolve by parallel transport on \mathcal{S}_2 . This definition of the frame is entirely analogous to that used in the description of geometric phases in optics: When polarized light is sent down an optical fibre^{5,6} with local tangent $\mathbf{t}(s)$, the polarization vector $\mathbf{n}(s)$ which is perpendicular to $\mathbf{t}(s)$ also evolves by parallel transport. Berry has shown that in this problem the rotation of the plane of polarization of the light is given by the area enclosed by the trajectory $\mathbf{t}(s)$ on the sphere, a result entirely analogous to that of Fuller for the writhe of DNA. We see at once that Fuller's result is equivalent to the geometric phase for photons. The advantage of this formulation using a parallel transport frame rather than the Frenet frame is that it remains valid even for trajectories which are non-smooth as is the case for DNA.

For short molecules the sphere \mathcal{S}_2 can be approximated by its tangent space, so that the probability distribution of writhe for an open molecule tends to the Levy distribution⁷ for area enclosed by a random walk. This distribution is non-Gaussian, with exponential wings.

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References

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