

## Topological Defects in Twisted Bundles of Two-Dimensionally Ordered Filaments

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Twisted assemblies of filaments in ropes, cables, and bundles are essential structural elements in both macroscopic materials and living organisms. We develop the unique, nonlinear elastic properties of twisted filament bundles that derive from generic properties of two-dimensional line-ordered materials. Continuum elasticity reveals a formal equivalence between the elastic stresses induced by bundle twist and those induced by the positive curvature in thin, elastic sheets. These geometrically induced stresses are screened by fivefold disclination defects in the lattice packing, and we predict a discrete spectrum of elastic-energy ground states associated with integer numbers of disclinations in cylindrical bundles. Finally, we show that elastic-energy ground states are extremely sensitive to the defect position in the cross section, with off-center disclinations driving the entire bundle to buckle and writhe.

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From the textile fibers in our clothing to the steel cables that suspend the Brooklyn Bridge, twisted filament assemblies are familiar structural elements of everyday life. This deceptively simple geometric motif, a dense packing of helical filaments with a constant pitch and varying radius, underlies several unique mechanical properties of ropes and fibers. The twist of a rope or yarn transmits tension to lateral compression, binding together multiple short strands into a single cohesive element of arbitrary length [1]. For the case of wire ropes, composed of continuous filaments, a helical pretwist allows one to build a material with a high tensile strength while maintaining remarkable flexibility from an assembly of relatively inextensible elements [2]. It is not surprising that nature has evolved many ways to take advantage of the mechanical fidelity of ropes, at much smaller length scales, by way of supermolecular assemblies of protein filaments in living organisms. Bundles of cytoskeletal filaments, *f*-actin or microtubules, are implicated in a variety of cellular processes in eukaryotic life, from cell division to mechanosensing [3]. Fibers of extracellular proteins, like collagen, are ubiquitous mechanical components of plant and animal tissue [4]. Because biological filaments are helically structured molecules, intermolecular forces between densely packed filaments generate intrinsic torques in bundle assemblies. Indeed, there is clear evidence of spontaneous twisting of a variety biological filament bundle types [5–7], pointing to yet another function of twist in these self-organized bundles. The frustration between two-dimensional packing and interfilament twist generically gives rise to a mechanism of self-limited radial bundle growth [8–10], suggesting that spontaneous bundle twist plays a necessary role in shaping the structure and mechanics of biological filament assemblies.

While mechanical considerations of ropes and fibers date back to as early as Galileo, very little is known about the role that the cross-sectional ordering plays in determining the global elastic properties of twisted bundles. In this

Letter, we describe a continuum approach to the unique, nonlinear elasticity of two-dimensionally (2D) ordered filament bundles, revealing a fundamental coupling between the presence and location of topological defects in the lattice packing and the global twist of the bundle. We discover a precise equivalence between the in-plane stresses created by twisting a bundle and the long-range stresses introduced into a 2D elastic sheet by forcing it to adopt a spherically curved geometry. Because of the accumulation of elastic stresses, we show that a sufficiently large and twisted bundle becomes energetically unstable to the incorporation of a finite number of fivefold disclination defects in its cross section. We predict a spectrum of discrete low-elastic-energy states of twisted bundles, associated with an integer number of disclinations as a function of increasing bundle twist. Finally, we show that the global geometry of the low-energy states of bundles is extremely sensitive to the location of disclinations in the cross section. Displacing a disclination from the bundle center leads to a complex class of structures that buckle, writhing out of the plane, ultimately folding the entire bundle into a compact helical configuration.

Consider a bundle of semiflexible filaments of infinite length that is organized into a regular array perpendicular to mean filament orientation along the  $\hat{z}$  direction. Interactions between filaments favor a constant neighbor spacing,  $d_0$ , much smaller than the radius of the bundle,  $R$ , which is approximately cylindrical in shape. The zero energy state of these interactions is a hexagonal packing of straight filaments. Deviations from the uniform spacing as well as filament bending are described by the energy [10],

$$E = \frac{1}{2} \int d^3x \{ \lambda (u_{ii})^2 + 2\mu u_{ij}u_{ij} + K_b [(\hat{\mathbf{t}} \cdot \nabla) \hat{\mathbf{t}}]^2 \}. \quad (1)$$

Here,  $\lambda$  and  $\mu$  are elastic constants that penalize compressive and shear distortions of the array and  $u_{ij}$  is the elastic strain tensor of the 2D filament bundle. This strain is constructed from displacements of filament positions,

$\mathbf{u}(\mathbf{x})$ , in the  $xy$  plane, and the projection of the local filament orientation,  $\hat{\mathbf{t}}(\mathbf{x})$ , into the  $xy$  plane,

$$u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i - t_i t_j). \quad (2)$$

The nonlinear contribution to strain from filament tilt is a direct consequence of the invariance of the elastic energy under rotation about an axis in the  $xy$  plane [11], and can be intuitively understood to measure distances between neighbor filaments perpendicular to the filament tangent, that is, the distance of closest approach. The final term in  $E$  describes the bend elasticity of filaments, with  $K_b$  proportional to the stiffness of filaments.

To study low-energy configurations of twisted filament bundles possessing defects in cross-sectional order, we focus on configurations for which the shear and compressive contributions to Eq. (1) are constant along filaments. In these structures,  $\mathbf{u}(\mathbf{x})$  and  $\hat{\mathbf{t}}_\perp(\mathbf{x})$  differ along  $z$  only by uniform rotations around an axis in the  $xy$  plane, and at some reference plane ( $z = 0$ ), the in-plane tilt field is described by  $\hat{\mathbf{t}}_\perp(\mathbf{x}) \simeq \mathbf{\Delta} + \Omega(\hat{\mathbf{z}} \times \mathbf{x})$  where  $\mathbf{x} = 0$  is the center of the bundle,  $\mathbf{\Delta}$  is a constant tilt in the plane, and  $\Omega$  is the rate of torsion. Initially, we restrict our analysis to  $\mathbf{\Delta} = 0$ , in which filaments wind around the geometrical center of the bundle.

For fixed  $\Omega$ , configurations are determined by  $\partial_i \sigma_{ij} = 0$  subject to stress-free boundary conditions at the surface of the bundle. As we have reduced the problem to solving for the stress  $\sigma_{ij} = \delta E / \delta u_{ij}$  in a single 2D plane, it is convenient to determine the stress tensor in terms of an Airy stress function,  $\chi$  [12]. By construction,  $\sigma_{ij} = \epsilon_{ik} \epsilon_{jl} \partial_k \partial_l \chi$  is divergenceless, and the Airy stress is determined by the ‘‘compatibility relation,’’ which relates  $\chi$  to the definition of elastic strain, Eq. (2),

$$K_0^{-1} \nabla_\perp^4 \chi = \sum_\alpha s_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) - \frac{1}{2} \nabla_\perp \times [(\nabla_\perp \times \hat{\mathbf{t}}_\perp) \hat{\mathbf{t}}_\perp - (\hat{\mathbf{t}}_\perp \times \nabla_\perp) \hat{\mathbf{t}}_\perp], \quad (3)$$

where  $K_0 = 4\mu(\lambda + \mu)/(\lambda + 2\mu)$  and  $\nabla_\perp \times \hat{\mathbf{t}}_\perp = \epsilon_{ij} \partial_i t_j$  is the 2D curl. Here,  $s_\alpha = \pm 2\pi/6$  denotes the topological charge of a disclination at position,  $\mathbf{x}_\alpha$ , in the cross section of the bundle where the local bond angle,  $\theta(\mathbf{x}) = \epsilon_{ij} \partial_i u_j / 2$ , rotates around singular points. Disclinations represent lattice sites of five- (positive) and sevenfold (negative) symmetry in the otherwise sixfold symmetric packing. The second line of Eq. (3) describes the nonlinear contribution from in-plane tilts to the strain in the bundle, deriving from the fact that in 2D ordered chains, twisted configurations of tangents necessarily introduce gradients in nearest neighbor orientation, lying in a perpendicular plane [13]. For the case of a twisted bundle where  $\nabla_\perp \times \hat{\mathbf{t}}_\perp = \pm 2\Omega + \mathcal{O}[(\Omega r)^3]$ , the second line reduces to  $-K_{\text{eff}} = -\epsilon_{ij} \epsilon_{kl} \partial_i \partial_k t_j t_l / 2 = -3\Omega^2$ , a uniform and negative source of Airy stress in the bundle.

An analogous compatibility equation describes the nonlinear elasticity of 2D crystalline membranes, known as the

Föppl–von Kármán theory of thin plates [12]. In that case, the coupling between in-plane strain and out-of-plane bending generates a source of the Airy stress,  $-K$ , where  $K$  is the Gaussian curvature of the surface. Hence, we find the surprising result that the twist of the filament bundle generates precisely the same source of stress as stretching a 2D elastic sheet over a positively curved, spherical surface of radius  $R_{\text{eff}} = (\sqrt{3}\Omega)^{-1}$ . Seung and Nelson showed that the far-field stresses created by Gaussian curvature in 2D crystalline membranes are precisely of the form to be ‘‘screened’’ by the presence of pointlike disclination defects in the membrane [14]. For the case of 2D filament bundles, Eq. (3) shows that positively charged, fivefold disclinations are able to partially screen the elastic stresses of twisted bundles.

The elastic energy of twisted bundles with an arbitrary distribution of disclinations can be computed by solving Eq. (3) for  $\chi$  subject to vanishing normal stress at  $r = R$  by multipole expansion [15]. These expansions can be summed to compute the effective theory for the elastic energy,

$$\frac{E}{VK_0} = \sum_\alpha \frac{s_\alpha^2}{32\pi^2} \left(1 - \frac{\rho_\alpha^2}{R^2}\right)^2 - \frac{3(\Omega R)^2}{2} \sum_\alpha \frac{s_\alpha}{32\pi} \left(1 - \frac{\rho_\alpha^2}{R^2}\right)^2 + \frac{3(\Omega R)^4}{128} \left(1 + \frac{3}{32\gamma}\right) + \frac{1}{2} \sum_{\alpha \neq \beta} s_\alpha V_{\text{int}}(\mathbf{x}_\alpha, \mathbf{x}_\beta) s_\beta, \quad (4)$$

where  $V$  is the volume of the bundle and  $\rho_\alpha$  is the radial distance the  $\alpha$ th disclination. The first term describes the self-energy of a disclination in the bundle, which, notably, has the same radial dependence as the interaction between disclinations and twisted-induced stress described by the second term. The third term describes the twist dependence of elastic energy in the defect-free state, where  $\gamma \equiv K_0 R^2 / K_b$ , that measures the relative importance of in-plane elastic energy to bend elasticity. The final term gives the effective interaction between disclination pairs in cylindrical crystals,

$$V_{\text{int}}(\mathbf{x}_\alpha, \mathbf{x}_\beta) = \frac{1}{16\pi^2} \left(1 - \frac{\rho_\alpha^2}{R^2}\right) \left(1 - \frac{\rho_\beta^2}{R^2}\right) + \frac{|\mathbf{x}_\alpha - \mathbf{x}_\beta|^2}{8\pi^2 R^2} \ln \left( \frac{|\mathbf{x}_\alpha - \mathbf{x}_\beta|}{|\mathbf{x}' - \mathbf{R}|} \right), \quad (5)$$

where  $|\mathbf{x}' - \mathbf{R}|^2 = R^2 + \rho_\alpha^2 \rho_\beta^2 / R^2 - 2\rho_\alpha \rho_\beta \cos\theta$ , with  $\theta$  the angular separation between disclinations  $\alpha$  and  $\beta$ . The minimum-energy configurations of bundles with fivefold ( $s_\alpha = +2\pi/6$ ) disclinations are shown in Fig. 1 for  $\Omega R \leq 1.25$  and for negligible bending energy,  $\gamma^{-1} = 0$ . For these results we find that the elastic energy of a filament bundle is unstable to the incorporation a finite number of disclinations when the twist of a bundle exceeds  $|\Omega_c R| = \sqrt{2/9} \simeq 0.471$ , at which point the lowest energy is accomplished by placing a single fivefold defect at the center. Upon further twist, this single defect structure gives way to lower-energy states with 2, 3, 4, 5, ... disclinations.

Evidently, along with crystals on curved surfaces, twisted bundles belong to the unusual class of frustrated materials in which defects are necessary components of ground state configurations. We note that although sevenfold disclinations are not necessary to screen the twist-induced stresses in a bundle, we expect these defects to appear in low-energy configurations when  $R \gg d_0$ . On large spherical crystals [16] fivefold disclinations are unstable to breaking up into extended strings of alternating five- and sevenfold defects of a net positive charge, so-called grain boundary scars. By analogy, we anticipate similar extended defect configurations in the elastic-energy ground states of large twisted bundles.

The elastic energy in Eq. (4) demonstrates an important and previously unknown coupling between the in-plane stresses created by lattice defects and bundles twist: fivefold disclinations screen the twisted-induced stresses and vice versa. Hence, the elastic energy of bundles with an excess of fivefold disclinations (relative to sevenfold) can always be lowered by twisting a finite amount. The right- or left-handed spontaneous twist of a bundle is the analog of the upward or downward buckle of a crystalline membrane induced by the presence of fivefold defects in the hexagonal order [14]. The degree of “torsional buckling” is sensitive to the relative costs of filament bending and in-plane elastic energies. We find that an optimal degree of twist,  $\Omega_1$ , for a bundle with a single centered, fivefold disclination has the form  $(\Omega_1 R)^2 = (3 + 32/\gamma)^{-1}$ . For small bundles of rigid filaments,  $\gamma \rightarrow 0$ , the pitch of the bundle is sensitive to the bending of the elastic moduli and insensitive to size,  $2\pi/\Omega_1 \propto \sqrt{K_0/K_b}$ . While for bundles much larger than this characteristic size,  $\gamma \rightarrow \infty$ , the tilt angle of the outer filament is predicted by the continuum theory to achieve a universal value,  $\Omega_1 R \rightarrow \sqrt{1/3} \approx 0.577$ .

We now consider filament bundles for which  $\Delta \neq 0$ , with successive vertical layers rotated and shifted by a constant amount in the  $xy$  plane. From the continuum theory we derive the mean torque on the filaments due to the presence of twist- and defect-induced stress,

$$\begin{aligned} \frac{\partial E}{\partial \Delta i} &= - \int d^3x \sigma_{ij} t_j \\ &= - \frac{VK_0\Omega}{8\pi} \sum_{\alpha} s_{\alpha} \left[ 1 - \frac{\rho_{\alpha}^2}{R^2} - 2 \frac{\rho_{\alpha}^2}{R^2} \ln\left(\frac{\rho_{\alpha}}{R}\right) \right] (\hat{z} \times \mathbf{x}_{\alpha})_i, \end{aligned} \quad (6)$$

where  $\sigma_{ij}$  is the stress in the  $\Delta = 0$  state. Hence, in a bundle with a single off-center, fivefold defect, the elastic energy decreases most rapidly by tilt in a direction  $\pi/2$  away from the radial location of the dislocation. When  $\Delta \neq 0$ , the center of rotation in the bundle is not the central filament, and Eq. (6) shows that this rotation center, for which  $\hat{\mathbf{t}}_{\perp}(\mathbf{x}) = 0$ , migrates from the bundle center towards the off-center disclination by a distance  $|\Delta|/\Omega$ , demonstrating that the low-energy state of the bundle adopts a globally writhing and helical configuration.

To investigate the ground states of bundles with off-center disclinations, we introduce a discrete, numerical model of cylindrical bundles of fully flexible filaments with preferred hexagonal order. Bundles are described arrays of filaments at positions,  $\mathbf{x}_{\alpha}$ , and filament tangents corresponding to  $\hat{\mathbf{t}}_{\perp}(\mathbf{x}) = \Delta + \Omega(\hat{z} \times \mathbf{x})$ . The elastic energy in a vertical cross section of height  $\Delta z$  is constructed following the bead-spring model of Ref. [14],

$$\Delta E = \frac{k}{2} \sum_{\langle \alpha \beta \rangle} (|(\mathbf{x}_{\alpha} - \mathbf{x}_{\beta})_{\perp}| - d_0)^2 \Delta l_{\alpha\beta}. \quad (7)$$

Here,  $k$  parametrizes a harmonic restoring force for distortions in the packing and  $(\mathbf{x}_{\alpha} - \mathbf{x}_{\beta})_{\perp} = \mathbf{x}_{\alpha} - \mathbf{x}_{\beta} - \hat{\mathbf{t}}(\mathbf{x}_{\alpha} - \mathbf{x}_{\beta}) \cdot \hat{\mathbf{t}}$  is the projection of the filament spacing perpendicular to the local tangent direction, thereby measuring distances of closest approach for weakly bent filaments. The interactions are weighted the lengths of elements  $\Delta l_{\alpha\beta} = \Delta z (\hat{\mathbf{t}} \cdot \hat{z})^{-1}$  which vary with in-plane tilt in the cross section. To study the ground states numerically, we generate a fivefold disclination in an unrelaxed, infinite hexagonal array. This disclination is offset to a distance,  $\rho$ , from the center of the bundle at a given azimuthal angle. Lattice positions within a radial distance,  $r \leq R = 10d_0$ , are triangulated and used as initial in-plane coordinates of filaments in the bundle. The elastic energy per total filament length is numerically minimized by relaxing filament positions,  $\Omega$  and  $\Delta$ .

The geometry of energy-minimizing configurations is plotted in Fig. 2 in terms of the rate of torsion,  $\Omega$ , and the helical radius of the geometric center of the bundle,  $r_h$ , both of which reveal a striking sensitivity of global bundle geometry of the bundle to disclination position. The center of helical rotation migrates rapidly from  $r_h = 0$  when  $\rho = 0$  to a position nearly at the boundary of bundle,  $r_h \approx 9.7d_0$  when  $\rho = 5d_0$ , adopting a globally helical conformation. More surprising, the degree of spontaneous rotation,  $\Omega$ , steeply increases as the disclination position is offset from the bundle center. The helical pitch of the bundle decreases

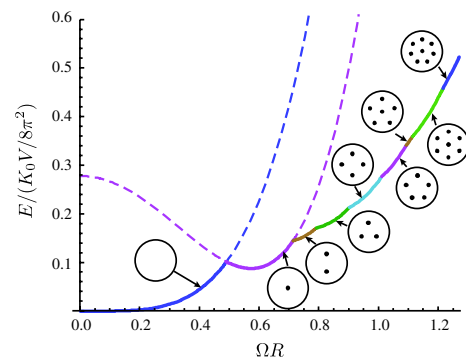


FIG. 1 (color online). Solid curves show the elastic energy of 2D bundle ground states as a function of twist times bundle radius,  $\Omega R$ , for  $K_b = 0$ . The cartoons depict the energy-minimizing configurations of multiple fivefold disclinations. The dashed lines show the metastable branches of the disclination-free and single-disclination bundle energy.

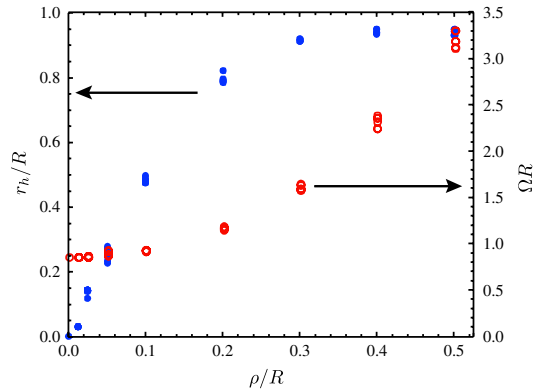


FIG. 2 (color online). The ground state geometry of the elastic energy of Eq. (7), for  $R = 10d_0$  bundles possessing a single disclination at radius  $\rho$ . The filled, blue circles show the helical radius of the geometrical center of the bundle and the open, red circles show the rate of torsion around the  $z$  axis. The data for each  $\rho$  correspond to disclinations at 6 azimuthal angles:  $0, \pm 2\pi/6, \pm 4\pi/6, \text{ and } \pi$ .

more than threefold as the disclination is moved from  $\rho = 0$  to  $\rho = 5d_0$ . Remarkably, the writhing and contorted bundle geometries shown in Fig. 3 provide a more uniform filament spacing than can be achieved in straight bundles. For disclinations at radial positions,  $\rho \geq 6d_0$ , we find that bundle ground states are self-intersecting and, therefore, cannot be modeled without the inclusion of either bend elasticity or excluded-volume constraints.

In summary, we have demonstrated a coupling between nonlinear elastic stresses that arise from the twisting of a

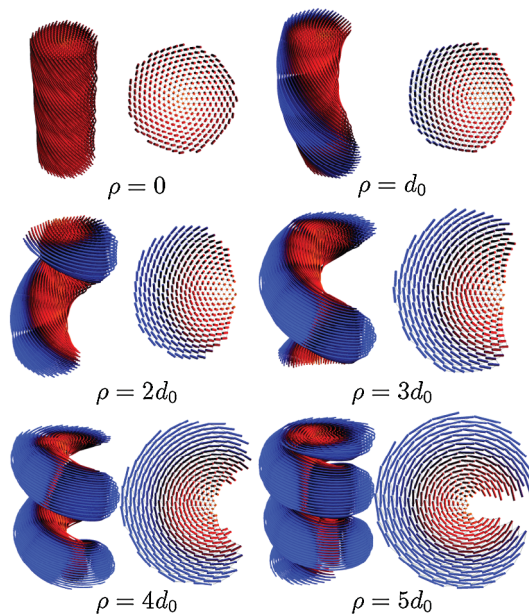


FIG. 3 (color). Cross-sectional (constant  $z$ ) and side views of energy-minimizing bundles for the disclination positions,  $\rho \leq 5d_0$ . Filament colors correspond to radial distance from center of rotation in the  $xy$  plane, from yellow  $r = 0$  to blue  $r = 20d_0$ .

filament bundle and orientational defects in the lattice packing. Thus, fivefold disclinations are necessary components of low-energy configurations of sufficiently twisted and large bundles of continuous filaments. We expect this finding to be particularly relevant to the self-assembled bundles and fibers of biological filaments, whose chiral molecular structure leads to a generic preference for inter-filament twist in compact assemblies. Indeed, cylindrical collagen fibrils derived from certain tissue types show pronounced twist, along with considerable evidence from small-angle scattering of localized disorder in their cross-sectional organization [6,17]. In light of these observations, we speculate that the unique properties of these self-organized collagen fibrils—the well-defined diameter, the twisted structure, and their “almost crystalline” order—may all find a common origin in generic properties of the nonlinear elasticity of filament assemblies.

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