

Mechanics of disclination emergence in three-dimensional active nematics

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Active nematics have served as model systems for studying defect dynamics for decades, yet the general mechanism of defect formation in three dimensions (3D) remains unclear. Here, we introduce the principal-plane framework to study disclination-loop nucleation in 3D active nematics. This approach intuitively captures the 3D director field around disclinations and connects perturbative instability analysis with geometric characterization. With particle-based simulations, we further reveal that disclinations arise from the bend instability, while their tilt reflects the competition between activity and elasticity. We show that an activity-dependent effective stiffness $\kappa_{\text{eff}} = \kappa / (1 + 2f_a^2)$ governs both defect morphology and the system's steady behavior. Together, these results establish a unified picture of disclination-loop emergence and provide design principles for controlling defect-driven dynamics in orientational materials.

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I. INTRODUCTION

Topological defects are key to understanding structure in ordered media [1,2]. In nematic liquid crystals, disclinations induced by external fields or boundaries reveal the geometry and energy distribution of the director field [3]. Recently, there has been much attention paid to defects in active nematics, where self-driven nematogens break local time-reversal symmetry and drive the system out of equilibrium [4–7]. This interest arises for two reasons. First, activity overcomes energy barriers and enables the spontaneous creation of disclinations, which does not occur in passive systems. Second, this continual defect generation makes active nematics a uniquely fertile setting for studying general defect mechanics.

In two-dimensional (2D) nematics, the dominant topological features are point defects, whose energy, interactions, and morphology have been extensively investigated in both passive [2] and active [8] systems. In three dimensions (3D), defects mainly appear as disclination lines, with far richer topological properties [1,5,9–12], complex structures [5,13–20], and dynamic evolution [5,13–15,21–24]. Yet, a fundamental question, how initial disclination loops emerge in 3D active nematics, has been examined only in restricted or simplified cases [5,13,17,25], leaving the general mechanisms largely uninvestigated.

One major challenge in studying the onset of defect loops is interpreting the complex 3D director field $\hat{\mathbf{n}}$ around them. Currently, two main approaches address this problem. The first examines the $\hat{\mathbf{n}}$ field along normal cross sections

intersecting nascent loops [2,3,5,13,25,26] [Fig. 1(a)]. This method resolves the local geometry of $\hat{\mathbf{n}}$ along the loop but offers little insight into the structure at the scale of the loop. The second analyzes continuum theories of active nematics via perturbation methods to identify unstable modes of $\hat{\mathbf{n}}$ [17,25,27,28]. Although this approach captures global features of the $\hat{\mathbf{n}}$ field, it lacks explicit defect information and is difficult to compare with observed defects.

In this Article, we propose an approach bridging the two methods above. As in earlier work, we analyze $\hat{\mathbf{n}}$ through cross sections of initial loops, but instead of normal sections, we introduce *principal planes*, a class of coordinate systems that inherently reflect the surrounding $\hat{\mathbf{n}}$ field. As we show, this natural coordinate system allows us to identify an approximately 2D configuration on each principal plane for 3D loops, offering an intuitive and coherent view of the overall $\hat{\mathbf{n}}$ structure near the loop. Moreover, the definition of principal planes directly links to the local perturbation analysis of $\hat{\mathbf{n}}$, enabling immediate comparison with continuum theory.

To study defect-loop nucleation in 3D active nematics, we apply our framework to large-scale particle-based simulations of active semiflexible polymers. This approach avoids parameter ambiguities of continuum models, while still providing cleaner and better resolved data than experiments. With principal planes, we develop a 2D-analog theory extending prior limited cases. Our simulations show that the phenomenology is predominantly governed by a microscopic parameter, κ_{eff} , which sets the competition between the timescales of loop nucleation and twist deformations. This framework can be regarded as a descriptive language to capture the universal mechanism of loop emergence in 3D active nematics.

II. INSTABILITY

We consider the emergence of an isolated disclination loop from a uniform ordered background. The initial state is characterized by uniform director $\hat{\mathbf{n}}_0$. Under activity or external fields, $\hat{\mathbf{n}}$ deforms and undulates, eventually overcoming the

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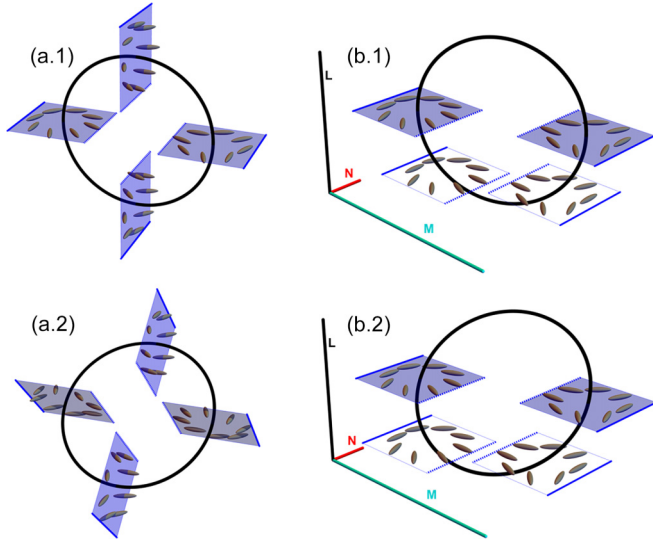


FIG. 1. Schematic comparing initial defect loops in two views: (a) normal cross sections and (b) principal planes. Loops in each row correspond to the same surrounding $\hat{\mathbf{n}}$ field. In the first row, variations of $\hat{\mathbf{n}}$ along the planes arise solely from the separation between the in-plane 2D defects pair, so the loop is perpendicular to the principal planes. In contrast, the second row exhibits an added twist deformation from a shear of the principal planes, thereby tilting the loop.

elastic energy barrier to form defects that, due to the topological constraints of 3D nematic field, can only appear as small loops [2,3].

We now outline the perturbative framework, where the concept of principal planes also emerges. Since $\hat{\mathbf{n}}$ is weakly deformed before loop nucleation, we assume small fluctuations around $\hat{\mathbf{n}}_0$, mainly along a spontaneously chosen perturbation $\delta\hat{\mathbf{n}}$. Thus, we obtain $\hat{\mathbf{n}} \approx \hat{\mathbf{n}}_0 + \epsilon(\mathbf{r}, t)\delta\hat{\mathbf{n}}$, with $\epsilon \ll 1$. With the Fourier expansion of the perturbation, $\epsilon(\mathbf{r}, t) = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}(t) \sin(\mathbf{k} \cdot \mathbf{r})$, the time-evolution equation extracted to leading order in ϵ yields the conditions under which these perturbations evolve.

For example, in this Article we focus on 3D dry extensible active nematics, whose dynamics results from a balance between Stokesian friction and active stress: $\zeta \mathbf{v} = \nabla \cdot \sigma_a$, with $\sigma_a = -\alpha \hat{\mathbf{n}} \hat{\mathbf{n}}$ and active strength $\alpha > 0$ [29]. For high-aspect-ratio nematogens, $\hat{\mathbf{n}}$ obeys the Leslie-Erickson equation [2]: $\partial_t \hat{\mathbf{n}} = \mathbf{\Omega} \cdot \hat{\mathbf{n}} + \mathbf{E} \cdot \hat{\mathbf{n}} + \mu \nabla^2 \hat{\mathbf{n}}$, where $\mathbf{\Omega} = [(\nabla \mathbf{v})^T - \nabla \mathbf{v}]/2$ and $\mathbf{E} = [(\nabla \mathbf{v})^T + \nabla \mathbf{v}]/2$ are the vorticity and strain-rate tensors, and $\mu \nabla^2 \hat{\mathbf{n}}$ penalizes deformations. The linearized perturbation equation is $\partial_t \epsilon_{\mathbf{k}}(t) = [\alpha \cos^2(\hat{\mathbf{k}} \cdot \hat{\mathbf{n}}_0) - \mu] \|\mathbf{k}\|^2 \epsilon_{\mathbf{k}}(t)$, which implies a competition between torques of activity $\sim \alpha$ and elasticity $\sim \mu$ and $\hat{\mathbf{k}} = \mathbf{k}/\|\mathbf{k}\|$. The growth rate peaks at $\hat{\mathbf{k}} = \hat{\mathbf{n}}_0$, corresponding to the bend mode [3], consistent with previous findings [4,8,25,27,30]. Details of the instability analysis and continuum model are provided in the Supplemental Material [31].

III. PRINCIPAL PLANES

The instability further deforms the $\hat{\mathbf{n}}$ field and generates defects. Once an initial loop forms, we consider a small box

enclosing it. The second moment of $\hat{\mathbf{n}}(\mathbf{r})$ within this box, $\langle \hat{\mathbf{n}} \hat{\mathbf{n}} \rangle_{\text{box}}$, has eigenvectors $\hat{\mathbf{N}}$, $\hat{\mathbf{M}}$, and $\hat{\mathbf{L}}$ corresponding to the largest, intermediate, and smallest eigenvalues. $\hat{\mathbf{N}}$ represents the average orientation of $\hat{\mathbf{n}}$ within the box and approximates $\hat{\mathbf{n}}_0$ [2], as the loop remains confined by the ordered background. Likewise, $\hat{\mathbf{M}} \approx \delta\hat{\mathbf{n}}$ captures the main deviation of $\hat{\mathbf{n}}$ from $\hat{\mathbf{n}}_0$. Although the $\epsilon \delta\hat{\mathbf{n}}$ term in $\hat{\mathbf{n}}$ is no longer small because $\hat{\mathbf{n}}$ rotates by π around defects, the component along $\hat{\mathbf{L}}$ can still be neglected; otherwise, substantial deformation would occur. This assumption is supported by observations from our simulations discussed later. Consequently, the directors predominantly form 2D patterns within the $\hat{\mathbf{N}}-\hat{\mathbf{M}}$ planes, which we define as the *principal planes* [see examples in Fig. 1(b)]. Scanning the loops along these planes therefore enables a quasi-2D view of the 3D $\hat{\mathbf{n}}$ field, revealing its dominant features (see Video S3 in the Supplemental Material [31]).

Furthermore, the wave vector $\mathbf{k}$ from the perturbation analysis can also be represented by principal planes. Variations in $\hat{\mathbf{n}}$ across planes are minimized if $\mathbf{k}$ lies within the principal planes. In this case, defect positions on different planes remain similar, differing only in the spacing between defect pairs on each plane [Figs. 1(a.1) and 1(b.1)]. When $\mathbf{k}$ deviates from principal planes, and assuming defect shapes vary little across planes due to elastic cost, the variation in $\hat{\mathbf{n}}$ manifests as relative shifts in defect positions, effectively shearing the structure and tilting the loop [Figs. 1(a.2) and 1(b.2)].

In summary, the principal-plane framework interprets the 3D $\hat{\mathbf{n}}$ field around disclination loops through the defect morphologies observed on successive principal planes and the resulting loop tilt. It further enables direct comparison with perturbative analysis in continuum theories.

IV. SIMULATION MODEL

Using the principal-plane framework, we study particle-based simulation results of 3D active nematics to unpack the mechanism of emergence of initial disclination loops in this system. The simulations, built on our earlier 2D model, capture the collective dynamics of active semiflexible filaments and preserve the essential behaviors and symmetries of active nematics [32]. Each filament is modeled as a bead-spring chain, with the monomer coordinates $\mathbf{r}_i$ governed by a Langevin equation of the form $m \ddot{\mathbf{r}}_i = \mathbf{f}_{a,i} - \xi \dot{\mathbf{r}}_i - \nabla_{\mathbf{r}_i} U + \mathbf{R}_i(t)$, where $\mathbf{f}_{a,i}$ is the active force for i th monomer, $\mathbf{R}$ is a Gaussian thermal noise with variance $6\xi k_B T$, U is the potential energy, and ξ is the friction coefficient. The coefficients of these terms are chosen such that inertia relaxes much faster than all other timescales, rendering the system overdamped (see Supplemental Material [31]). The stiffness of filaments is given by the pairwise additive potential $\bar{\kappa}(\pi - \vartheta)^2$, where ϑ is the angle between adjacent bonds and $\bar{\kappa}$ is the elastic modulus. $\mathbf{f}_a$ is modeled by self-propulsion on each monomer directed along the local filament tangent $\hat{\mathbf{t}}$ with $\|\mathbf{f}_a\| = \bar{f}_a b$, where $\bar{f}_a$ is the strength of activity and b is the bond length. The nematic symmetry of activity is ensured by reversing $\mathbf{f}_a$ in random time intervals, synchronously for all monomers within each filament (see Supplemental Material [31]). Figures 2(a) and 2(b) show an active filament and a schematic representation of the bead-spring model. To integrate the Langevin dynamics, we modified LAMMPS [33] to include activity [34].

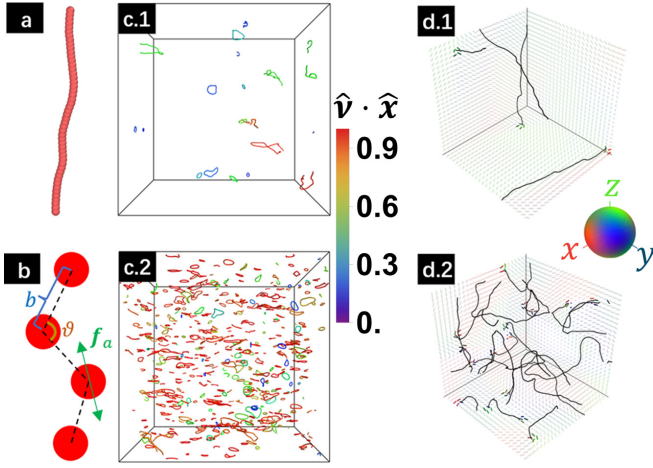


FIG. 2. The microscopic model and phenomenology. (a) Illustration of an active filament. (b) Schematic of the filament model, where nematic active forces act along the local tangent (see Videos S1(a)–S1(c) in the Supplemental Material [31]). (c) Initial disclination loops, colored by the alignment between the loop’s normal $\hat{\mathbf{v}}$ and the direction of initial order $\hat{\mathbf{x}}$. (d) Steady state: Enlarged views of the disclination network at long times, with directors on the boundary planes color coded by orientation. (c.1), (d.1) Activity and stiffness $f_a = 1500$, $\kappa = 2$ (effective stiffness $\kappa_{\text{eff}} \equiv \kappa/(1 + 2f_a^2) = 167.8$). (c.2), (d.2) $f_a = 1500$, $\kappa = 3.5$ ($\kappa_{\text{eff}} = 58.8$). All parameters are reported in dimensionless units defined in Sec. IV.

In this Article, we employ the LJ units, where length, energy, and mass units are set by the monomer diameter σ , $k_B T$, and monomer mass m , respectively. To probe the instability, we initialize the system in an aligned nematic state and simulate a broad range of stiffness and activity values, reported in dimensionless form as $\kappa \equiv \bar{\kappa}/k_B T \in [100, 1500]$ and $f_a \equiv \bar{f}_a \tau / \xi \in [1-10]$, covering steady states from chaotic to nearly static flow. For analysis, we coarse grain the system into the tensor order parameter field $\mathbf{Q}$, whose largest eigenvalue and eigenvector defines order S and director $\hat{\mathbf{n}}$. Details of the coarse graining and parameter choices are given in the Supplemental Material [31].

V. PHENOMENON

The initially ordered system evolves through three stages. (1) *Instability*: filaments deform and reorient, causing a drop of the order parameter S . (2) *Loops*: local director distortions further grow and generate disclination loops [Fig. 2(c)]. (3) *Isotropy*: the disclinations merge into dynamical networks [Fig. 2(d)], leading to the steady state, which has stationary statistics and is independent of the initial condition [31].

Our previous 2D studies showed that the macroscopic behavior of the nematic field is governed by a single parameter, the activity-dependent stiffness κ_{eff} , hereafter termed the *effective stiffness*. We confirm that this result also holds in 3D, with $\kappa_{\text{eff}} = \kappa/(1 + 2f_a^2)$, as macroscopic quantities expressed in κ and f_a collapse onto a single curve defined by κ_{eff} (Fig. 3). We therefore focus on how loop emergence depends on κ_{eff} . Heuristically, κ_{eff} reflects filament softening by both thermal noise $\sim k_B T$ (1 in our units) and active stress $\sim f_a^2$. The latter scale as the product of active force $\sim f_a$ and collision

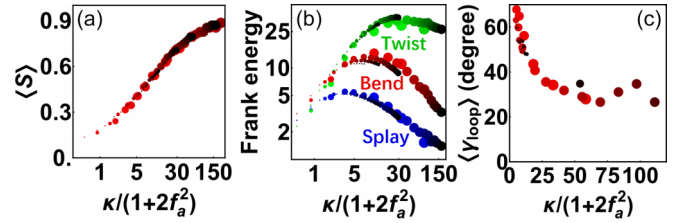


FIG. 3. (a), (b) Mean order parameter S and the total Frank elastic deformation, both analyzed in the steady state. (c) Average γ of all initial loops. These values collapse with effective stiffness κ_{eff} . Darker points indicate higher stiffness and larger points indicate lower activity.

frequency $\sim f_a/l$, where l is the mean spacing between microunits. Details of the statistical analysis are provided in the Supplemental Material [31].

VI. INITIAL DISCLINATIONS

We propose a unified picture of bend-induced loop formation via principal-plane scans, based on our simulation observations. Figure 4(a) shows that loops stem from the bend instability, consistent with our perturbation analysis. Given that active forces are extensile and aligned with $\hat{\mathbf{n}}$, bending induces a unit active force approximately along $\hat{\mathbf{M}}$, distorting the field and creating a pair of $\pm 1/2$ 2D-like defects on each principal plane [Fig. 4(b)]. Defects on successive planes collectively connect to form the initial disclination loop.

We now discuss the dependence of initial loops on κ_{eff} in our observations. At low κ_{eff} , variations of $\hat{\mathbf{n}}$ along the principal planes appear only through the spacing between the 2D defects within each plane, making the loop perpendicular to the principal planes [Fig. 4(b.1)]. At high κ_{eff} , defect positions differ, tilting the loop [Fig. 4(b.2)]. As discussed previously, this tilt implies that the dominant wave vector $\hat{\mathbf{k}}$ approaches $\hat{\mathbf{L}}$ as κ_{eff} grows. We quantify this tilt by the topological parameter γ , the angle between the loop normal $\hat{\mathbf{v}}$ and the rotation vector $\hat{\Omega}$, which is defined as the axis that the surrounding directors rotate along [5]. Since $\hat{\mathbf{n}}$ forms a quasi-2D structure, $\hat{\Omega}$ is nearly normal to the principal planes and aligned with $\hat{\mathbf{L}}$. Consequently, at large κ_{eff} , the loop tilt shifts $\hat{\mathbf{v}}$ away from the principal planes and reduces γ . Figure 4(c) and Video S4 in the Supplemental Material [31] illustrate loop emergence and tilt mechanics. Across simulations, the average $\langle \gamma \rangle$ collapses onto a single, monotonically decreasing curve as a function of κ_{eff} [Fig. 3(c)].

This tilt configuration can also be described by additional twist. At high κ_{eff} , the significant variations of $\hat{\mathbf{n}}$ across principal planes reflect effective shear. This deformation, where $\hat{\mathbf{n}}$ differs across planes within the quasi-2D structure, represents *twist*, a feature unique to 3D nematics and absent in 2D. Hence, loops at low κ_{eff} arise mainly from the pure-bend mode, whereas those at high κ_{eff} incorporate substantial twist.

Since our system dynamics always starts with the bend instability, we interpret the loop tilt as a competition between two timescales: τ_{nuc} , when the first loop nucleates, and τ_{twi} , when the deformation transitions from bend to other modes. In Fig. 5, the vertical black lines denote τ_{nuc} , which we measured independently, while the curves represent the time

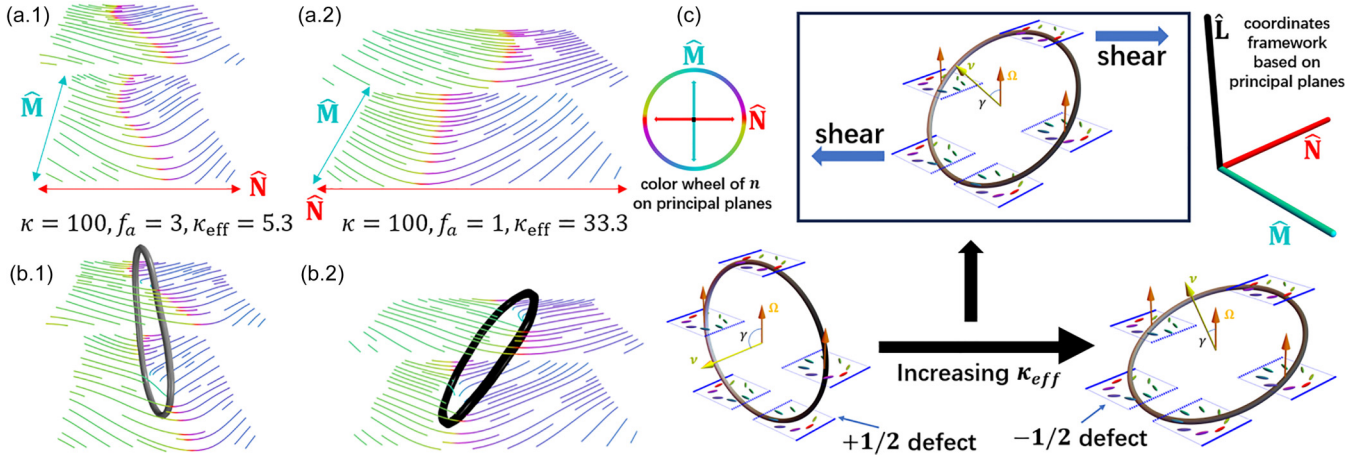


FIG. 4. Phenomenology of the emergence of initial disclination loops. (a) Visualization of $\hat{\mathbf{n}}$ (color coded by orientations) projected onto the principal planes before loop formation, from simulations at $\kappa_{\text{eff}} = 5.3$ (left) and 33.3 (right). (b) The initial loops emerge from the configurations shown in panel (a). Each principal plane exhibits a pair of bend-induced $\pm 1/2$ 2D-like defects. (c) Schematic illustration of the initial loops, showing idealized structures corresponding to panel (b). The diagram highlights how increasing κ_{eff} shears the bend pattern, adds twist, and thereby reduces the angle γ between the loop's normal $\hat{\mathbf{n}}$ and the rotation vector $\hat{\Omega}$. The coordinate frame of the schematic loops and $\hat{\mathbf{n}}$ color wheel are also shown.

dependence of the largest Fourier coefficients of $\mathbf{Q}_{xy}$ and $\mathbf{Q}_{xz}$, which are the leading order terms of the instability, so the peaks of these curves mark τ_{twi} . At low κ_{eff} , the active stress is sufficient to induce defects during bend instability ($\tau_{\text{nuc}} < \tau_{\text{twi}}$), with loops normal to principal planes. In contrast, at high κ_{eff} , larger distortions must build up before defect nucleates. By then, significant twist has developed ($\tau_{\text{nuc}} > \tau_{\text{twi}}$), resulting in tilted loops with smaller γ .

VII. DISCUSSION

The key innovation of this work is the introduction of *principal planes*, as natural coordinate systems that borrow nomenclature from the Frenet framework for curves, to represent $\hat{\mathbf{n}}$ fields near defects particularly in active nematics. Here, “natural” means that our analysis relies solely on *local* information around the loops, unlike earlier studies that implicitly

invoked principal planes but relied on the far-field $\hat{\mathbf{n}}$ pinned by *global* boundary conditions [13,26,35,36]. Our framework thus captures the intrinsic bulk behavior of 3D active nematics and elucidates the *local* mechanisms underlying the spontaneous defect creation. Moreover, because the principal-plane formulation is purely geometric, it applies to any orientational field with small perturbations, making it broadly relevant to disclination loops and lines in systems from passive nematics to ferromagnets [2].

Although our simulation is built for extensile systems undergoing a bend instability, its validity generalizes to other cases. If the system is made contractile or key parameters, such as the flow-alignment parameter and elastic moduli, are adjusted, a splay instability may dominate [25,30,31,37]. However, in that regime our framework predicts minimal changes in loop emergence as $\hat{\mathbf{k}}$ remains within the principal planes, but now aligns with $\delta\hat{\mathbf{n}}$ instead of $\hat{\mathbf{n}}_0$ [2]. More broadly, the loop emergence mechanics remain valid once $\hat{\mathbf{k}}$ lies in the principal planes, differing only by the orientation of the $\pm 1/2$ 2D-like defect pairs [8,38]. Moreover, when $\hat{\mathbf{k}}$ deviates from the principal planes, effective shear induced by additional twist emerges due to $\hat{\mathbf{n}}$ gradients across multiple planes (Fig. 4). In particular, when $\hat{\mathbf{k}}$ is nearly to the principal planes (pure twist mode), the quasi-2D description breaks down. A more unified framework encompassing these regimes is under development [39].

The initial loops can also be investigated by the established formalism of normal cross sections [2,3,5,10]. Compared with our framework, this approach directly captures the local topological properties of point defects. For example, the collapse of $\langle \gamma \rangle$ indicates that increasing κ_{eff} transforms the loops from wedge twist type to pure twist. The advantage of the principal-plane representation is that it provides an intuitive understanding of the $\hat{\mathbf{n}}$ structure on larger scales (Fig. 1) and connects naturally with perturbative analyses. This connection reveals the structure and formation mechanisms of loops,

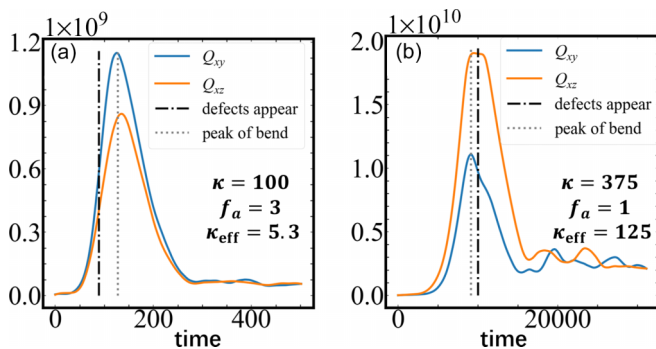


FIG. 5. Interplay between Frank distortions and loop emergence. The colored lines denote the largest Fourier coefficients of $\mathbf{Q}$. The time of each peak (gray lines), τ_{twi} , denotes the timescales of growth of twist. The black lines give the nucleation timescale τ_{nuc} when the first loop appears. This implies that high κ_{eff} results in $\tau_{\text{nuc}} > \tau_{\text{twi}}$.

which arise from the competition between Frank elasticity and active stress, manifested by the tilt of the principal planes.

In this work, the power of principal planes is also reflected in how they allow us to extend the existing bend-induced theory of loop formation. Previous theory predicts that initial loops are exclusively born with $\gamma \approx 90^\circ$ [5,13], and it has remained untested whether this scenario is universal, in part because the 3D structure of nascent loops is difficult to resolve. Using principal planes, we show that tilted loops can naturally arise from a similar mechanism, modulated by a nontrivial timescale competition between nucleation and twist development. Consequently, our analysis provides a more general and complete description of defect-loop morphogenesis beyond current theory.

With principal planes, we systematically investigate the emergence of disclination loops in 3D active nematics. Our particle-based simulations provide key insights into the microscopic mechanisms that govern large-scale defect formation, exhibiting behaviors akin to 3D active nematics experiments composed of microtubules [5]. Compared with continuum simulations, our approach is both more realistic and more general, representing a minimal model that captures the key microscopic behaviors of nematogens: interparticle alignment, activity, and semiflexibility. Relative to experiments, our simulations yield large-scale, noise-free data suitable for quantitative analysis. We find that an activity-dependent effective stiffness κ_{eff} controls defect mechanics, morphology, and steady-state behavior, enabling precise control over the system's emergent behavior. This insight opens a path toward the design of self-regulating active fluids and bioinspired materials with tunable transport properties.

In conclusion, we have introduced the principal-plane framework as an intuitive tool to holistically analyze $\hat{n}$ fields around disclination loops in the bulk of 3D active nematics. Linked to perturbation theory, it reveals how loops arise from the bend instability and how their tilt reflects the balance between activity and elasticity. Our simulations show that loop formation and steady-state properties are governed by an activity-dependent effective stiffness κ_{eff} . These results advance the understanding of nonequilibrium defect dynamics and offer principles for controlling emergent structures in orientationally ordered materials.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [40,41].

The modified LAMMPS with the active force is available in Ref. [40] and the data files and scripts associated with the results are available in Ref. [41].

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