

# Density-selected topological pathways in the melting of single-particle-thick stripes

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The melting of stripe-forming systems involves changes in connectivity that are not fully captured by conventional structural and orientational descriptors. We investigate a two-dimensional model with competing interactions whose low-temperature phase consists of one-particle-thick stripes. Molecular dynamics simulations along seven heating isochores are analyzed using thermodynamic, orientational, dynamical, and graph-based observables. Heating produces a multistage reconstruction in which the loss of stripe alignment and the reorganization of filament connectivity occur over distinct temperature ranges. Density controls whether the disordered filaments fragment into finite polymerlike clusters or remain joined in a dynamically fluid, system-spanning network. The topological observables distinguish these outcomes, which are not resolved by the thermodynamic and orientational responses alone. Thus, the same ordered stripe microphase can melt into topologically distinct fluids selected by density.

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## I. INTRODUCTION

Competing interactions provide an economical route from isotropic building blocks to spatially modulated matter. When aggregation or local packing at one length scale is frustrated by a second interaction scale, macroscopic phase separation can be replaced by finite-wavelength organization into clusters, stripes, lamellae, bubbles, and interconnected networks [1–5]. This mechanism appears in systems as diverse as magnetic films, Langmuir monolayers, block copolymers, protein solutions, and colloidal suspensions. In colloids, this phenomenology is commonly associated with short-range attraction and long-range repulsion (SALR), but modulated structures can also arise from purely repulsive core-softened potentials possessing two competing particle separations. Early studies by Jagla showed that core collapse in two dimensions can be preempted by nontriangular ground states, including chains, squares, hexagonal motifs, and quasicrystalline arrangements [6,7]. Subsequent studies established stripe and lamellar formation as generic consequences of isotropic repulsive length-scale competition [8–11]. Such isotropic models are therefore minimal platforms for separating the generic consequences of length-scale competition from chemical or particle-specific details.

The phase behavior generated by competing interactions is by now well established theoretically and computationally. Mesoscopic theories connect SALR fluids with Brazovskii-

type free-energy functionals and predict a generic sequence of periodic morphologies [2,12]. Particle-resolved simulations have identified equilibrium and metastable cluster fluids, lamellae, cylindrical domains, percolated networks, and gyroidlike phases [3,13–16]. In two dimensions, where thermal fluctuations and defects are especially important, stripes can form either from competing attraction and repulsion or from an isotropic repulsive shoulder [8,13,17]. Recent work has further shown that changes in composition, confinement, substrate modulation, and particle anisotropy can select among straight, modulated, labyrinthine, and fragmented stripe patterns [18–21]. These results demonstrate that a stripe is not specified solely by a peak in the structure factor: its thickness, continuity, curvature, branching, and global connectivity constitute independent structural degrees of freedom.

Experimental realizations confirm both the relevance and the complexity of this picture. Small-angle scattering and microscopy have revealed finite clusters in protein solutions and colloid-polymer mixtures [22], while particle-resolved confocal experiments found anisotropic cluster growth and network formation when attraction and electrostatic repulsion compete [23]. Tunable magnetic dispersions provide a more recent route for controlling attraction and repulsion *in situ* and directly observing the continual reconfiguration of two-dimensional colloidal assemblies [24,25]. More direct realizations of filamentous self-assembly have been obtained with core-corona and polymer-grafted colloids. Isotropic colloidal building blocks have been assembled into chain phases at interfaces [26,27], while weakly charged polymer-grafted particles with competing attraction and repulsion form isolated linear and branched polymerlike clusters in aqueous suspension [28,29]. Experiments have also produced single-particle-wide colloidal lines [30], showing that filamentary morphologies need not possess a bulklike interior. At this limiting thickness every particle belongs to the boundary and the

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local coordination is essentially that of a chain. Consequently, bending, end formation, reconnection, and loop closure can replace the interfacial and bulk mechanisms that dominate the evolution of thicker lamellae.

The relation between stripes and finite particle chains is particularly suggestive. Simulations of colloidal systems have shown that quasi-one-dimensional aggregation may precede branching and gel formation [31,32], and inverse design has demonstrated that isotropic potentials can stabilize single-stranded “colloidomers” as equilibrium or ergodic assemblies [33]. Cluster morphology is also known to influence whether competing-interaction fluids remain ergodic, undergo cluster-glass arrest, or percolate into a network [34–36]. These observations suggest that a melted stripe state should not automatically be regarded as a homogeneous disordered fluid. Depending on the balance between end formation and reconnection, its chainlike constituents may form finite polymerlike clusters or remain joined into a percolated network. These alternatives can possess comparable local packing and mobility while differing fundamentally in their global topology.

Melting adds a second layer of complexity. For ordinary two-dimensional crystals, the Kosterlitz-Thouless-Halperin-Nelson-Young framework relates melting to the unbinding of topological defects [37–40]. Colloidal experiments have provided direct tests of this defect-mediated scenario and have also shown that the pathway depends on the interaction and anisotropy [41–43]. Microphase-forming systems are not ordinary crystals, however: translational and orientational order coexist with an emergent connectivity at the domain scale. Simulations of stripe-forming particles have accordingly found intermediate regimes, defect-rich stripes, and nontrivial melting sequences [44,45]. At the coarser level of continuous domain patterns, the expression “topological melting” has previously been used to describe the reorganization of magnetic stripes into polygonal, bubble, and labyrinthine morphologies [46]. That description concerns the topology of continuous domains, however, rather than the particle-resolved connectivity, branching, and loop structure of one-particle-thick filaments considered here. In our previous study of the present core-softened model, the one-particle-thick stripe phase displayed a gradual loss of order and pronounced mobility along the stripes [47]. What remained unresolved was whether melting this ordered phase necessarily destroys its system-spanning topology, and whether the resulting fluid topology is uniquely inherited from the stripe state or selected by density.

This question cannot be answered completely by conventional scalar order parameters. Pair correlations and bond-orientational order quantify positional and angular organization, but they do not distinguish a system-spanning stripe from a finite chain, a branched object, or a closed loop when these structures have comparable local packing. Graph and topological approaches offer the required complementary description by encoding connected components, independent cycles, percolating or winding objects, and cyclic backbones. More broadly, computational topology has detected phase changes and structurally relevant length scales in statistical models and soft materials [48–50], while network-based analyses have related mesoscale connectivity to heterogeneous relaxation in colloidal matter [51]. Nevertheless, the

temperature-resolved coupling among stripe curvature, graph topology, filament statistics, and particle mobility has received little attention. In particular, it remains unclear whether the same one-particle-thick stripe phase follows a universal fragmentation pathway or can melt into topologically distinct fluids as density changes.

Here we address this problem using molecular dynamics simulations of a two-dimensional Lennard-Jones–Gaussian system [52,53]. We study seven densities spanning the region in which the one-particle-thick stripe morphology is stabilized, including the density of optimal stripe stability [54], and follow continuous isochoric heating paths from identically ordered stripe configurations. Orientational descriptors are combined with a graph representation of the instantaneous particle structure. The first Betti number, periodic winding, the graph 2-core, cluster- and cycle-size distributions, filament conformations, bond persistence, long-time self-diffusion, and connectivity-conditioned mobility resolve how bending, opening, branching, reconnection, and fragmentation reorganize the stripe backbones.

## II. MODEL AND SIMULATION DETAILS

### A. Interaction model and simulation protocol

We consider a two-dimensional monodisperse system of particles interacting through the Lennard-Jones plus Gaussian (LJG) pair potential [52,55]

$$U(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] + A\varepsilon \exp \left[ - \left( \frac{r - r_0\sigma}{c\sigma} \right)^2 \right], \quad (1)$$

where  $\varepsilon$  and  $\sigma$  set the energy and length scales, respectively. We use  $A = 5.0$ ,  $r_0 = 0.7$ , and  $c = 1.0$ , corresponding to the shoulder-ramp core-softened model investigated in our previous studies [47,54]. The interaction was truncated at  $r_{\text{cut}} = 3.5\sigma$  and shifted so that  $U(r_{\text{cut}}) = 0$ . Lennard-Jones reduced units are used throughout [56]: lengths, energies, temperatures, and times are expressed in units of  $\sigma$ ,  $\varepsilon$ ,  $\varepsilon/k_B$ , and  $\tau = \sqrt{m\sigma^2/\varepsilon}$ , respectively, with particle mass  $m = 1$ .

The molecular dynamics simulations were performed with ESPRESSO [57]. The Lennard-Jones contribution was evaluated with the native ESPRESSO interaction, thereby preserving its short-range divergence, while only the smooth Gaussian contribution was tabulated. The two contributions were combined to reproduce Eq. (1) with the stated cutoff and shift. Periodic boundary conditions were applied in  $x$  and  $y$ . Motion along  $z$  was constrained for every particle and the  $z$  direction was nonperiodic.

The equations of motion were integrated with the velocity-Verlet algorithm using a time step  $\Delta t = 0.002\tau$ . Temperature was controlled by a Langevin thermostat with friction coefficient  $\gamma = 1.0 m/\tau$ . The main simulations contained  $N = 4096$  particles at the seven number densities,  $\rho = \frac{N}{L_x L_y} = 0.395, 0.405, 0.415, 0.425, 0.435, 0.445, \text{ and } 0.455$ . This interval spans the region in which the one-particle-thick stripe morphology is stabilized in the previously determined phase diagram [54].

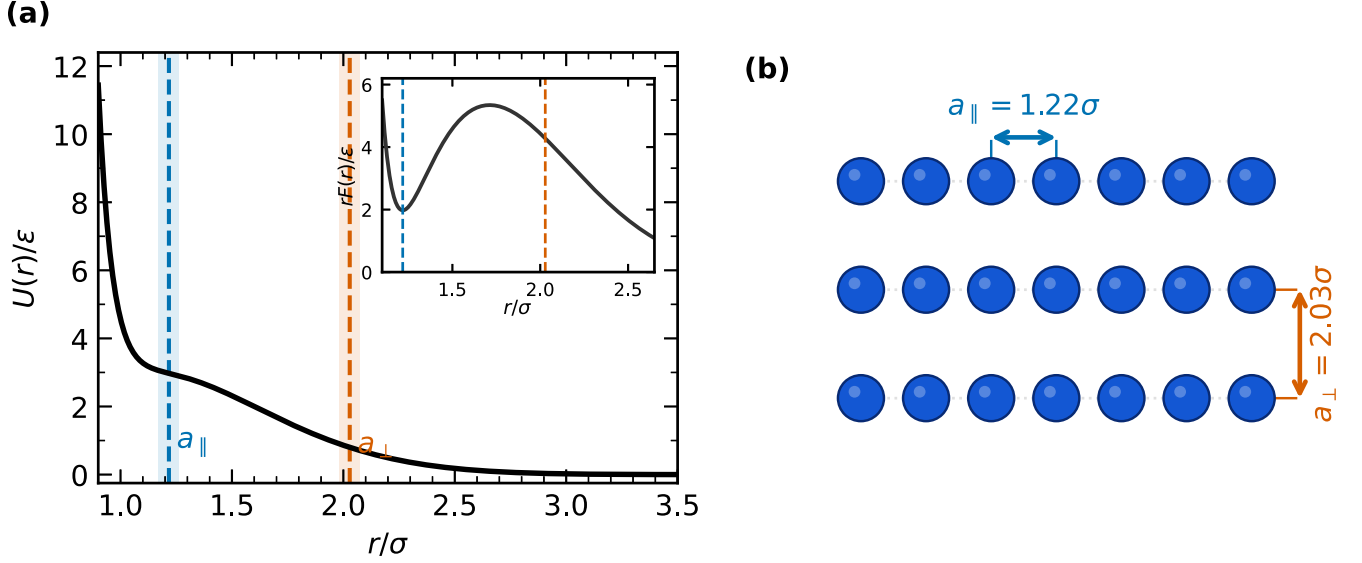


FIG. 1. Interaction model and microscopic organization of the stripe phase. (a) Lennard-Jones–Gaussian pair potential  $U(r)/\epsilon$  used in the simulations. The black and orange dashed lines identify the longitudinal and transverse separations at  $\rho = 0.405$ :  $a_{\parallel} = 1.22\sigma$  and  $a_{\perp} = 2.03\sigma$ , respectively; the shaded regions are visual guides to these structural scales. The inset shows the corresponding distance-weighted radial force,  $rF(r)/\epsilon$ . (b) Schematic representation of the one-particle-thick stripe arrangement. The short separation organizes particles along each stripe, whereas the long separation separates adjacent stripes.

Each run was initialized as a defect-free array of one-particle-thick stripes. The  $N = 4096$  configuration contained  $n_x = 64$  particles along each stripe and  $n_y = N/n_x = 64$  stripes. If  $a_{\parallel}$  and  $a_{\perp}$  denote the particle separations parallel and perpendicular to a stripe, respectively, we imposed

$$\frac{a_{\perp}}{a_{\parallel}} = \frac{2.0}{1.2} = \frac{5}{3}, \quad a_{\parallel} = \left[ \rho \left( \frac{a_{\perp}}{a_{\parallel}} \right) \right]^{-1/2}, \quad (2)$$

and used  $L_x = n_x a_{\parallel}$  and  $L_y = n_y a_{\perp}$ . This construction places consecutive particles along a stripe near the short structural scale and separates adjacent stripes by the longer scale. Across the simulated density interval,  $a_{\parallel}$  decreases from  $1.232\sigma$  to  $1.148\sigma$ , while  $a_{\perp}$  decreases from  $2.054\sigma$  to  $1.914\sigma$ . Simultaneous matching to the reference separations  $a_{\parallel} = 1.2\sigma$  and  $a_{\perp} = 2.0\sigma$  occurs at  $\rho_{\text{match}} = (1.2 \times 2.0)^{-1} \simeq 0.417$ . The density scan therefore probes both stretched and compressed stripe geometries relative to the two interaction-selected structural scales.

Figure 1 summarizes the relation between the interaction and the microscopic stripe geometry. The pair potential is monotonic, but the distance-weighted force  $rF(r)$  displays a broad softened region that permits distinct local separations [Fig. 1(a)]. The marked values  $a_{\parallel}$  and  $a_{\perp}$  are therefore structural scales rather than two minima of  $U(r)$ . As illustrated in Fig. 1(b), the shorter separation organizes consecutive particles along a one-particle-thick stripe, whereas the longer separation separates adjacent stripes. The schematic uses  $\rho = 0.405$ , for which  $a_{\parallel} = 1.217\sigma$  and  $a_{\perp} = 2.029\sigma$ .

Initial velocities were drawn independently from a Maxwell distribution at  $T = 0.04$ , and their center-of-mass contribution was removed. Four independent realizations were simulated at each density. Continuous isochoric heating paths

were followed from  $T = 0.04$  to  $0.20$  in increments of  $\Delta T = 0.005$ . The initial state point was equilibrated for  $10^7$  integration steps. At every subsequent temperature, the final configuration and velocities from the preceding state point were retained and the system was equilibrated for  $3 \times 10^6$  steps. Production trajectories comprised  $5 \times 10^7$  steps at each temperature. This protocol preserves the thermal history of the heating trajectory without regenerating the configuration at each state point. Particle configurations were stored every 5000 steps, corresponding to  $\Delta t_{\text{GSD}} = 10\tau$ , and the total energy was sampled every 1000 steps during production.

For each independent realization, we calculated the mean energy per particle  $e(T) = \langle E \rangle / N$ . The isochoric heat capacity per particle shown in the main text was obtained from the canonical energy-fluctuation estimator

$$c_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{NT^2}, \quad (3)$$

where  $k_B = 1$  in reduced units. The numerical derivative  $\partial e / \partial T$  was used as an independent consistency check. See Supplemental Material (SM) [58] for complete definitions of the observables, the robustness against the graph connectivity cutoff, the thermodynamic response along the heating isochores, and the system-size analysis.

System-size dependence was examined at the densities  $\rho = 0.405, 0.425, 0.435$ , and  $0.445$ , using  $N = 1024, 4096$ , and  $16384$ . The corresponding initial configurations contained  $n_x = 32, 64$ , and  $128$  particles along each stripe, respectively, with  $n_y = n_x$ . Thus,  $\rho, a_{\perp}/a_{\parallel} = 5/3$ , the box aspect ratio, and all interaction and thermostat parameters were preserved as the system size changed. The resulting finite-size analysis is presented in SM [58].

### B. Structural, topological, and dynamical observables

The instantaneous particle configurations were represented as undirected graphs in which particles constitute the vertices and an edge connects each pair separated by less than  $r_c^{\text{graph}} = 1.5\sigma$ . This construction maps the one-particle-thick stripes onto filamentous networks and permits their connectivity, branching, fragmentation, and periodic wrapping to be followed during heating. Robustness with respect to the graph cutoff is demonstrated in SM [58].

For a graph bond with polar angle  $\theta_{ij}$ , global nematic alignment was measured by

$$S_2 = \left| \frac{1}{|E|} \sum_{(i,j) \in E} e^{2i\theta_{ij}} \right|, \quad \langle |\psi_2| \rangle = \frac{1}{N'} \sum_{i:k_i > 0} \left| \frac{1}{k_i} \sum_{j \in \mathcal{N}(i)} e^{2i\theta_{ij}} \right|, \quad (4)$$

where  $\mathcal{N}(i)$  and  $k_i$  are the neighbor set and degree of particle  $i$ , and  $N'$  is the number of nonisolated particles. Thus,  $S_2$  measures alignment throughout the sample, whereas  $\langle |\psi_2| \rangle$  measures the anisotropy of individual neighbor environments without requiring their directors to be mutually aligned. At degree-2 vertices, local bending was measured from the turning angle  $\vartheta_i$  between the two outward bonds and the discrete curvature  $\kappa_i = \vartheta_i / [(|\mathbf{u}_i| + |\mathbf{v}_i|)/2]$ ; the reported rms curvature is  $\kappa_{\text{rms}} = \langle \kappa_i^2 \rangle^{1/2}$ .

The degree also identifies endpoints ( $k_i = 1$ ), filament-backbone particles ( $k_i = 2$ ), and branches or junctions ( $k_i \geq 3$ ). If  $C$  is the number of connected components, the number of independent graph cycles is the first Betti number

$$\beta_1 = |E| - |V| + C. \quad (5)$$

To distinguish local loops from periodic connectivity, image offsets were accumulated around closed graph paths. Their net periodic displacement defines an integer winding vector  $\mathbf{w} = (w_x, w_y)$ . A component was classified as winding if it contained at least one path with  $\mathbf{w} \neq (0, 0)$ , irrespective of winding direction. We define  $\beta_1^{\text{wind}}$  as the sum of the cycle ranks of all such components and  $\beta_1^{\text{nonwind}}$  as the corresponding sum for finite components. Consequently, a local cycle contained in an already winding network contributes to  $\beta_1^{\text{wind}}$  even if that particular cycle is contractible. The 2-core, obtained by recursively removing vertices of degree smaller than two, identifies the particle population supported by closed or multiply connected backbones.

A finite nonwinding object is a component for which all closed paths have  $\mathbf{w} = (0, 0)$ ; it may be an open filament with  $\beta_1 = 0$  or contain a contractible loop with  $\beta_1 > 0$ . By *original winding backbones* we mean the initially prepared stripes, which close through the periodic cell and have  $\mathbf{w} = (1, 0)$  in the present construction. A commensurate tilted stripe can instead have, for example,  $\mathbf{w} = (1, 1)$ , but it is assigned to the same winding category. The winding vector records the homology class on the torus, whereas  $\beta_1$  records the number of independent cycles. Representative examples of finite open filaments, finite nonwinding loops, and axis-aligned and tilted winding backbones are provided in Fig. S1 of SM [58].

Cluster-size distributions, the largest-cluster fraction, and the winding probability  $P_{\text{wind}}$  distinguish finite aggregates from system-spanning networks. Filament statistics were

evaluated for finite, nonwinding, unbranched open components. Their contour length  $L_c$  is the sum of their bond lengths, their end-to-end distance is  $R_{\text{ee}}$ , and their tortuosity is  $\mathcal{T} = L_c/R_{\text{ee}}$ , equal to unity for a straight filament and larger than unity for a curved one. Tangent correlations measure orientational memory along the contour, while fundamental-cycle lengths characterize the geometrical scale of graph loops. Complete implementation details and definitions are given in SM [58].

Fluctuations of the global orientational order were quantified by

$$\chi_2 = \frac{N}{T} (\langle S_2^2 \rangle - \langle S_2 \rangle^2), \quad (6)$$

and the temperature derivative  $\mathcal{R}_2 = -\partial \langle S_2 \rangle / \partial T$  was used as an orientational response function. Together with  $c_V$ , these quantities locate the structural and thermodynamic response interval without assuming a particular order for the transition.

Particle transport was characterized by the long-time self-diffusion coefficient obtained from the two-dimensional Einstein relation

$$D_{\text{MSD}} = \lim_{t \rightarrow \infty} \frac{\langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \rangle}{4t}. \quad (7)$$

The coupling between connectivity and motion was probed through the short-time mobilities of degree-1 endpoints and degree- $k \geq 3$  branch particles relative to degree-2 backbone particles, denoted  $R_{\text{end}}$  and  $R_{\text{branch}}$ , respectively. Bond survival over one stored-frame interval measures the accompanying renewal of the neighbor network.

Definitions of the correlation functions, mobility ratios, numerical derivatives, uncertainty estimates, and the detailed cluster- and cycle-distribution protocols are provided in SM [58].

### III. RESULTS AND DISCUSSION

The thermal evolution of the one-particle-thick stripe phase is summarized in Fig. 2. The representative configurations at  $\rho = 0.405$  [Figs. 2(a)–2(d)] and  $\rho = 0.445$  [Figs. 2(e)–2(h)] were selected at the same temperatures to expose the two reconstruction pathways without conflating density and thermal history. Both systems begin as nearly straight and mutually aligned stripes, consistent with the ordered state previously identified for this model [47]. On heating, the contours acquire curvature and lose their common orientation. Their final morphologies, however, are qualitatively different: the lower-density stripes open and fragment into finite polymerlike clusters, whereas the higher-density system retains an interconnected structure after stripe alignment has disappeared.

The orientational observables show that the initial loss of stripe order is nevertheless similar in the two pathways. The global nematic order  $S_2$  decreases sharply over a narrow temperature interval [Fig. 2(i)], while the local twofold order  $\langle |\psi_2| \rangle$  remains comparatively high [Fig. 2(j)]. The midpoint temperature of the  $S_2$  decay first increases from approximately 0.128 at  $\rho = 0.395$  to 0.139 at  $\rho = 0.415$ –0.425, and then decreases to 0.117 at  $\rho = 0.455$ . Thus, the extended density range reveals a nonmonotonic stability of global stripe

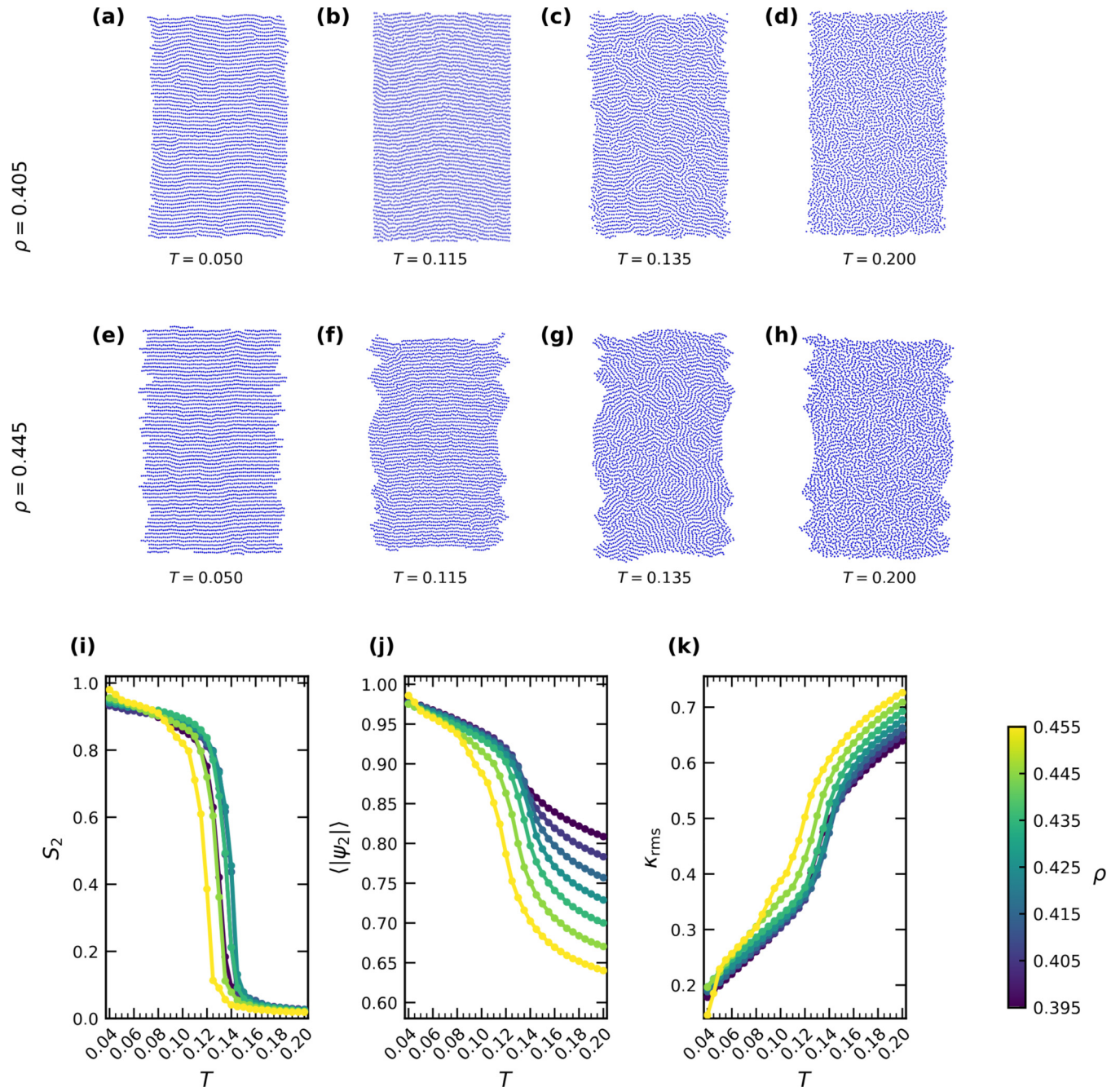


FIG. 2. Density-selected pathways in the melting of one-particle-thick stripes. Representative configurations are shown for  $\rho = 0.405$  in (a)–(d) and  $\rho = 0.445$  in (e)–(h), at  $T = 0.050, 0.115, 0.135$ , and  $0.200$  from left to right. Panels (i)–(k) show, respectively, the global nematic order  $S_2$ , the local twofold order  $\langle |\psi_2| \rangle$ , and the rms contour curvature for all seven densities. Symbols and shaded bands denote averages and standard errors over four independent runs.

alignment rather than the continuous upward shift suggested by the three central densities alone. At these midpoints,  $\langle |\psi_2| \rangle$  remains between approximately 0.81 and 0.90. Local anisotropic environments therefore survive the decay of global alignment throughout the density interval.

The simultaneous increase of the rms curvature [Fig. 2(k)] identifies bending as the geometrical precursor of this loss of alignment. Because the stripes are only one particle thick, they have no bulklike interior that can disorder independently of their boundaries. Thermal fluctuations act directly on their contours, making bending, end formation, reconnection, and

fragmentation the relevant relaxation modes. This differs from finite-width stripes, for which internal disordering and intrastripe motion can precede large-scale breakup [45]. Figures 2(i)–(k) consequently establish a common orientational melting process, but the configurations in Figs. 2(d) and 2(h) already indicate that its topological outcome depends strongly on density.

The connectivity observables in Fig. 3 clarifies this point. Most importantly, the nonmonotonicity of  $\beta_1$  is itself density dependent: the curves do not represent a common sequence translated along the temperature axis. For  $\rho = 0.395$ – $0.415$ ,

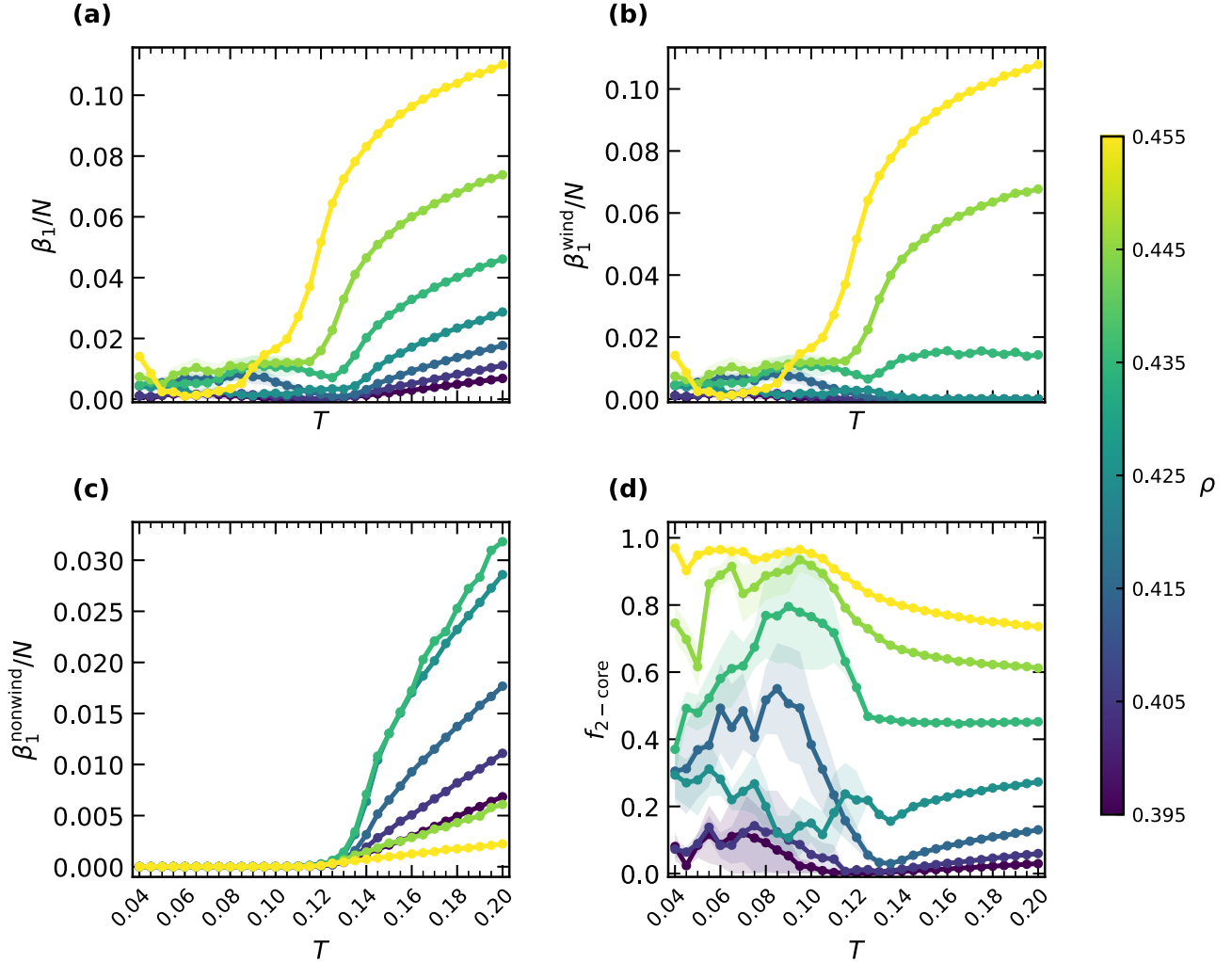


FIG. 3. Topological reconstruction during heating for the seven densities. (a) First Betti number per particle,  $\beta_1/N$ . Contributions to the cycle rank from components (b) with and (c) without nonzero periodic winding; cycles counted in (b) need not individually wind around the box. (d) Fraction of particles in the graph 2-core. Symbols and shaded bands denote averages and standard errors over four independent runs.

the total cycle density first displays a low-temperature shoulder, then decreases to a pronounced minimum, and finally increases again [Fig. 3(a)]. The minima occur near  $T = 0.110, 0.115$ , and  $0.130$ , respectively. At the two highest densities, by contrast, the dominant feature is the strong increase of  $\beta_1/N$  through and beyond the loss of orientational order. The intermediate densities connect these limits in a nontrivial way.

The winding decomposition is essential for identifying the origin of these different curve shapes. At low temperature, essentially the entire  $\beta_1$  is carried by components with nonzero periodic winding [Fig. 3(b)], while the nonwinding contribution remains negligible [Fig. 3(c)]. The initial shoulder at the three lower densities therefore does not originate from compact loops in a cluster fluid. It reflects opening, closure, and reconnection within the system-spanning stripe pattern. Since every stripe is only one particle thick, a local reconnection can immediately change the cycle rank of the spanning component even while  $S_2$  and  $\langle |\psi_2| \rangle$  remain large. The ordered stripe state is consequently not topologically inert.

For  $\rho = 0.395\text{--}0.425$ , further heating removes the winding contribution and replaces it with cycles belonging to finite, nonwinding objects. The two contributions become equal at  $T_{\text{cross}} \simeq 0.115, 0.123, 0.128$ , and  $0.132$ , respectively. Around this crossover, destruction of the original winding backbones is not yet compensated by the proliferation of local loops, producing the minimum or weak-cycle interval in the total  $\beta_1$ . The structures are therefore predominantly open and curved: they preserve chainlike local packing but have lost most of the global connectivity of the stripe state. We use *topological intermediate* for this connectivity regime without implying a separate thermodynamic phase. Its finite temperature width shows that opening a winding stripe and closing new loops among its fragments are distinct processes.

The evolution at  $\rho = 0.435$  is qualitatively mixed. The winding contribution decreases from  $\beta_1^{\text{wind}}/N \simeq 0.0106$  at  $T = 0.10$  to approximately  $0.0065$  at  $T = 0.125$ , but then increases again to approximately  $0.0156$  at  $T = 0.16$ . Nonwinding cycles grow simultaneously and become dominant only at  $T_{\text{cross}} \simeq 0.155$ , after the main decay of  $S_2$ . Thus, this

density does not merely postpone fragmentation. It samples a competition between the production of finite loops and the reconstruction of cycles inside components that remain system spanning.

This second mechanism becomes dominant at  $\rho = 0.445$  and  $0.455$ . For  $\rho = 0.445$ ,  $\beta_1^{\text{wind}}/N$  grows from approximately 0.012 at  $T = 0.10$  to 0.068 at  $T = 0.20$ ; for  $\rho = 0.455$ , it grows from approximately 0.0165 to 0.108 over the same interval. Much of this growth occurs after the maxima of the orientational response, when the straight stripe alignment has already disappeared. No winding-nonwinding crossover is reached by  $T = 0.20$ , and the corresponding nonwinding contributions are only about 0.0061 and 0.0022. Heating therefore does not simply preserve a progressively weakened remnant of the initial stripe pattern. It produces additional independent cycles within a winding, orientationally disordered network.

Here  $\beta_1^{\text{wind}}$  denotes the cycle rank of every connected component that has nonzero periodic winding; an individual cycle contributing to this quantity need not itself traverse the box. Its postmelting growth can thus be generated when branch formation and reconnection add short local loops to an already winding backbone. This distinction reconciles the rapid increase of  $\beta_1^{\text{wind}}$  with the coexistence of short and system-scale cycles shown below: the high-density fluid is simultaneously locally reticulated and globally connected.

The 2-core fraction in Fig. 3(d) independently measures how much of the structure belongs to a cyclic backbone. At  $T = 0.20$ , it increases from approximately 0.029 at  $\rho = 0.395$  to 0.273 at  $\rho = 0.425$ , 0.452 at  $\rho = 0.435$ , and 0.612 and 0.736 at  $\rho = 0.445$  and  $0.455$ . The low-density increase of  $\beta_1$  is therefore produced by numerous small loops involving a limited particle fraction, whereas the high-density increase is accompanied by an extensive cyclic backbone. The density dependence of  $\beta_1$  thus separates two physically different outcomes of melting: finite loop-bearing filaments and a multiply connected winding fluid.

This interpretation extends defect-based descriptions of stripe melting [44] by distinguishing the opening of winding backbones, the creation of local cycles, and the reticulation of a spanning component. More generally, experiments on two-dimensional colloidal melting demonstrate that the production and evolution of topological defects need not coincide with a single loss-of-order temperature [68].

The filament statistics in Fig. 4 connect this topological distinction to the geometry of the aggregates. The endpoint fraction increases throughout the reconstruction [Fig. 4(a)], but its final value decreases markedly with density, from approximately 0.34 at  $\rho = 0.395$  to 0.19 at  $\rho = 0.425$  and 0.095 at  $\rho = 0.455$ . End formation is therefore the dominant outcome on the low-density side, whereas it is progressively suppressed as the connected network becomes favored. The characteristic contour length simultaneously decreases by orders of magnitude [Fig. 4(b)], showing that loss of system-spanning stripe order produces shorter connected segments in both regimes.

The opposite density trends of the endpoint and 2-core fractions expose the local operations responsible for the two topological outcomes. On the low-density side, opening a winding contour removes particles from the cyclic backbone and creates two mobile ends; the large endpoint fraction and

small 2-core fraction at  $T = 0.20$  are the cumulative signatures of this process. On the high-density side, contacts between bent filaments create junctions and alternative paths. End production is then suppressed while the 2-core expands, and the newly formed loops remain attached to a winding component. The change between these limits is therefore not merely a variation in cluster size: density selects whether bond rearrangements terminate a filament or reticulate the network.

The conformational evolution is not a direct collapse into compact isotropic aggregates. The mean tortuosity rises from values close to unity to approximately 1.2–1.3 [Fig. 4(c)], while the tangent correlation at contour separation  $s = 10$  loses its initial long-range coherence [Fig. 4(d)]. Near the topological intermediate, the contours are already substantially curved although many remain much longer than the final clusters. The subsequent weak decrease of tortuosity at the highest temperatures does not represent a recovery of straight stripes; it follows from the shortening of the available contour over which large-scale bending can develop.

At lower density, the loss of tangent coherence accompanies the conversion of long open filaments into flexible finite polymerlike clusters. At higher density, the same local loss of coherence occurs without global fragmentation: the measured contours are flexible strands connecting junctions inside a multiply connected network. Hence similar local chain statistics can coexist with opposite global topologies. Linear growth followed by branching is a known route to network formation in colloids with competing interactions [31], and both linear and branched aggregates have been observed in experiments and particle-based models [28,29]. The present results show that the balance between these motifs is continuously selected by density during the melting of an initially ordered stripe phase.

The two final morphologies are dynamically fluid. The long-time diffusion coefficient increases smoothly through the reconstruction interval [Fig. 5(a)] and remains only weakly density dependent. At  $T = 0.20$ ,  $D_{\text{MSD}}$  decreases modestly from  $0.1645 \pm 0.0009$  at  $\rho = 0.395$  to  $0.1496 \pm 0.0010$  at  $\rho = 0.455$ . In particular, the percolated structures at  $\rho = 0.445$  and  $0.455$  have diffusion coefficients comparable to those of the finite-cluster fluids. Their persistent connectivity should therefore not be interpreted as network arrest or gelation; it characterizes the topology of a continuously restructuring fluid. It is relevant because competing interactions can also produce arrested cluster and network states [34]; here, the finite diffusivity demonstrates that percolation and arrest are separated.

Conditioning the displacement on local graph environment reveals dynamical heterogeneity that is hidden in the bulk diffusivity. Filament ends are more mobile than degree-2 backbone particles [Fig. 5(b)]. Their relative mobility  $R_{\text{end}}$  first increases, then forms a broad plateau near 1.3–1.5, and finally approaches unity. The initial enhancement shows that terminations are mobile defects of the stripe pattern. At the lower densities, this enhancement precedes and overlaps the collapse of  $\beta_1^{\text{wind}}$ : opening a spanning contour simultaneously creates an end and releases a locally undercoordinated particle. As endpoints proliferate and the degree-2 segments themselves become mobile, the end environment becomes less exceptional, accounting for the plateau and subsequent

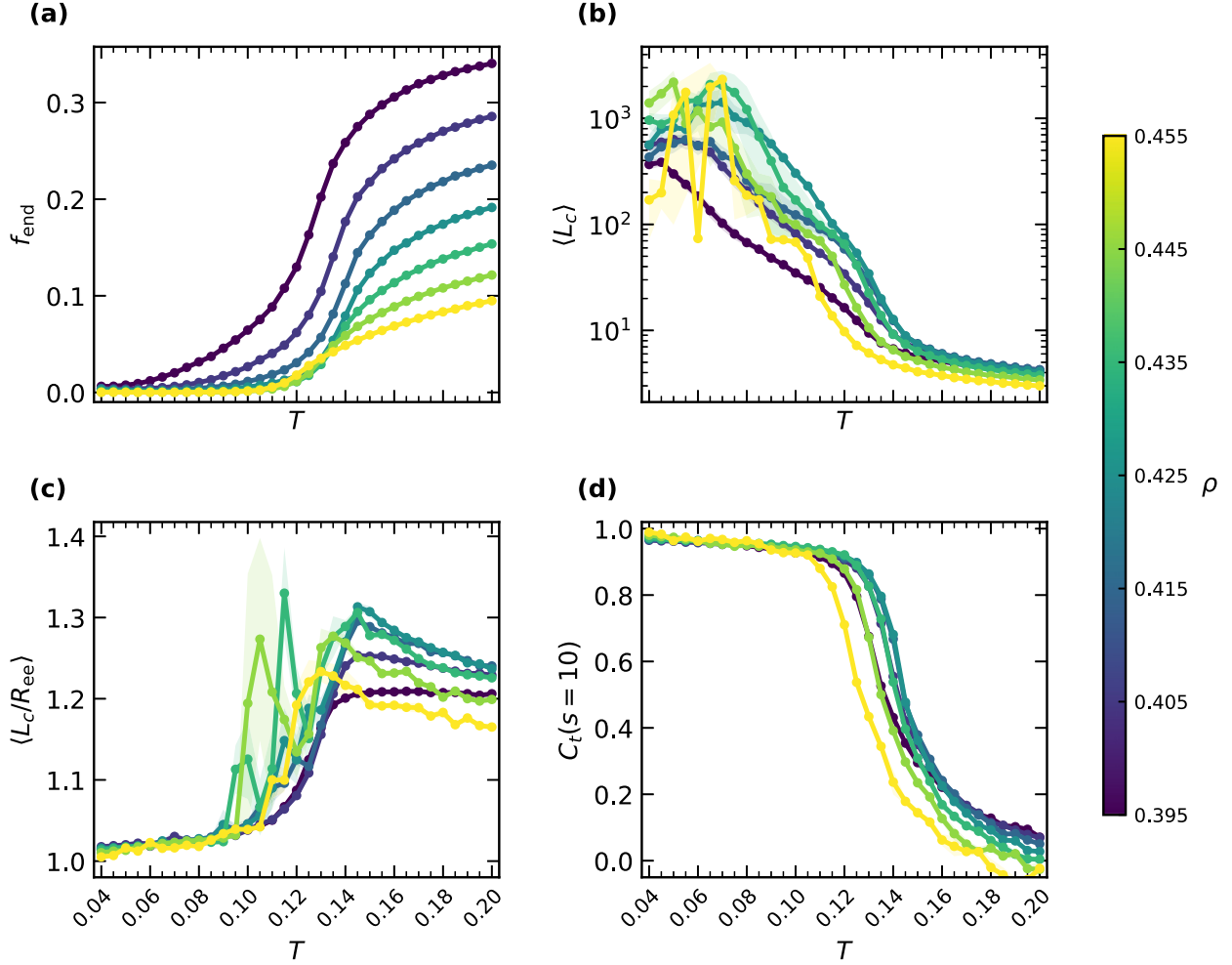


FIG. 4. Evolution of filament geometry during heating. (a) Endpoint fraction, (b) mean contour length, (c) mean tortuosity  $\langle L_c/R_{\text{ee}} \rangle$ , and (d) tangent correlation at contour separation  $s = 10$ . Symbols and shaded bands denote averages and standard errors over four independent runs.

decay of the mobility contrast. At the highest densities, the endpoint population is negligible in the low-temperature stripe phase. We therefore report  $R_{\text{end}}$  only when all four replicas contain, on average, at least one complete endpoint pair per stored configuration. This population criterion removes ratios formed from an effectively absent conditioning class and does not affect the reconstruction interval.

Branch particles display a distinct temporal hierarchy [Fig. 5(c)]. On the low-density side, a statistically resolved branch population appears only after fragmentation has begun, with an initial mobility close to twice that of the backbone. Increasing density makes junctions abundant at lower temperature and simultaneously suppresses the production of endpoints. Branches are consequently not the direct product of bond breaking: they arise when bent contours contact, merge, or reconnect, and become the elements that maintain connectivity in the dense network fluid. Their initial mobility, approximately 1.6–2 times that of the backbone, identifies junctions as active reconstruction sites rather than permanent crosslinks. At  $\rho = 0.445$  and 0.455, the interval

with a well-developed branch signal is also the interval in which  $\beta_1^{\text{wind}}$  grows rapidly. The structural and dynamical evidence therefore support the same mechanism: mobile contacts create alternative paths and local loops while retaining the system-spanning component. Their mobility contrast, like that of the endpoints, decays toward unity at high temperature, when bond rearrangements are no longer localized at a special coordination environment.

The bond-survival probability decreases from nearly one to values between approximately 0.53 and 0.58 [Fig. 5(d)]. Its strongest variation overlaps the loss of tangent coherence and the redistribution between winding and nonwinding cycles. The persistent high-density network is therefore not a fixed set of bonds. It maintains global connectivity while its individual connections are continually renewed, consistent with the comparable diffusivities in Fig. 5(a). At low density this renewal primarily advances fragmentation; at high density it changes the internal cycle structure of the winding component without destroying its global connectivity. Similar connections between mesoscale connectivity and heterogeneous dynamics

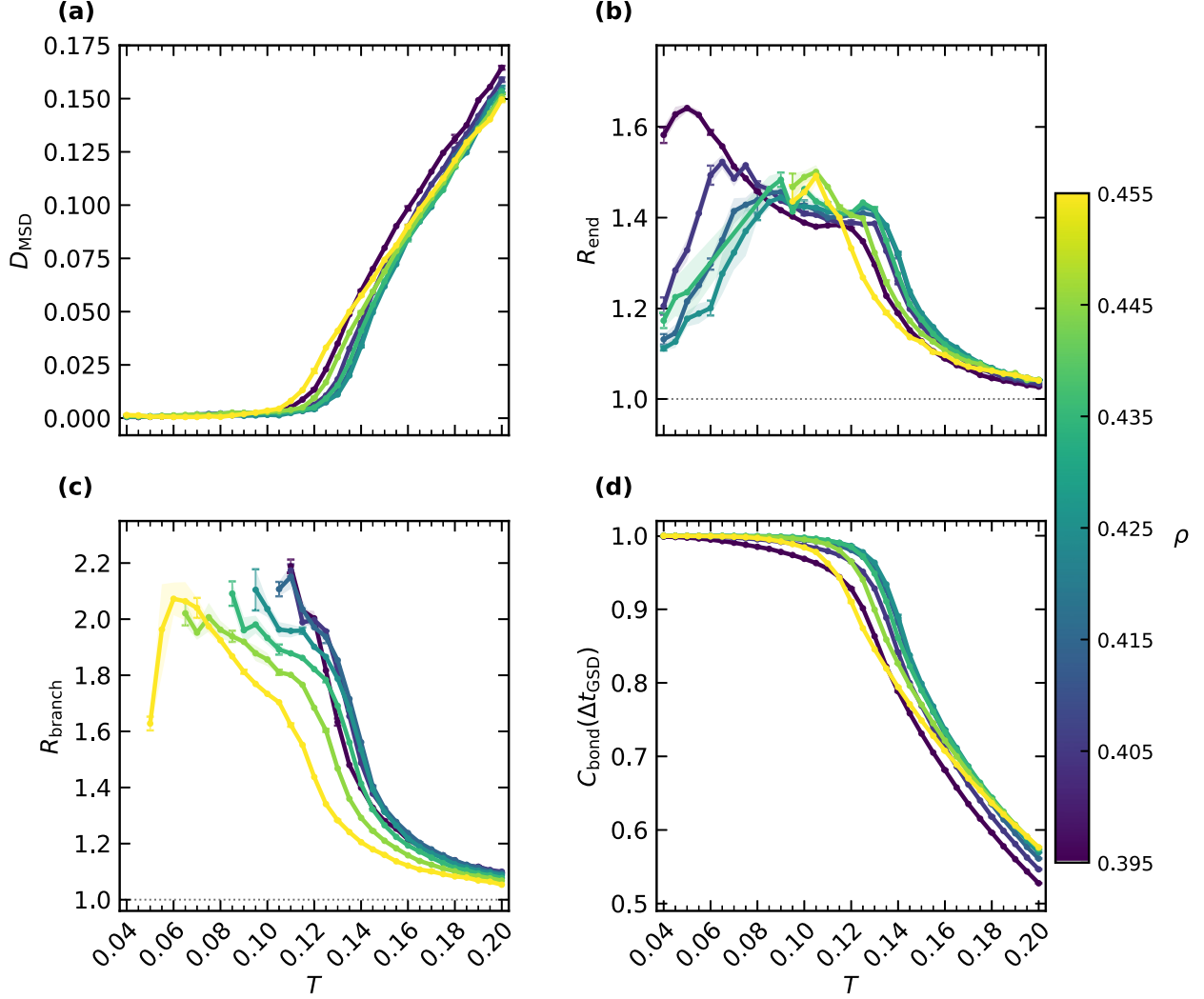


FIG. 5. Coupling between local connectivity and dynamics. (a) Long-time diffusion coefficient  $D_{\text{MSD}}$ , (b) mobility of filament ends relative to the degree-2 backbone,  $R_{\text{end}}$ , (c) relative mobility of branch particles,  $R_{\text{branch}}$ , and (d) bond-survival probability over one stored-frame interval. Topology-conditioned mobility ratios are reported only when all four replicas contain, on average, at least two particles of the corresponding class per stored configuration. Shaded bands and sparse error bars denote standard errors over independent replicas.

have been reported for colloidal networks and competing-interaction fluids [25,51].

The distributions in Fig. 6 establish the length scales and spanning character of the two fluids. The particle-weighted cluster-size distributions at  $T = 0.20$  [Fig. 6(a)] shift continuously toward larger objects as density increases. For  $\rho \leq 0.425$ , the distributions decay before the system size, confirming a fluid of finite clusters. At  $\rho = 0.445$  and  $0.455$ , they instead retain most of their weight near the system size, consistent with a dominant connected network. The strong density dependence is consistent with the general sensitivity of cluster morphology and percolation to thermodynamic conditions in competing-interaction fluids [3,66].

The spanning-cluster measures in Fig. 6(b) make this crossover explicit. At  $\rho = 0.425$ , the percolation probability is only 0.012 and the largest cluster contains approximately 14% of the particles. At  $\rho = 0.435$ , these quantities increase to 0.468 and 0.511, respectively, identifying a crossover

regime in which finite and spanning structures are both sampled. At  $\rho = 0.445$ , the percolation probability is already 0.989 and the largest component contains about 87% of the particles; at  $\rho = 0.455$ , the corresponding values are 1.0 and 95%. Because percolation is sensitive to finite size and to the connectivity cutoff, these results do not by themselves locate a sharp density-driven transition. They robustly distinguish, however, the finite-cluster and percolated-network limits on opposite sides of the crossover.

The cycle-size distributions further show that the distinction is not captured solely by the presence of one large cluster. At  $\rho = 0.405$  [Fig. 6(c)], the low-temperature distribution is concentrated near the stripe winding length. This feature disappears during heating, and by  $T = 0.20$  the median fundamental-cycle length is three particles, with a 90th percentile of approximately nine. The renewed high-temperature growth of  $\beta_1$  at this density therefore originates from short local loops in finite aggregates.

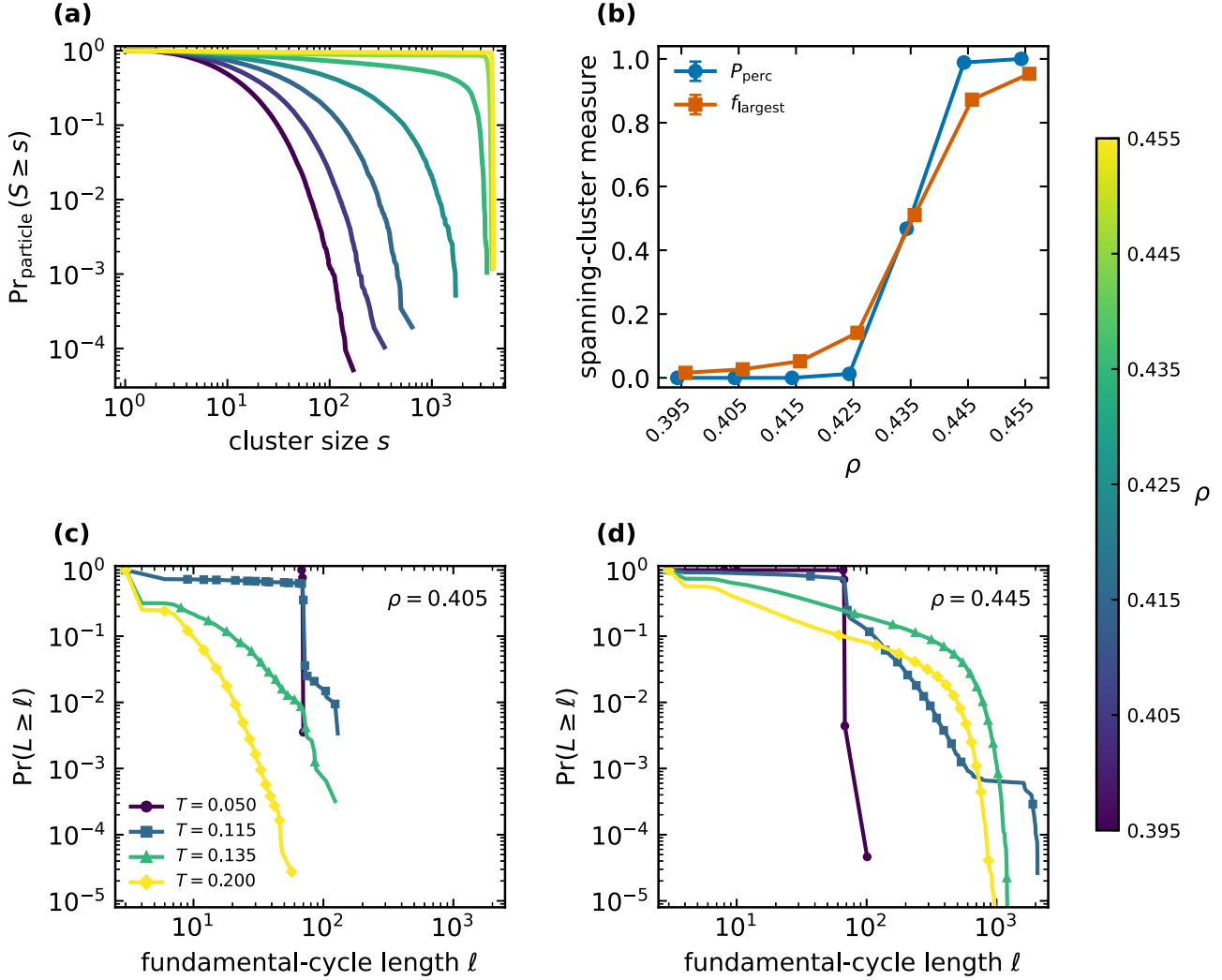


FIG. 6. Density-selected topology of the high-temperature fluid. (a) Particle-weighted cluster-size complementary cumulative distributions at  $T = 0.20$ . (b) Percolation probability and fraction of particles in the largest cluster at the same temperature. Number-weighted complementary cumulative distributions of fundamental cycle lengths at selected temperatures for (c)  $\rho = 0.405$  and (d)  $\rho = 0.445$ . Error bars in (b) are standard errors over four independent runs and are smaller than the data points.

At  $\rho = 0.445$  [Fig. 6(d)], short cycles also become numerous after loss of stripe order, but they coexist with a much broader tail. At  $T = 0.20$ , the median cycle length is approximately 7, the 90th percentile is about 65, and rare cycles extend to more than  $10^3$  particles. Local restructuring and system-spanning connectivity therefore coexist in the dense fluid. Because short loops attached to the percolated backbone contribute to  $\beta_1^{\text{wind}}$ , this broad, two-scale distribution provides the geometrical counterpart of its post-melting increase in Fig. 3(b). Branching points can mediate restructuring between locally ordered aggregate segments [69]; in the present system, increasing density converts this local reconnection mechanism into the means by which a winding network survives orientational melting.

The relation between the structural, topological, and thermodynamic temperature scales is collected in Fig. 7. The orientational response  $\mathcal{R}_2$  has a well-defined maximum at

every density [Fig. 7(a)]. The susceptibility  $\chi_2$  [Fig. 7(b)] and the heat capacity  $c_V$  [Fig. 7(c)] peak in the same temperature interval within the resolution  $\Delta T = 0.005$ . Their common density dependence is nonmonotonic: the characteristic temperature increases from approximately 0.13–0.135 at  $\rho = 0.395$  to 0.14–0.145 around  $\rho = 0.415$ –0.425, and then decreases to 0.12 at  $\rho = 0.455$ .

The characteristic-temperature map in Fig. 7(d) demonstrates that coincidence of the orientational and thermodynamic responses does not imply a simultaneous topological conversion. Up to  $\rho = 0.425$ ,  $T_{\text{cross}}$  rises toward the response line while remaining slightly lower. At  $\rho = 0.435$ , it instead moves to approximately 0.155, above the maxima of  $\mathcal{R}_2$ ,  $\chi_2$ , and  $c_V$ . At  $\rho = 0.445$  and 0.455, a winding-to-nonwinding crossover is not reached within the simulated temperature interval, as indicated by the open triangles. The thermodynamic signature is thus associated primarily with loss of stripe

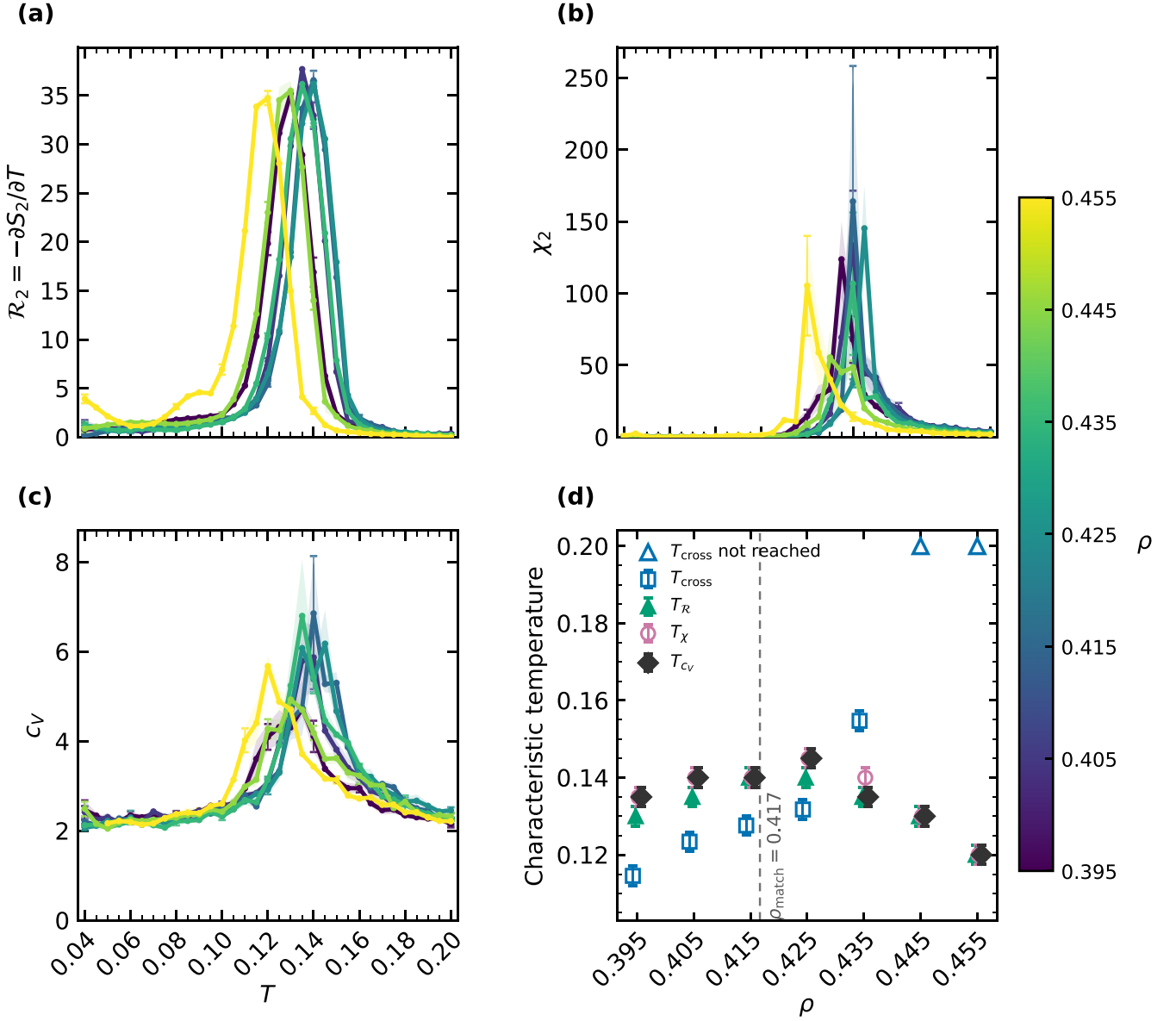


FIG. 7. Structural and thermodynamic response across density. (a) Orientational response  $\mathcal{R}_2 = -\partial S_2/\partial T$ , (b) orientational susceptibility  $\chi_2$ , and (c) heat capacity per particle  $c_V$ . The two lowest-temperature state points at  $\rho = 0.455$  are omitted from panel (c) because the energy records retain nonstationary relaxation of the prepared initial configuration; they are not thermodynamic fluctuation estimates. (d) Density dependence of the winding-nonwinding crossover temperature  $T_{\text{cross}}$  and the maxima of the three response functions. The vertical dashed line marks  $\rho_{\text{match}} = (1.2 \times 2.0)^{-1} \simeq 0.417$ . Open triangles at  $T = 0.20$  identify densities for which  $T_{\text{cross}}$  was not reached. Shaded bands and sparse error bars in (a)–(c) denote standard errors over independent replicas; temperature error bars in (d) represent half the simulated temperature increment.

orientational order, whereas the topology of the disordered fluid is selected by density and can remain winding well beyond that loss.

The nonmonotonic response line can be related to the two geometrical scales of the stripe construction. With  $a_\perp/a_\parallel = 5/3$ , simultaneous matching to  $a_\parallel = 1.2\sigma$  and  $a_\perp = 2.0\sigma$  occurs at  $\rho_{\text{match}} = (1.2 \times 2.0)^{-1} \simeq 0.417$ , indicated by the vertical dashed line in Fig. 7(d). The maximum of the orientational and thermodynamic response temperatures lies close to this reference. Moving to either side stretches or compresses both imposed separations relative to these interaction-selected values, providing a natural source of geometric frustration. This geometrical matching is consistent with the observed

nonmonotonic density dependence of stripe stability, although it should be regarded as a structural reference rather than an independent determination of a phase boundary. The conversion to the connected high-density fluid occurs only beyond this matching point. For example,  $a_\perp$  decreases from approximately  $2.00\sigma$  at  $\rho = 0.415$  to  $1.94\sigma$  at  $\rho = 0.445$ , increasing the opportunity for contacts and reconnections between neighboring filaments. Such sensitivity of modulated morphologies to competing scales and geometric frustration is a generic feature of stripe-forming systems [1,2].

At fixed  $N$ , increasing density also reduces both periodic box lengths as  $\rho^{-1/2}$ ; between  $\rho = 0.395$  and  $0.455$  the reduction is about 6.8%. This can enhance the probability

that a connected object closes through a periodic boundary and therefore contributes to the measured winding and percolation probabilities. It is not, however, equivalent to reducing the number of particles along a stripe, which remains fixed in the present construction. We consequently interpret the interval  $\rho = 0.435\text{--}0.445$  as a finite-size-broadened connectivity crossover between cluster- and network-dominated fluids rather than assign a sharp density-driven transition to it.

The system-size analysis reported in the Supplemental Material shows that the high-density network is not generated solely by periodic closure in a small simulation box. At  $\rho = 0.445$  and  $T = 0.18$ , the winding probability remains above 0.979, while the largest connected component contains approximately 89% of the particles for  $N = 1024, 4096$ , and 16384. Moreover,  $\beta_1/N$  and the 2-core fraction closely collapse for the three sizes. In contrast, the winding probability and largest-cluster fraction decrease with  $N$  on the low-density side. These findings support a robust distinction between the finite-cluster and winding-network regimes, while confirming that the intermediate density range remains a finite-size-broadened connectivity crossover.

The winding label is used here as a finite-system diagnostic of macroscopic connectivity, not as an intrinsic bulk order parameter. The specific winding vector of the prepared state depends on the periodic cell and on the commensurate orientation of the stripes. Likewise, the absolute number and length of its low-temperature winding cycles are cell dependent. This contribution is subextensive,  $\beta_1^{\text{wind}}/N \sim N^{-1/2}$ , and is therefore separated explicitly from the extensive local cycle population. The evidence distinguishing the two disordered regimes does not rely on the absolute cycle count associated with the (1,0) initial array: on the low-density side the cluster distribution converges to finite objects and  $P_{\text{wind}}$  vanishes with increasing size, whereas at  $\rho = 0.445$  an approximately size-independent fraction of 0.89 of all particles belongs to a single connected object and the intensive 2-core and cycle densities converge. In a finite experimental field of view with open boundaries, the corresponding distinction would be between bounded clusters and a connected backbone spanning opposite sides of the observation window; the local measures of endpoints, branches, loops, curvature, and 2-core membership require no periodic boundary. The present protocol follows the same well-defined initial winding sector at all densities; it does not test kinetic memory across distinct commensurate  $(p, q)$  preparations.

#### IV. CONCLUSION

The thermal disordering of one-particle-thick stripes proceeds through coupled but distinct structural, topological, and dynamical changes. Upon heating, the initially aligned stripes bend and lose global orientational coherence while retaining substantial local twofold organization. The orientational

response, susceptibility, and heat capacity identify a common thermal interval for this loss of stripe order, whereas connectivity evolves over a broader and density-dependent temperature range. Stripe melting is therefore not a single transformation in which all signatures of order disappear simultaneously.

Density determines the topology selected after orientational melting. At lower densities, winding stripe backbones open and fragment into finite polymerlike clusters containing predominantly short, nonwinding loops. At higher densities, branching and reconnection preserve a cycle-rich, system-spanning network, with intermediate densities displaying a crossover between these outcomes. This distinction also explains the density-dependent nonmonotonicity of  $\beta_1$ : its high-temperature increase reflects local cyclization within finite clusters at low density, but reticulation of a winding network at high density, rather than recovery of the ordered stripe topology. Both regimes remain diffusive, so the persistent high-density network is a continuously restructuring fluid rather than an arrested gel.

Topology-conditioned mobilities provide a microscopic picture of this reconstruction. Endpoints become mobile before the principal orientational transformation, whereas branches emerge later through contacts and reconnections between curved filament segments. This close coupling between contour fluctuations and connectivity follows from the one-particle thickness of the stripes, which leaves no bulklike interior that can disorder independently of their boundaries. More broadly, the results show that orientational and thermodynamic observables alone do not determine the connectivity of the melted state. Combining them with graph topology and particle dynamics provides a general framework for describing the melting of narrow filamentary microphases.

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#### DATA AVAILABILITY

The data that support the findings of this study were generated by numerical simulations. The source code and parameters used to generate the simulations and to analyze the trajectories are publicly available in [70].

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