Matter self-assembling into layers generates unique properties, including structures of stacked surfaces, directed transport, and compact area maximization that can be highly functionalized in biology and technology. Smectics represent the paradigm of such lamellar materials—they are a state between fluids and solids, characterized by both orientational and partial positional ordering in one layering direction, making them notoriously difficult to model, particularly in confining geometries. We propose a complex tensor order parameter to describe the local degree of lamellar ordering, layer displacement and orientation of the layers for simple, lamellar smectics. The theory accounts for both dislocations and disclinations, by regularizing singularities within defect cores and so remaining continuous everywhere. The ability to describe disclinations and dislocation allows this theory to simulate arrested configurations and inclusion-induced local ordering. This tensorial theory for simple smectics considerably simplifies numerics, facilitating studies on the mesoscopic structure of topologically complex systems.

Layered materials are key components in many technological, biological and fluidic systems. Graphene, MXene and other two-dimensional materials are composed of atomistically thin sheets with only weak out-of-plane bonding. Moreover, layering is a widespread strategy for increasing the surface area of organs, as in the friction ridges that make up fingerprints (Fig. 1a), convolutions within the cortex of human brains, and the enormous surface area of intestinal villi. At the subcellular level, the Golgi apparatus, rough endoplasmic reticulum, and cristae in mitochondria all possess many folds and creases. Layered fluids include liquid crystalline cholesterics which form “pseudolayers” via their helicity and, most plainly, smectics composed of stacks of orientationally aligned molecules that maintain fluidic disorder within each layer.

The lamellar structure of stacked layers produces fascinating properties. The smectic ground state consists of flat, equally spaced, layers for which both translational and rotational symmetries are broken. Because layers locally break translational symmetry, dislocation-type defects are allowed, while broken rotational symmetry of the layering direction results in a singularity of the layer normal, allowing disclination-type defects (Fig. 1b). This makes smectics excellent systems for exploring self-assembly and topology, especially in confining geometries or in contact with micropatterned structures.

However, the very properties that make these lamellar phases so interesting also contrive to make them challenging to model. Any order parameter that contends to describe simple smectics, i.e., lamellar phases without underlying nematic order, must explicitly include three pieces of information: (i) the degree of ordering, (ii) dilation/contraction of layers’ spacing and (iii) the direction/bending of layers, either through its instantaneous value or gradients. Since the 1970s, it has thus been recognized that a complex scalar order parameter can be employed to incorporate this information, which leads to a strong analogy to superfluids and superconductors. However, such a complex order parameter faces many difficulties. Fundamentally, these issues arise because complex scalar order parameters assume a global layer normal direction is known and that the layers only vary about this well-defined direction.

To circumvent this shortcoming, theoreticians have modeled smectic-A liquid crystals by coupling models of smectic ordering to the nematic order parameters for the orientation of rod-like molecules. While sensible for smectic liquid crystals with inner-layer nematic ordering, this does not fundamentally solve the issue for many non-
Fig. 1 | A catalog of defects in 2D smectics. a Single defects marked on a high resolution photo of a fingerprint. +1/2 disclination, −1/2 disclination and edge dislocation marked by red cross, yellow trilateral and red circle, respectively. b Schematics of (left) +1/2 disclination, (center) −1/2 disclination and (right) dislocations. c–k Simulations of defects for model parameters $\lambda = -1$ (lamellar state), $C = 2$ and $\kappa^2 = 0.75$ in circular domains with boundary conditions requiring single defects. Columns present three defect types: (first column) +1/2 disclination; (second) −1/2 disclination; (third) edge dislocation. Rows show plots of: c–e layer visualization $\text{Re}[\Psi]$; f–h modulus $|\psi|$ with N overlaid; i–k phase $\phi$ with N.

nematic lamellar materials, which have their own intrinsic rotational symmetry breaking. Furthermore, these approaches model smectics at the microscopic level, resolving each layer at length scales comparable to the molecular size. This makes such models computationally expensive for mesoscale and hydrodynamic modeling.

Recent studies of defect annihilation in block copolymer films\(^\text{32,33}\) and confined smectic colloidal liquid crystals showing unique pairs of quarter-charge topological defects connected by domain wall bridges\(^\text{34,35}\) motivate the need for alternative theoretical descriptions for simple smectics that allow simulations to tackle more topologically complex structures without relying on micr..
In this article, we propose a tensorial order parameter field for simple, lamellar smectics. The tensor $E(r, t)$ is complex, symmetric, traceless and globally gauge invariant. It incorporates the extent of layering and relative layer displacement, as well as the layer normal orientation. It encompasses the advantages of tensor formalism providing to nematics but for simple smectics. Here, we exclusively consider the simplest smectics, with only lamellar broken translational symmetry and layer-normal broken rotational symmetry. Such simple lamellar ordering is observed in systems with little-to-no nematic ordering, such as the striped phases of short-range attraction and long-range repulsion colloidal systems, colloidal liquid crystals and active fluids, by treating defects as locally disordered cores, rather than singularities. Explicitly, the tensor $Q$ describes mesoscopic variations of the scale of individual layers, these issues can be avoided with negligible cost, akin to a membrane curvature free energy density. We again consider a Landau free energy expansion. The total free energy density $f$ is the sum of bulk and two deformation (compression and curvature) terms. All contributions to the free energy must be real, requiring pairings of $E$ and its complex conjugate $\bar{E}$. Furthermore, the free energy should not depend on $E$ in a manner that is equivalent to a direct dependence on the phase, since it can be globally shifted.

### Results

In this article, we propose a tensorial order parameter field for simple, lamellar smectics. The tensor $E(r, t)$ is complex, symmetric, traceless and globally gauge invariant. It incorporates the extent of layering and relative layer displacement, as well as the layer normal orientation. It encompasses the advantages of tensor formalism providing to nematics but for simple smectics. Here, we exclusively consider the simplest smectics, with only lamellar broken translational symmetry and layer-normal broken rotational symmetry. Such simple lamellar ordering is observed in systems with little-to-no nematic ordering, such as the striped phases of short-range attraction and long-range repulsion colloidal systems, colloidal liquid crystals and active fluids, by treating defects as locally disordered cores, rather than singularities. Explicitly, the tensor $Q$ describes mesoscopic variations of the scale of individual layers, these issues can be avoided with negligible cost, akin to a membrane curvature free energy density. We again consider a Landau free energy expansion. The total free energy density $f$ is the sum of bulk and two deformation (compression and curvature) terms. All contributions to the free energy must be real, requiring pairings of $E$ and its complex conjugate $\bar{E}$. Furthermore, the free energy should not depend on $E$ in a manner that is equivalent to a direct dependence on the phase, since it can be globally shifted.

### Bulk

Since $E$ is traceless, the bulk smectic free energy density can be written

$$f_{\text{bulk}}(E, N) = \frac{A}{2} \varepsilon_2 E_{ij} E^{ij} + \frac{C}{4} \left( E_{ij} E^{ij} \right)^2 + \ldots$$

where $C > 0$, and Einstein summation convention is adopted. Lamellar order is established when $A < 0$, but the fluid is isotropic when $A > 0$. The bulk free energy does not depend on phase or layer normal, but only on $|\psi|$. This form is consistent with scalar-based bulk free energies (see Methods). In the mean-field limit, Eq. (2) predicts a second order phase transition.

### Compression

Lamellae possess two deformation modes: (i) compression, and (ii) curvature of the layers. We consider first compression free energies, which involve derivatives of the tensor order parameter. The simplest such term is $E_{ij} E_{ij}$, where $k$ denotes the direction of the gradient. Additional real terms could be constructed through combinations of similar forms, which would allow different deformation modes to possess differing elastic moduli. For clarity, we make a one-constant approximation

$$f_{\text{cl}} = b_1 E_{ij,k} \varepsilon_{ij,k},$$

where $b_1$ is a layer compression elastic constant. Equation (3) accommodates first order distortions of the layer normal, as well as contributions due to gradients of the complex amplitude $\psi$. In a vector-based model, defects would create topological singularities in the layer normal field, making gradient terms in Eq. (3) irregular; however, $E$ regularizes the singularities and Eq. (3) is continuous.

### Curvature

Distortions from uniformly aligned layers come with a free energy cost, akin to a membrane curvature free energy density. We again make a one-constant approximation and keep only the simplest term

$$f_{\text{curv}} = b_2 E_{ij,k} \varepsilon_{ij,k},$$

where $b_2$ is a bending modulus.
By inserting the eigenvalue and associated eigenvector via Eq. (1) into the free energy contributions (Eqs. (2)–(4)), one can directly compare E-theory to existing models of smectics (Methods). When the lamellae phase is free of deformations, minimizing the free energy produces the equilibrium value

$$|\psi|^2 = \begin{cases} \sqrt{-\frac{\Lambda}{\sigma}} & \text{if } A \leq 0 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

where $\sigma = (d - 1)/d$, which is in agreement with complex scalar Landau models. In our model, $\mathbf{E}$ is a hydrodynamic-scale field that does not involve layer spacing, so imposing an equilibrium wave number would require that covariant derivatives replace gradients. At equilibrium, the free energy density is $\mathcal{F}_t = -\frac{\sigma}{4}(1 - \frac{\Lambda}{\sigma})$. In contrast to nematics, the free energy possesses two material length scales: (i) coherence length $\xi = \sqrt{b_i/\Lambda}$ and (ii) penetration depth $\lambda = \sqrt{b_i/\xi}$. The coherence length $\xi$ characterizes the defect core size and the ratio of $\kappa = \Lambda/\xi$ is a Ginzburg parameter. As in superconductors, $\kappa \leq 1/\sqrt{2}$ is a type-I system, while $\kappa > 1/\sqrt{2}$ is type-II. We also take the strong anchoring limit by fixing $\mathbf{E}$ at solid surfaces.

Proven numerical schemes exist for minimizing the free energy of real $\mathbf{Q}$ tensors. The numerical difficulty lies in extending the methodology to allow for complex tensor elements. We employ a gradient descent time evolution of $\mathbf{E}(\mathbf{r}, t)$ in 2D (see Methods). Defining the total free energy $F(t) = \int \mathcal{F}(\mathbf{E}(\mathbf{r}, t), \mathbf{V}(\mathbf{E}(\mathbf{r}, t)))$ we adopt a time-dependent Ginzburg-Landau model

$$\mu \frac{\partial \mathbf{E}}{\partial t} = -\frac{\delta \mathcal{F}}{\delta \mathbf{E}} + \mathbf{A}_{\psi}, \tag{6}$$

where $\mu$ is a mobility coefficient and $\mathbf{A}$ constrains $\mathbf{E}$ to be traceless and normal (see Methods). It should be stressed that $\mathbf{E}(\mathbf{r}, t)$ is the sole subject of all calculations—the complex amplitude $\psi(\mathbf{r}, t)$ and layer normal $\mathbf{N}(\mathbf{r}, t)$ are only found ex post facto. Both $|\psi|$ and $\phi$ are calculated directly from contractions of $\mathbf{E}$ with itself, while $\mathbf{N}$ is found via eigen-decomposition (see Methods). Defects are identified from the $\mathbf{N}$ and $\phi$ fields (see Methods). While our approach circumvents the ambiguity of $\mathbf{N}$ as a double-valued function $\text{Re}[\mathbf{N}] \pm \text{Im}[\mathbf{N}]$, the post-processing visualizations based on $\text{Re}[\mathbf{N}]$ introduce aberrations that $\mathbf{E}$ itself does not possess. It is clear that these aberrations (see Fig. 1c–e, Fig. 2 and Methods) are not visible in the $|\psi|$ or $\phi$ fields, appearing only as a result of reintroducing the microscopic layer structure.

**Discussion**

The ability of $\mathbf{E}$-theory to model simple smectics is probed by simulating a variety of confining geometries (Fig. 2). We first demonstrate that individual aspects of the order parameter can vary independently. In a long slit with $\mathbf{N}$ strongly anchored parallel to the walls, a temperature gradient is modeled via a linear increase of the bulk free energy (Eq. (2)) parameter $A$ from $-1$ to $1$ (Fig. 2a). This causes $|\psi|_r$ to decrease, going from an ordered lamellar state on the left to the isotropic state with $|\psi|_r = 0$ on the right, in agreement with Eq. (5), and without variation of $\phi$ or $\mathbf{N}$. After minimization of the free energy, $\text{Re}[\mathbf{N}]$ visualizes the lamellar structure and the layer normal reflects the direction of layering (Fig. 2a). Similarly, the phase $\phi_\mathbf{r}$ can be varied within a long slit without variation of $|\psi|_r$ or $\mathbf{N}$ by linearly increasing the phase over a narrow region of the channel walls (Fig. 2b). Again, $\mathbf{N}$ is strongly anchored parallel to the walls, which causes compressional distortion—the layers to dilate, as seen from $\text{Re}[\mathbf{N}]$. The final pure type of deformation is distorting $\mathbf{N}(\mathbf{r})$. To create this deformation, the smectic is confined within an annulus with strong homeotropic anchoring of the layer normal (Fig. 2c). This geometry produces pure bend distortion with no compression that changes $\phi$. Not all geometries allow the aspects of the order parameter to vary independently, as accomplished by Fig. 2a–c; in general, we expect some interplay between deformation modes as in Fig. 3.

There are two classes of defects in smectic systems (Fig. 1). The first relates to singularities in the layer normal $\mathbf{N}$, in which $\mathbf{N}$ rotates by $2\pi n\mathbf{N}$, $\mathbf{N}$, we show this occurring in two ways: (i) A $m_\mathbf{N} = -1/2$ disclination with a 180-degree folding of smectic layers around the defect core (Fig. 1b; left) or a $m_\mathbf{N} = -1/2$ disclination in which the layers exhibit a trifold symmetry (Fig. 1b; center). (ii) An irregularity in the layer structure, which represents an insertion/deletion of layers at a point (Fig. 1b; right). To identify and measure the respective charges of these, we measure winding numbers using a closed contour integral (Methods). To explore the capacity of this model to describe smectic defects, consider a circular confining domain with boundary conditions requiring a single $+1/2$ disclination (Fig. 1c). After minimization of the free energy, $\text{Re}[\mathbf{N}]$ depicts the lamellar structure around the disclination (Fig. 1f). Since $\mathbf{N}$ is the layer normal, it mirrors the layers (Fig. 1f, i). The lamellar structure exhibits the expected symmetries of a $+1/2$ disclination and deformations are primarily bend on one side of
the defect and splay on the other\textsuperscript{2}. The lamellae are highly ordered away from the defect with $|\psi| \to |\psi|^\text{eq}$. However, $|\psi| \to 0$ in the defect core (Fig. 1d), verifying that $E$-theory permits a finite sized defect core. Crucially, $E$ remains continuous at the center of the defect, regularizing the singularity in $N$. The deformations are principally curvature distortions, rather than compression, which is reflected in a constant phase everywhere in the vicinity of the disclination (Fig. 1i). We find no evidence of any artificial order parameter melting where $\phi \to \phi$, suggesting that the non-physical line tension and associated free energy penalty observed in simulations of folded layers using two-dimensional scalar theories\textsuperscript{30} is absent (Supplementary Fig. 1). The situation is analogous for a $\pm 1/2$ disclination (Fig. 1d): The layers are visualized by Re[$\Psi$] (Fig. 1d), with perpendicular layer normals (Fig. 1g, j). The defect core is again seen to be locally disordered with no variation in phase, indicating negligible compression. In both $\pm 1/2$ disclinations, the free energy density is largest in the immediate vicinity of the cores (Supplementary Fig. 2). Not only is $f$ non-constant only at the core, but the deformation energy densities are strongly localized\textsuperscript{2}. In addition to half-integer disclinations, $E$-theory has the capacity to simulate $\pm 1$ disclinations that have been observed in theoretical and numerical studies\textsuperscript{23,24}. Energy density, $\Delta f(\{A\})$, for small ($14\times 14$) and large ($42\times 42$) systems. Shading represents the standard deviation. $f$-theory: since theories of $\phi$ alone cannot model independent disclinations and models that simulate $Q$ near the nematic-smectic transition cannot replicate dislocations. While disclinations and dislocations are considered separately in Fig. 1, they can co-reside in a single defect.

We now consider the role of defects in lamellar states evolving to equilibrium by simulating 2D systems with a deep quench from the isotropic to lamellar state, and periodic boundary conditions (Fig. 3). At first, the system is disordered (Fig. 3a), but relaxes through defect annihilation (Fig. 3b) to form many locally ordered domains (Fig. 3c). However, even at the longest times, the system remains disordered on mesoscopic scales: It is kinetically arrested into a glassy configuration\textsuperscript{17} with a non-zero number of defects (Fig. 3d). In this glassy state, domains for which $N$ is rotated by $\pi/2$ (Fig. 3c, g), which is allowed by $E$-theory, is the bridge-type line boundaries observed in 2D colloidal smectics\textsuperscript{14}.

To clarify this pinning of long-lived non-equilibrium structures, we compare simulations of large and small systems. While the small system routinely relaxes to the fully ordered lamellar state (Fig. 3e; inset and Supplementary Movie 1) with $\lim_{t \to \infty} |\psi| \to |\psi|^\text{eq}$, the large system never reaches the global equilibrium (Fig. 3c). Correspondingly, the free energy of the small system rapidly approaches $f^\text{eq}$, the equilibrium defect free value; whereas, the large system is inevitably trapped away from equilibrium (Fig. 3e). Snapshots and associated videos show that both disclinations and edge dislocations are pinned (Fig. 3f, g and Supplementary Movie 2). This highlights the importance of defects in lamellar ordering kinetics and the challenge posed for lamellar self-assembly\textsuperscript{20,21,22,23}. In contrast to the continual relaxation...
dynamics through annihilation in nematic liquid crystals, the kinetic arrest of coarsening and long-lived domains are associated with pinned defects (Fig. 3e). This implies an energy barrier associated with the sliding of dislocations with respect to the lamellar structure. This indicates the possibility of non-zero Peierls-Nabarro energy barriers, further validating of the E formulation.

The presence of inclusions embedded within the lamellar material can act to locally order layers or to induce additional defects. We evaluate boundary-induced lamellar ordering within an isotropic fluid (A > 0), due to strong anchoring to a circular inclusion (Fig. 4a). An inclusion with strong planar anchoring of N and \( \psi = e^{-\infty} \) locally layers the smectic but the ordering rapidly decays (Fig. 4a). By fitting an exponential to \( |\psi| \) in a channel geometry, we extract the decay length \( \xi \) (Fig. 4b). We see that the decay length varies inversely with the Ginzburg parameter \( \kappa \), indicating \( \xi \) varies linearly with lamellar coherence length \( \xi \). While strong anchoring locally orders the isotropic phase, it induces a pair of defects in the lamellar phase (Supplementary Movie 6). The steady-state can be seen from the layer normal field (Fig. 4c) or directly from the qualitative layer visualization via Re[\( \psi \)] (Supplementary Fig. 4a). The topological charge of the circular inclusion is neutralized by the two \(-1/2\) disclinations on opposite poles of the inclusion. The resemblance to a nematic system follows from their shared \( \pi \)-rotational symmetry. Outside of the defect cores, the smectic remains well ordered and the deformation free energy contributions are localized around the inclusion (Supplementary Fig. 5). This demonstrates the E-formalism can be employed for nontrivial geometries.

In strongly confined two-dimensional smectics composed of colloidal silica rods, it has recently been reported that half-charge \( \pm 1/2 \) disclinations can expand into grain-boundary lines capped by pairs of end-point \( \pm 1/4 \) charge defects. These quarter-charge defects have been numerically reproduced using microscopic density functional theory and explored using extensive Monte Carlo simulations but are yet to be described by a mesoscopic continuum theory. To demonstrate the complex tensor E description has the capacity to simulate such defect structures, a circular inclusion is once again embedded in a simple smectic (as in Fig. 4), but initialized with a significant difference of phase \( \phi \) at the inclusion surface compared to the bulk (Fig. 5b). This causes the \(-1/2\) disclinations seen in Fig. 4 to each split into two \(-1/4\) charge end-point defects capping a bridging line boundary. Such behavior is not expected nor observed in nematic liquid crystals, and does not arise in Q-tensor theories of nematics but can be reproduced by the E-tensor formalism for lamellar fluids. Both of the new quarter-charge end points are seen to possess disordered defect cores in which \( |\psi| \rightarrow 0 \) (Fig. 5a). The phase \( \phi \) changes discontinuously across the line boundary and a \( n/2 \) misalignment of the layer normal occurs (Fig. 5b). This can also be seen in the plots of Re[\( \psi \)] (Supplementary Fig. 4b). However, if the phase is integrated around the whole structure, rather than through the line boundary, the winding number of the phase of the structure is zero (Fig. 5d).

While the end-point defect cores have a free energy cost, no free energy cost is associated with the line boundary (Fig. 5c). In 2D, the eigenvalues of the traceless E differ by only a sign. This reflects the fact that a 2D smectic system can be described equally well by the layer normal N or the perpendicular layer tangent. Indeed, the layer normal and layer tangent can be swapped so long as \( \phi \rightarrow \phi + \pi \), thereby exchanging the signs of the eigenvalues. This suggests that such line boundaries are only possible in 2D, since the eigenvalue associated with the layer normal in 3D is distinct from the two degenerate eigenvalues associated with the pair of in-plane unit vectors.

Simulating the relaxation of a strongly anchored system in an annular confinement allows us to analyze the differing relaxation dynamics of both half- and quarter-charged disclinations. Systems initialized with no significant difference of phase \( \phi \) at the boundaries compared to the bulk see formation of half-charged disclination defects (Fig. 6a, b). Annihilation dynamics are consistent across repeated initializations with noise in \( \psi, \phi \) and N (Fig. 6b; inset). However, systems forming pairs of quarter-charge defect complexes (Fig. 6c, d) undergo much less consistent annihilation under equally varied initial conditions (Fig. 6d; inset), with 65% remaining after long times \((t > 150\mu)\). This is consistent with the dynamics observed in Fig. 3. By comparing the free energy density at times \( 5\mu \) before and after annihilation events, the mean free energy per unit area change for a pair of half-charge defects is \( (5.24 \pm 0.04) \times 10^{-13}/\mu \) compared to \( (3.8 \pm 0.5) \times 10^{-13}/\mu \). We note that quarter-charge defects are more costly per unit absolute topological charge than half-charge defects in these simulations, possibly accounting for their scarce creation in systems missing an enforced initial phase gradient of \( \phi \).

We have proposed a complex, symmetric, traceless, globally gauge invariant, normal, uniaxial tensorial order parameter \( E(r, \tau) \) for describing simple smectic phases at mesoscopic scales. As a second-rank tensor, \( E \) encodes the apolar nature of the layer normal in an arbitrary reference frame and circumvents the ambiguity of using a complex scalar order parameter. It does so without resorting to a microscopic approach, such as density functional theory, real-valued density variation or particle-based simulations, which also bypass such ambiguities but at a higher computational cost. While such microscopic models can simulate microscopic structure of individual layers, a numerically amenable framework for simulating the mesoscopic variations is advantageous for modeling configurations.
Phase b micropatterned substrates much like the introduction of grammable photoalignment and electrically reversible templating could be extended to simulate patterned defect arrays through programing photoalignment. For numerical modeling of nematics, we appeal and delve into more complex systems. Smectic textures in three dimensions can be idealized that does not require a well-defined nematic director as a prerequisite of spontaneous lamellar symmetry breaking. Liquid crystalline phases such as smectic-A or -C are composed of anisotropic molecules that also exhibit nematic ordering, and simulating these will require coupling of $E$ to $Q$, which is conceptually straightforward.

Additionally, the $E$-formalism should be extended to consider more complex systems. Smectic textures in three dimensions can be complex, appealing and difficult to model. The tensor theory could be extended to simulate patterned defect arrays through programable photoalignment, electrically reversible templating and micropatterned substrates. Much like the introduction of $Q$ helped expand the possibilities for numerical modeling of nematics, we expect this framework to be advantageous for simulating colloidal smectics, smectic-isotropic interfaces, smectic-smectic emulsions, smectics in contact with active material and swimming bacteria in smectics.

**Methods**

**Numerical methods**

We employ a gradient descent evolution of $E(r, t)$. This is to say that $E(r, t)$ obeys a time-dependent Ginzburg-Landau model, which follows the steepest decrease in global free energy under the constraints that it remain traceless and uniaxial. This is described by Eq. (6) in the main text and Eq. (16) in Methods.

The total free energy density is the sum of Eq. (2)-(4),

$$f = f^{\text{bulk}} + f^{\text{rel}} + f^{\text{surv}}$$

$$f^{\text{surv}} = \frac{A}{2} E_i E_i + \frac{C}{4} (E_i E_i)^2 + b_1 E_{i,k} E_{i,k} + b_2 E_{i,k,l} E_{i,k,l}.$$  

At each timestep, we use the instantaneous free energy density to calculate the right hand side of Eq. (6). The Lagrange multipliers can be found directly but the functional derivative term involves spatial derivatives. The system is discretised in space on a square grid of step size $\Delta r$. We employ a two-step Adams-Bashforth method to calculate $E$ at the next timestep, using a discrete time step of $\Delta t$. This is iterated for $T$ time steps. For Fig. 2, $\Delta t = 0.07C$, $\Delta t = 0.001\mu$. For Fig. 2, $T = 15000$, which amounts to a total simulation time of $15\mu$; for Fig. 1, $T = 20,000$.
choice of eigenvalue along each boundary and promulgate that numerical decision though the system. This decision prevents an artificial discontinuity in the layer normal along an arbitrary line due to a phase shift of $\pi$ swapping the signs of the eigenvalues, and hence the choice of corresponding eigenvector. This argument is avoided in 3D as the eigenvalues are $\psi_1, -\psi_2, -\psi_2$; so the eigenvalue with the largest modulus should always be chosen.

**Lagrange multipliers**

We enforced the fact that $E$ be traceless, uniaxial and a normal operator, which commutes with its own adjoint, in the numerics. This is essential for ensuring $E$ maintains real eigenvectors and allows us to interpret the $E$ after the simulations. These two conditions can be written as

$$g_1(E) = E_{ii} = 0$$

$$g_2(E) = \det\left(\begin{bmatrix} E & E^* \end{bmatrix}\right) = 0.$$  

where $[A, B] = AB - BA$ denotes the commutator. Using the Cayley–Hamilton Theorem and noting $g_2$ can be rewritten

$$g_2(E) = -\frac{1}{2} \text{tr}\left(\begin{bmatrix} E & E^* \end{bmatrix} E \right).$$

Decomposing $g_1$ into real and imaginary parts, $g_{1a} = \text{Re}[g_1]$ and $g_{1b} = \text{Im}[g_1]$, we introduce three real Lagrange multipliers, $\lambda_{1a}, \lambda_{1b}$ and $\lambda_2$, defined as

$$\lambda_{1a} = \text{Re}\left[\frac{1}{d} \frac{\delta F}{\delta E_{ii}} - \lambda_2 \frac{\delta g_2}{\delta E_{ii}}\right]$$

$$\lambda_{1b} = \text{Im}\left[\frac{1}{d} \frac{\delta F}{\delta E_{ii}} - \lambda_2 \frac{\delta g_2}{\delta E_{ii}}\right]$$

$$\lambda_2 = \frac{c_1}{c_2}.$$  

Where $c_1$ and $c_2$ are

$$c_1 = -\frac{\delta g_{1a}}{\delta Y_{ik}} X_{ik} Y_{jp} X_{pm} - Y_{ik} \frac{\delta F}{\delta X_{ik}} X_{jp} Y_{pm} + \frac{\delta F}{\delta X_{ik}} Y_{pm} - Y_{ik} \frac{\delta F}{\delta Y_{pm}} X_{jp} - Y_{ik} \frac{\delta F}{\delta Y_{pm}} Y_{jp}$$

$$+ \frac{\delta F}{\delta Y_{ik}} Y_{pm} + Y_{ik} \frac{\delta F}{\delta Y_{pm}} X_{jp} + Y_{ik} \frac{\delta F}{\delta X_{jp}} Y_{pm} + \frac{\delta F}{\delta X_{ik}} X_{jp} + \frac{\delta F}{\delta X_{jp}} Y_{pm} - \frac{\delta F}{\delta X_{ij}} Y_{jk} Y_{jp} X_{pm} - X_{ik} Y_{jk} Y_{jp} X_{pm} - X_{ik} Y_{jk} X_{jp} Y_{pm} - Y_{ik} X_{jk} X_{jp} Y_{pm}$$

$$c_2 = -\frac{\delta g_{1b}}{\delta Y_{ik}} X_{ik} Y_{kp} Y_{pm} - Y_{ik} \frac{\delta g_{1b}}{\delta Y_{kp}} Y_{pm} + Y_{ik} \frac{\delta g_{1b}}{\delta Y_{kp}} Y_{pm} + Y_{ik} \frac{\delta g_{1b}}{\delta Y_{pm}} Y_{kp} + \frac{\delta g_{1b}}{\delta Y_{ik}} Y_{kp} + \frac{\delta g_{1b}}{\delta Y_{kp}} Y_{pm} + \frac{\delta g_{1b}}{\delta Y_{kp}} X_{pm} + Y_{ik} Y_{jk} X_{kp} Y_{pm}$$

$$+ \frac{\delta g_{1b}}{\delta Y_{ik}} Y_{kp} Y_{pm} + X_{ik} Y_{jk} Y_{jp} Y_{pm} + X_{ik} Y_{jk} X_{kp} Y_{pm} + X_{ik} Y_{jk} X_{kp} Y_{pm} + Y_{ik} X_{jk} X_{kp} Y_{pm} + \frac{\delta g_{1b}}{\delta Y_{ik}} Y_{kp} Y_{pm}$$

$$+ \frac{\delta g_{1b}}{\delta Y_{ik}} Y_{kp} X_{pm} - X_{ik} Y_{jk} Y_{jp} Y_{pm} - X_{ik} Y_{jk} X_{kp} Y_{pm} - Y_{ik} X_{jk} X_{kp} Y_{pm} - X_{ik} Y_{jk} X_{kp} Y_{pm} - \frac{\delta g_{1b}}{\delta Y_{ik}} Y_{kp} Y_{pm}.$$  

and we have written $E = X + iY$ for real tensors $X$ and $Y$. We then introduce a dynamics that minimizes our free energy above with

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**Fig. 6** Annihilation of quarter- and half-charged disclinations exhibit different relaxation dynamics. Systems are initialized with (a, b) or without (c, d) a phase gradient between the bulk and boundary in annular confinements, leading to either two pairs of half-charged disclinations (a) or four pairs of quarter-charged disclinations (c). All parameters are as in Fig. 5. a The modulus $|\psi|$ for a system initialized to produce two pairs of half-charged disclinations at time $t=15\mu s$. b Temporal dependence of the free energy density, $\Delta f = f - f^0$, during the simulations with the a initialization. Black circles mark defect annihilation events. (inset) Temporal evolution of defect separation for each pair relative to the real tensor $N = \sum_i \text{Re}(\psi_i \psi_i^*)$ corresponds to one eigenvalue and $N^\perp = \sum_i \text{Re}(\psi_i \psi_i^*)$ to the other. c The $\phi$ field for a system initialized to produce four pairs of quarter-charged disclinations at time $t=15\mu s$. d Same as b but for quarter-charged annihilation dynamics.
respect to these constraints

$$\mu \frac{\partial E_{\alpha\beta}}{\partial t} = \frac{\delta F}{\delta E_{\alpha\beta}} + \delta_{\alpha\beta}(\lambda_{\text{Ia}} + \lambda_{\text{lb}}) + \lambda_2 \frac{\partial g_2}{\partial E_{\alpha\beta}}$$

(16)

With respect to the main text,

$$\lambda_{\alpha\beta} = \delta_{\alpha\beta}(\lambda_{\text{Ia}} + \lambda_{\text{lb}}) + \lambda_2 \frac{\partial g_2}{\partial E_{\alpha\beta}}.$$  

(17)

**Comparison to existing models**

Substituting the eigenvalue $\psi$ and vector $N$ into Eq. (1) produces explicit forms for the free energy densities in terms of $|\psi|$, $\nabla \psi$ and $N$. This allows us to compare to existing models. The bulk term (Eq. (2)) becomes

$$f_{\text{bulk}} = \frac{\sigma}{2} |\psi|^2 + \frac{C_0}{4} |\psi|^4,$$  

(18)

where $\sigma = (d - 1)/d$, which demonstrates the consistency between this complex tensor theory approach and scalar-based bulk free energies$^{67}$. Other possible real forms of the tensor $\sim (E + E)^T$ are zero, while terms of the form $\sim (E + E)^T (E + E)$ depend directly on $\phi$, which is non-physical. Therefore, such terms cannot be included in Eq. (2). The compression term (Eq. (3)) becomes

$$f_{\text{curv}} = \frac{\alpha}{2} |\psi|^2 |\nabla \psi|^2 + (\nabla \psi) \cdot (\nabla \phi) + (\nabla \nabla \psi) : (\nabla \nabla N),$$

(19)

where we have made use of the identity $N \nabla \nabla N = 0$, which is due to the fact that $N$ is a unit vector. Differentiating this again, we see that $(\nabla \nabla N) : (\nabla \nabla N) = (N \nabla \nabla N) = 0$, which we make use of below. Finally, the curvature term (Eq. (4)) is the most complicated, becoming

$$f_{\text{curv}} = \frac{\alpha}{2} \left[ |\nabla \psi|^4 - \frac{1}{|\psi|^2} (|\nabla \phi|^2 + 2 |\nabla \psi|^2) \right] + \frac{1}{2} \left[ \nabla \nabla \phi \cdot |\nabla \psi|^2 |\nabla \phi|^2 \right] + 4 \left( \frac{|\nabla \psi|^2}{|\psi|^2} \right) \cdot (\nabla \psi) \cdot (\nabla \phi) + \frac{1}{8} \left[ (\nabla \nabla \phi \cdot |\nabla \psi|^2 |\nabla \phi|^2) \right] + 4 \left( \nabla \nabla \phi \cdot |\nabla \psi|^2 |\nabla \phi|^2 \right)$$

(20)

where we have stated the contraction on the gradients in the last term using Einstein notation for clarity but have used vector notation elsewhere. It is worth re-emphasizing that none of the contributions to the free energy density depend directly on the phase $\phi$. In these forms, the E-tensor theory can be compared to existing models.

In the ground state equilibrium of flat, equally spaced, layers, the deformation free energy (Eq. (19) and Eq. (20)) are both zero. Only the bulk free energy $f_{\text{bulk}}$ (Eq. (18)) is non-zero and its form is consistent with scalar-based bulk free energies$^{66,67}$.

In the limit of fixed $\psi$ but variable $N$, only incompressible distortions are allowed. Taking $\psi$ to be constant, the deformation free energies (Eq. (19) and Eq. (20)) become

$$f_{\text{curv}} = \frac{\alpha}{2} |\psi|^2 |\nabla \psi|^2 + (\nabla \psi) \cdot (\nabla \phi) + (\nabla \nabla \psi) : (\nabla \nabla N),$$

(21)

$$f_{\text{curv}} = \frac{\alpha}{2} |\psi|^2 |\nabla \psi|^2 + (\nabla \psi) \cdot (\nabla \phi)$$

(22)

If we further only keep the lowest order term in the deformation free energy $\sim (\nabla \psi) \cdot (\nabla \phi)$, then this is precisely the nematic deformation free energy in the one-constant approximation$^{66}$. We note that this specifically does not lead to the Oseen constraint that twist be prohibited, a prevalent simplifying assumption in models of smectic materials, because we have explicitly made a one-constant elastic approximation for simplicity. In nematic models near the vicinity of the nematic-smectic A phase transition, the ratios of elastic constants significantly differ from unity$^{66}$. More intricate E-tensor theories that allow for differing elasticities will be able to make twist and bend of the layer normal (splaying of the layers themselves) come at an increased free energy cost.

We next presume that the layer normal is fixed globally along a constant axis and $|\psi|$ is constant, representing a smectic that is sufficiently deep within the lamellar phase. In this case, the deformation free energies (Eq. (19) and Eq. (20)) become

$$f_{\text{curv}} = \frac{\alpha}{2} |\psi|^2 |\nabla \psi|^2 + (\nabla \psi) \cdot (\nabla \phi)$$

(23)

$$f_{\text{curv}} = \frac{\alpha}{2} |\psi|^2 |\nabla \psi|^2 + (\nabla \psi) \cdot (\nabla \phi)$$

(24)

which together have the form $c_0 + B_1 |\nabla \psi|^2 + B_2 (|\nabla \phi|^2 + K (|\nabla \phi|^2)^2$ where we have included an arbitrary constant, assigned the $f_{\text{curv}}$ differing elastic coefficients, and absorbed $|\psi|^2$ into each coefficient. Moreover, for simplifying choics of constants, this becomes $f = B_1 (1 - (|\nabla \psi|^2)^2 + K (|\nabla \phi|^2)^2$, which is an existing model free energy density for smectics$^{66,70,77}$. We could also choose to write this in terms of a layer displacement $u = \phi - \phi_0$, making this free energy $f = B_1 (1 - (|\nabla u|^2)^2 + K (|\nabla \phi|^2)^2$. Models of this form are used to describe smectic systems$^{66}$ and are reminiscent of the de Gennes–McMillan form$^{70,71}$, although here we have made one-constant approximations for elasticity in the parallel and perpendicular directions. Furthermore, if the higher-order term $\sim (\nabla \psi) \cdot (\nabla \phi)^2$ term is neglected then Eqs. (23)-(24) reduces to the Brazovskii free energy, which is commonly employed to model lamellar diblock copolymers$^{60,70}$.

**Biaxiality**

In the present study, we have exclusively focused on 2D systems for which uniaxiality is maintained due to the tracelessness constraint (requiring eigenvalues to be equal and opposite). However, a degree of biaxiality could be conceived along a secondary direction in 3D. In three dimensional nematic liquid crystals, allowing biaxiality increases the number of degrees of freedom in the order parameter $Q$ from three in the uniaxial case to five. The two ancillary degrees of freedom represent the degree of biaxial alignment and the biaxial direction, constrained to be both a unit vector and orthogonal to the director. However, bulk biaxiality at equilibrium requires higher order terms in the expansion of the bulk free energy$^{70,71}$. The order terms were not included for biaxiality to naturally emerge in nematic defect core regions$^{70,71}$. This is because the three eigenvalues can be distinct in regions where the ordering goes to zero$^{70,71}$ and in strong confinements$^{70,71}$. Similarly, biaxiality in $E$ increases the degrees of freedom from four in the uniaxial case to seven. The three extra
degrees of freedom represent another degree of ordering, biaxial layer displacement and the secondary direction, constrained to be a unit vector orthogonal to $\mathbf{N}$. The biaxial case will not necessarily have a uniform complex phase across different components of the tensor and biaxiality at equilibrium would require higher order terms in the bulk free energy expansion (Eq. (2)).

**Defect identification**

To identify defects, we measure winding numbers

$$m_a = (2\pi)^{-1} \int_{\Gamma} \alpha \, da$$  \hspace{1cm} (25)

at each point over the smallest possible closed loop $\Gamma$, as a measure of topological charge. For dislocations, we measure the change in the layer normal azimuthal angle, $\alpha = \mathbf{N} \cdot dl$. Values of $m_a = \pm 1/2$ correspond to half-charge topological defects. For dislocations, $\alpha = \phi$ measures the displacement of layers and gives the strength of the Burgers vector.

**Layer visualization**

To visualize the layers, we use

$$\operatorname{Re}[\Psi] = |\psi| \cos(q_0 \mathbf{N} \cdot \mathbf{r} + \phi).$$  \hspace{1cm} (26)

Note however that this visualization technique does not respect the smectic symmetry; the focus is on providing an intuitive visual description of the layer structure. To calculate $\operatorname{Re}[\Psi]$, we use a Voronoi transformation of the plane into regions by defects and use the location of each defect as the origin for the dot product in Eq. (26). This numerical scheme gives good visualization of isolated defects in terms of layer structure (see Fig. 1c–e) but the transition from smooth $|\psi|$ and $\phi$ fields can introduce aberrations in defect-crowded regimes (see Fig. 3c). This is due to the ambiguity of the layer displacement that is not possessed when working in terms of $\mathbf{E}$ alone. Visualizations based on $\operatorname{Re}[\Psi]$ must necessarily re-introduce the shortcomings that $\mathbf{E}$ theory bypasses and so we generally avoid visualizations of $\operatorname{Re}[\Psi]$, except as a qualitative guide. Despite these disadvantages, we at times find it convenient to have an explicit, if rough, visualization of the layer configuration. The advantage of working with these fields can be seen in Fig. 3f, g and Supplementary Movies 2, 3. The resulting layer visualization is in Fig. 3c and Supplementary Movie 4.

**Data availability**

All data generated in this study are included in this published article (and its supplementary information files).

**Code availability**

Codes are available upon request.

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