Unifying polar and nematic active matter
Emergence and co-existence of half-integer and full-integer topological defects
Amiri, Aboutaleb; Mueller, Romain; Doostmohammadi, Amin

Published in:
Journal of Physics A: Mathematical and Theoretical

DOI:
10.1088/1751-8121/ac4abe

Publication date:
2022

Document version
Publisher’s PDF, also known as Version of record

Document license:
CC BY

Citation for published version (APA):
Unifying polar and nematic active matter: emergence and co-existence of half-integer and full-integer topological defects

To cite this article: Aboutaleb Amiri et al 2022 J. Phys. A: Math. Theor. 55 094002

View the article online for updates and enhancements.
Unifying polar and nematic active matter: emergence and co-existence of half-integer and full-integer topological defects

Aboutaleb Amiri¹, Romain Mueller² and Amin Doostmohammadi³, ∗

¹ Max Planck Institute for the Physics of complex systems, Dresden, Germany
² Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom
³ The Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark

E-mail: doostmohammadi@nbi.ku.dk

Received 10 August 2021, revised 21 December 2021
Accepted for publication 12 January 2022
Published 3 February 2022

Abstract
The presence and significance of active topological defects is increasingly realised in diverse biological and biomimetic systems. We introduce a continuum model of polar active matter, based on conservation laws and symmetry arguments, that recapitulates both polar and apolar (nematic) features of topological defects in active turbulence. Using numerical simulations of the continuum model, we demonstrate the emergence of both half- and full-integer topological defects in polar active matter. Interestingly, we find that crossover from active turbulence with half-to full-integer defects can emerge with the coexistence region characterized by both defect types. These results put forward a minimal, generic framework for studying topological defect patterns in active matter which is capable of explaining the emergence of half-integer defects in polar systems such as bacteria and cell monolayers, as well as predicting the emergence of coexisting defect states in active matter.

Keywords: active matter, topological defects, polar, nematic

(Some figures may appear in colour only in the online journal)

∗Author to whom any correspondence should be addressed.

Original content from this work may be used under the terms of the Creative Commons Attribution 4.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Topological defects denote singularities in the order parameter field, marking the regions where the order breaks down [1–3]. They are topological in the sense that no smooth local variation in the order parameter space can remove them [4, 5] and they are prevalent in various physical systems ranging from cosmic strings in particle physics model of early Universe [6] to vortices in superfluid helium films [1] and flux tubes in superconductors [7], to disclination lines in liquid crystals [8]. More recently, topological defects have been increasingly identified in biological systems. In analogy to liquid crystals, they mark singularities in the orientation field associated with the alignment of the constituents of biological systems. These range from topological defects in subcellular filaments such as actin [9, 10] or microtubules [11–13], to defects in bacterial alignment [14, 15], and topological defects in the orientation field associated with the elongation of fibroblasts [16], epithelial [17], and stem cells [18]. Remarkably, not only these topological defects are found within numerous biological systems, and across subcellular to multicellular scales, they appear to play an important role in various biological processes such as cell death and extrusion in epithelia [17], accumulation sites for bacteria and stem cells [15, 18, 19], and determinants of morphological features in bacterial colonies [20] and developing animal Hydra [21]. The distinguishing feature of these realizations of topological defects, compared to their counterparts in non-living systems, is that they are characterized by active flows continuously being generated due to the activity of the constituents of the living material (see [22, 23] for recent reviews of active topological defects).

Despite abundant and growing identifications of topological defects in various living biological systems, fundamental questions regarding their nature remain unanswered. One particularly puzzling observation is the abundance of half-integer defects (defects with nematic, head-tail, symmetry) in systems with an apparent polar symmetry such as motile bacteria [15, 19] and eukaryotic cells [17, 18, 24]. Polarity in this context determines the direction of motion of the self-propelled cell, and yet when multicellular collections of these polar entities are formed, such as in biofilm layers or epithelial monolayers, the emerging topological defects show half-integer charges—in systems with polar symmetry full-integer defects are expected [25, 26].

Indeed, continuum theories of polar active matter predict topological defects in the form of asters, vortices, and spirals that have a full-integer charge [26, 27] as has been reported for microtubule-motor protein mixtures [11, 28]. On the other hand, based on the emergence of half-integer defects in several cellular systems, most of existing continuum models treat these as active nematics, describing the coarse-grained alignment of constituent particles through nematic tensor, modeling activity through a stress term proportional to this nematic tensor, and neglecting polarity altogether. It is not clear how these distinct yet relevant symmetries compete in a real biological system, nor why half-integer defects emerge in active polar systems. Various coarse-grained models of self-propelled particles have been considered introducing separate equations for polarity vector and nematic tensor fields [29–33], and while recent experiments and agent-based models have reported coexisting polar waves and nematic bands in actomyosin motility assay [34], the study of topological defects in systems with mixed polar-nematic symmetry is non-existent and a generic theoretical framework for describing defect dynamics in such systems is lacking.

Here we address this problem by introducing a continuum formulation for polar active entities that shows the emergence of both half-integer and full-integer defects within one framework. Moreover, compared to the current active nematics models based on tensorial equations for the nematic orientation, we introduce a vector-based model that holds all the essential features and allows for recovering both polar and nematic topological defects.

We begin by describing a force balance equation governing both self-propulsion and active stress generation in the same active system. We describe the direction of self-propulsion by
a local polarity vector $\vec{p}$ such that each active particle generates a polar force $\vec{F}_{\text{pol}} = \alpha \vec{p}$, where $\alpha$ controls the force strength. In addition to this polar force, each particle generates a dipolar contribution to the active stress that can be described at leading order by the stresslet $\sigma^\text{active} = - \zeta \left( \vec{p} \vec{p}^T - p^2 \mathbf{I} / 2 \right)$ [35, 36], where $\mathbf{I}$ is the identity tensor, and $\zeta$ is the activity coefficient. The active contributions, from the polar force and active stress, are balanced by viscous and elastic passive stresses and any existing friction with the underlying substrate through the momentum equation

$$\rho \left( \partial_t \vec{u} + \vec{u} \cdot \nabla \vec{u} \right) = \vec{F}_{\text{pol}} + \nabla \cdot \sigma^\text{active} + \nabla \cdot \sigma^\text{passive} - \xi \vec{u},$$

(1)

where $\rho$ is the fluid density, $\vec{u}$ the velocity field that satisfies incompressibility condition ($\nabla \cdot \vec{u} = 0$), and $\xi$ the friction coefficient. The passive stress $\sigma^\text{passive} = -p \mathbf{I} + \sigma^\text{elastic} + \sigma^\text{viscous}$ comprises pressure $p$, elastic stress $\sigma^\text{elastic}$, and viscous stress $\sigma^\text{viscous} = 2\eta \mathbf{E} = 2\eta (\nabla \vec{u})^S$, where $\eta$ is the shear viscosity and $\mathbf{E}$ is the rate of strain tensor characterizing the symmetric part of the velocity gradient. The elastic stress $\sigma^\text{elastic} = \lambda_1 \vec{h} \vec{h}^T + \lambda_2 (\nabla \vec{h} - \frac{1}{2} (\vec{h} \cdot \vec{h}) \mathbf{I})$, is described in terms of the polarity field and its conjugate field $\vec{h}$ known as the molecular field (defined below), with $\lambda$ denoting the flow alignment parameter [4]. For completeness, we have retained all inertial terms and passive stresses in equation (1). In many biological realizations of active matter, including microscopic active particles, the inertia is negligible compared to strong viscous dissipation, and as such, the lhs of (1) drops out. Furthermore, elastic stresses are normally dominated by active contributions and are commonly neglected in studies of active systems [37, 38].

The velocity field is coupled to the spatio-temporal evolution of the polarity vector through:

$$\partial_t \vec{p} + \vec{u} \cdot \nabla \vec{p} + \lambda \mathbf{E} \cdot \vec{p} + \Omega \cdot \vec{p} = \frac{1}{\gamma} \vec{h},$$

(2)

where the flow alignment parameter $\lambda$ characterizes the response of the polar alignment to the symmetric and anti-symmetric parts of the velocity gradient tensor (denoted by the rate of strain $\mathbf{E}$ and vorticity $\Omega$ tensors, respectively), and $\gamma$ is the rotational viscosity that controls the relaxation of the polar alignment to the minimum of the free energy $\mathcal{F}$ through the molecular field $\vec{h} = -\delta \mathcal{F} / \delta \vec{p}$. The free energy is described as

$$\mathcal{F} = \int d\mathbf{x} \left\{ A \left( -\frac{p^2}{2} + \frac{p^4}{4} \right) + \frac{K_p}{2} (\nabla \vec{p})^2 + \frac{K}{2} \left( \nabla \left( \vec{p} \vec{p}^T - p^2 \mathbf{I} / 2 \right) \right)^2 \right\},$$

(3)

where the first term under the integral controls the isotropic-polar transition favoring the emergence of finite polarity at $|\vec{p}| = 1$. The nature of alignment interactions in our model is embedded in the gradient expansion terms in the elastic free energy in terms of order parameter $\vec{p}$ (the polarity field) given in equation (3). Physically, the second term in equation (3) means that any configuration rather than alignment of directions should cost energy, the amount of which is controlled by the parameter $K_p$. This is analogous to the gradient term in the mean-field description of Ising model (the term $(\nabla \vec{m})^2$, where $\vec{m}$ is the magnetisation) that penalises deviations from alignments of the neighboring spins [39]. However, by virtue of the symmetry, the additional third term in the definition of free energy is allowed and can be understood in a similar fashion: it accounts for energetic cost, characterised by $K$, of any configuration rather than alignment of orientations. Note that, unlike the polarity direction, the orientational alignment is head-tail symmetric, which is reflected in the construction $\vec{p} \vec{p}^T - p^2 \mathbf{I} / 2$, which forms the second moment of the polarity direction to make head and tail indistinguishable. As we show
here, the competition between the additional nematic elasticity, controlled by $K$, and the regular polar elasticity, controlled by $K_p$, allows for continuous transition between polar and nematic topological defects. As such the model presented here provides, generic, minimal continuum formulation of active self-propelled particles, with emergent polar and nematic properties.

We simulate equations (1) and (2) using a hybrid lattice-Boltzmann method, combining finite-difference method for the evolution of polarity vector equation (2), and the lattice-Boltzmann method for solving the Navier–Stokes equation equation (1) with $\rho = 40$ and $\eta = 1/6$ in lattice Boltzmann units, ensuring that the Reynolds number in the simulations is negligible $Re \ll 1$ [40,41]. Simulations are initialized by setting quiescent velocity field and random polar alignments and periodic boundary conditions are used on the domain of the size $L_x \times L_y = 1024 \times 1024$. We also repeated the simulations on both coarser and finer grids ($512 \times 512$ and $2048 \times 2048$, respectively). We find that for the resolution that we have used in the paper the formation of defects is independent of the discretization. The dimensionless ratio of the viscosities is fixed $\eta/\gamma = 1/6$, the alignment parameter is $\lambda = 0.1$, and the dimensionless activity $\bar{\zeta} = \zeta/A$ and elasticities $K_p/K$ are varied throughout this study. The winding angle approach is employed to identify topological defects in the system [42]. To verify the robustness of our defect detection method, we have compared this method with an alternative approach based on diffuse charge density [43] definition in previous studies [17,20] and have confirmed that they yield identical results.

We begin by investigating the case of pure apolar elasticity $K_p/K = 0$, setting the polar elasticity to zero ($K_p = 0$). Unless stated otherwise, we also set the polar force and friction to zero $\alpha = 0$, $\xi = 0$. Including such terms will allow for the emergence of flocking state and as such present interesting questions in terms of transitions between active turbulence to active flocking and possible co-existence between them, which is not the focus of the current study. Here, in this study, setting the polar force and friction to zero $\alpha = 0$, $\xi = 0$ reduces the number of parameters while still retaining the minimal physics that shows topological defect formation and the decisive role of the new apolar elastic term. As shown in figure 1(a), at statistical steady-state, the system evolves into active turbulence characterized by chaotic patterns of polar ordering and flow vortices [44,45]. Remarkably, the orientation field associated with the polarity vectors demonstrates the emergence of half-integer topological defects in the form of comet-shaped $+1/2$ and trefoil-shaped $-1/2$ defects, interleaving the vorticity patterns in the velocity field. This is striking since the emergence of such half-integer defects has so far been only associated to continuum active nematics where a nematic tensor is described to account for coarse-grained orientation of active particles [22, 46–48]. More importantly, measuring the average velocity field around the emergent half-integer defects confirms their self-propulsive feature and produces flow patterns in agreement with experimentally measured flow fields for twitching bacteria [15] and epithelial and progenitor stem cell layers [17,18,49] (see figure 1(b)). Additionally, the isotropic stress patterns characterizing the compressive and tensile stresses around the self-propelled defect are in agreement with the experimentally measured stresses for epithelial monolayers of Madine Darby canine kidney (MDCK) cells (figure 1(b)). Together, these results show that, at the limit of zero polar elasticity $K_p = 0$, our proposed minimal model reproduces the emergence and active dynamics of half-integer topological defects, from spatio-temporal evolution of the polarity vectors and without revoking any dynamic evolution for an additional nematic tensor.

We find that at the other limit of zero apolar elasticity $K = 0$ and finite polar elasticity $K_p/K = \infty$, the minimal model recovers the emergence of active turbulence interleaved by full-integer topological defects in the form of spiral vortex $+1$ and anti-vortex $-1$ defects (figure 2(a)). The existence of such full-integer defects in active polar systems has been predicted theoretically [26] and shown experimentally in motility assays of actin or microtubule
filaments where the motion is generated by motor proteins [9, 28, 50]. Furthermore, numerical studies have explored the hydrodynamics of interactions between pairs of full-integer defects in active polar systems [27], however—surprisingly—the emergence and dynamics of active turbulence interleaved with full-integer defects are not well-understood. In particular, earlier studies of the active polar systems did not find any full-integer defects in the active turbulence phase [51] and only recently it has been shown numerically that such defects can mark the transition from active polar turbulence to phase turbulence upon increasing polarity [52].

Importantly, when both polar and apolar elasticities are finite and non-zero, the minimal model predicts the emergence of an active topological state with a mixed symmetry. Here, the active turbulence, characterized by the emergence of vortices and jets in the flow profile, is accompanied by the emergence of both half-integer and full-integer topological defects in the orientation of the polar director field. Therefore, varying the ratio of polar and apolar elasticities \(K_p/K\) from a purely apolar elasticity \((K_p = 0)\) to a purely polar elasticity \((K = 0)\) results in a cross-over region where half-integer comet-like and trefoil-like defects coexist with their full-integer counterparts (figure 2(b)). This is a hallmark of a state with mixed symmetry and indicates that the minimal model unifies both polar and nematic active turbulence. To explain this more clearly using first principles, the formation of defects with half-integer and full-integer charges can be explained in terms of the energetic costs of forming such defects based on the two contributions in equation (3): without the third term in equation (3), i.e. when \(K = 0\), the lowest energy excitations in the polarity field are the full integer topological defects in the form of vortex (or aster) and anti-vortex pairs, as is well-established for vectorial order parameter both in active matter [26] and also in classic XY models and ferroelectric liquid
Figure 2. Emergence of active polar turbulence and active turbulence state with mixed symmetry. The colormaps are the same as in figure 1 and only a zoomed-in section of the entire simulation domain is shown. The full-integer $+1, -1$ topological defects are marked by orange asters and green squares, while the half-integer $+1/2, -1/2$ topological defects are marked by red comets and blue triangles, respectively.

Figure 3. Stability-diagram in the activity-relative elasticity phase space. Colormap indicates the average charge of the system with 0 corresponding to no topological defect, 0.5 to half-integer, and 1.0 to full-integer topological defects, with values between 0.5–1.0 marking the co-existence region. (lower panel) A cut in the phase space marked by dashed black line corresponding to activity value $\zeta = 3.5$. 
Figure 4. Turbulent flow characteristics. (a) Kinetic energy spectrum and (b) vorticity–vorticity correlation function for the activity value \( \zeta = 3.5 \). The wave number \( \kappa \) and length \( r \) are normalised by the integral length \( \kappa / \int d\kappa E(\kappa) / \kappa / \int d\kappa E(\kappa) \).

Now, in the other limit when \( K_p = 0 \) the elastic free energy is identical to the one for nematic liquid crystal with the nematic tensor defined as \( Q = \mathbf{p} \mathbf{p}^{T} - p^2 \mathbf{I} / 2 \). In this case, the energy of a topological defect with charge \( \kappa = \pm 1/2, \pm 1, \ldots \) can be estimated as [4]:

\[
F_{\text{def.}}^\kappa = \kappa^2 \pi K \ln \left( \frac{R}{a} \right),
\]

where \( R \) is the defect range and \( a \) is the size of the defect core. Because of the square-dependence of the energy on the defect charge \( \kappa \), it can be seen that two half-integer defects will have less energetic cost compared to a full-integer one and therefore in the absence of the second term in equation (3) \( (K_p = 0) \) the lowest energy excitations will be of half-integer charge.

To quantify the emergence of mixed symmetry and transition from states with half-integer to full-integer topological defects, we measure the absolute value of the topological charge of the system \( \langle |q| \rangle_{x,t} \), averaged over space and time, for varying dimensionless relative elasticity \( K_r = (K_p - K) / (K_p + K) \). As such, if all defects are half-integer \( \langle |q| \rangle_{x,t} = 1/2 \) and if all defects are polar \( \langle |q| \rangle_{x,t} = 1 \). As evident from figure 3 upon increasing the relative elasticity \( K_r \) the active system continuously crossovers from active nematic turbulence, characterized by apolar half-integer topological defects, to an active turbulence state with mixed polar and apolar symmetry, where half- and full-integer defects coexist, and to active polar turbulence, characterized by only polar full-integer topological defects. While recent studies have suggested the existence of universal scaling behaviors in active turbulence [45], the precise role...
of topological defects in setting turbulent flow characteristics in active fluids remains largely unexplored. We further characterize the flow properties of active turbulence states by measuring their associated kinetic energy spectrum and vorticity–vorticity correlation functions (figure 4). Interestingly, moving from active nematic turbulence to active polar turbulence is accompanied by an enhanced decay of the kinetic energy toward smaller scales and leads to lower vorticity correlation length, indicating that the nature of topological defects can have a marked impact on active turbulent flows. The reason behind this smaller vorticity length scale for the polar case compared to the nematic case, remains unclear, but we conjecture that it is due the different molecular field contributions to the passive elastic stresses. A detailed characterisation of the differences in collective flow features will be the focus of our future studies.

The minimal model presented herein is the first to show how apolar, half-integer, topological defects can emerge in a continuum representation of polar active matter. This presents a significant reduction in the complexity compared to the current active nematic formulation, which is based on the tensorial representation of the orientation and overcomes the limitation of active nematics by capturing the impact of the polarity of the particles. This is important because the majority of biological living systems such as bacterial suspensions or cellular monolayers for which half-integer topological defects have been identified [15–19], are composed of polar entities that continuously self-propel in the direction of polarity. Without the polar self-propelled forces, the current active nematic framework is basically modeling shakers that do not move but actively generate flows around themselves. Additionally, our findings provide a first characterization of the active turbulence with coexisting half- and full-integer defects. As such our approach unifies active polar and active nematics systems in one framework and provides testable predictions for observing states with mixed symmetry in the experiments. Indeed, recent experiments on motility-assays have shown how modifying the interaction between the filaments can result in the coexistence of phases with polar and nematic symmetry in the absence of topological defects [34]. Future experiments could investigate the active turbulence generation in a dense system of polar filaments-motor protein mixtures and probe the coexistence of half- and full-integer topological defects within the active turbulence. Moreover, although recent experiments on epithelial monolayers have identified half-integer defects in the orientation field corresponding to the deformable shape of the cells [17, 24, 49], earlier studies on epithelial monolayers have consistently reported the emergence of ‘rosette’ structures, which closely resemble full-integer topological defects [56, 57], though their associated orientation field is yet to be fully characterized. We conjecture that epithelial monolayers could realize the active turbulence with mixed half- and full-integer topological defects and hope that our study triggers further experiments analyzing biological states with such mixed symmetry.

Finally, it is worth noting that the framework developed here is applicable to passive systems such as ferroelectric nematic liquid crystals, which only recently have been experimentally realised [58, 59]. In this vein, our framework could be easily adapted to accommodate the coupling to the external electric field [60] to further investigate the emergent co-existence of full- and half-integer topological defects.

Acknowledgments and Funding

AD acknowledges support from the Novo Nordisk Foundation (Grant No. NNF18SA0035142), Villum Fonden (Grant No. 29476), and funding from the European Union’s Horizon 2020 research and innovation program under the Marie Sklodowska-Curie Grant Agreement No.
847523 (INTERACTIONS). AA acknowledges support from the Federal Ministry of Education and Research (Bundesministerium für Bildung und Forschung, BMBF) under Project 031L0160.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

ORCID iDs

Aboutaleb Amiri © https://orcid.org/0000-0001-7874-5123
Amin Doostmohammadi © https://orcid.org/0000-0002-1116-4268

References

[34] Huber L, Suzuki R, Krüger T, Frey E and Bausch A R 2018 Science 361 255
[38] Blanch-Mercader C and Casademunt J 2017 Soft Matter 13 6913
[41] Doostmohammadi A, Shendruk T N, Thijssen K and Yeomans J M 2017 Nat. Commun. 8 1
[49] Balasubramaniam L et al 2021 Investigating the nature of active forces in tissues reveals how contractile cells can form extensile monolayers Nat. Mater. 20 1167
[57] Razzell W, Wood W and Martin P 2014 Development 141 1814