The lattice Hamiltonian modeling for active nematic liquid crystals with disclinations and oriented surfaces

L V Elnikova¹, V V Belyaev²,³

¹Alikhanov Institute for Theoretical and Experimental Physics, Moscow, Russia
²Moscow Region State University «MRSU», Very Voloshinoy str., 24, Mytishi, 141014, Russia
³RUDN University (Peoples’ Friendship University of Russia), 6 Miklukho-Maklay St., Moscow, 117198, Russia

E-mail: elnikova@itep.ru

Abstract. We study the system of colloid active nematic liquid crystals evolving with transformation of the structure of surface linear topological defects. We estimate numerically the SO(2) Hamiltonian of the BKT model for disclinations on the surfaces connected with flows, which can participate in the defect ordering transitions.

1. Introduction

In the recent review [1] and reference therein, we can find a description of dissipative systems of liquid crystals (LCs), so called, active LCs, which are characterized by self-propelling motion, collective behavior, and broken rotation symmetry of assembled component particles. They are of any symmetry classes of LCs, e.g. nematics, hexatic, smectics etc. Phases of active LC may be suspension of molecular motors in organic media [2, 3], bacterial colonies, colloidal solutions, etc. [1]. These particles flow at low Reynolds numbers (their speed is about 1-200 μm/s), and the active particle flow is always mutually causal by creation and annihilation of topological defects.

An active force of self-propelled particles [1] may be induced by electrical or magnetic pumping of the sample, by the presence of different obstacles at the flow of particles, by chemical reactions or biological wiggling depending on the concrete system.

The theory of active nematics (ANs) is formulated more than 20 years ago from the pioneer Viscek model [4] of the macroscopic bird flocks with ferromagnetic ordering and next following works by Tu, Toner [5], and Vitelli (so called the VGT model) [6, 7] and by many other followers. Active LC particle motion obeys to the systems of hydrodynamic and nematodynamic equations [7]. In [8], their Hamiltonian representation was given, for example, in the light of quantum analogy and gauge of currents of self-propelled particles. The spin models of universality classes 2D Ising, XY [5], spin-glass etc. are applicable for analysis of the phase transitions, structure and thermodynamical properties both in active and passive regimes including Lagrangians of topological defects [9, 10].

The experimental observations of evolution of 2D and 3D disclinations in ANs were recently reported in [11, 12] etc.

Here we focus on the behavior of disclinations on colloid surfaces at the flow regime, which is induced by an active force, i.e. in the initially nonequilibrium system. The hydrodynamics of such defects was proposed in [9] and references therein.
We use the formalism of differential calculus on a lattice and calculate the energy and the declination currents for such configurations. This modeling allows us to predict the phase portraits and thermodynamical properties of active LCs for their possible applications in optical, electronic and spintronic devises, sensors, actuators etc.

2. The modeling of moving disclinations

We base on the concept of disclinations in active liquid crystals formulated by Ryskin and Kremenetsky [10] and the SO(3)⊗T(3) gauge Lagrangian representation by Osipov [13] and by Kadić and Edelen [14] in the elasticity theory.

In spirit of the scheme [9], we study disclinations with topological charge ±1/2 in a spherical surface of an AN, were the 2D BKT (Berezinsky-Kosterlitz-Thouless) scenario is established to be valid [9].

During the melting transition, these disclinations behave differently: the +1/2 defects are responsible for self-propelling flow, and the -1/2 disclinations are nonmotile and diffusive [9]. But they are topologically constrained in the way:

\[ \tilde{\dot{\xi}} \cdot (\nabla \times \mathbf{v}) = 2\pi \rho. \]  

(1)

Here \( \mathbf{v} \) is velocity of the \( i \)th ±1/2 defect, \( \rho = (n_+ - n_-)/2 \) is the always conserving topological charge density.

Due to [15], the Hamiltonian describing active particles, appearing from the Euler-Lagrange field equations, can be written as

\[ H = \sum_i \frac{1}{2} \dot{r}_i^2 + \frac{1}{2} \sum_i \omega_i + \frac{1}{2} \sum_{ij} U(r_{ij}) - \frac{1}{2} \sum_i J(r_i) \cos \theta_i, \]

(2)

where \( \mathbf{r}_i \) is a position of the \( i \)th spin, \( \theta_i \) is a spin angle of the XY model, \( \omega_i = \dot{\theta}_i \), \( U(r_{ij}) \) is a repulsive potential, \( J(r_i) \) is a ferromagnetic coupling.

On the other hand, the motion of disclinations for +1/2 and -1/2 charged defects are [9]:

\[ \ddot{r}_i^+ = \mathbf{v}_i + \gamma \mu \mathbf{K} \cdot \mathbf{v} + \sqrt{2\mu T} \xi_i(t), \]

(3a)

\[ \ddot{r}_i^- = -\gamma \mu \mathbf{K} \cdot \mathbf{v} + \sqrt{2\mu T} \xi_i(t), \]

(3b)

where \( \gamma \) is the defect mobility and \( \xi_i(t) \) is unit white noise. \( \mathbf{v} \) is the 2D Levi-Civita tensor, \( \mathbf{K} \) is the Frank elastic constant.

On the other hand, dynamics of disclinations on curved fluctuating surfaces may be described [13] as

\[ S = S_{el} + S_{gauss} + S_{fl}, \]

where \( S_{el} \) describes elastic properties of media, \( S_{gauss} \) includes the self-action field of disclinations, and \( S_{fl} \) is the Helfrich-type action for the energy of a free fluctuating surfaces, which may be associated with \( \xi \) in (3).

The dislocation currents violate the translation symmetry [9], so we take into account only SO(3) Lagrangians, but in the case of absent broken rotation symmetry in the normal to the colloidal surface direction, we can reduce the gauge group to SO(2) [16].

The continual Lagrangian of disclinations with two terms of surface displacements is described in SO(2) [13] and [16]. Then the curvature matrix is composed of 2-forms, which do not depend of choice of an oriented orthonormal basis, and, therefore, defines a global 2-form on the manifold \( M^2 \) [17]. The Hamiltonian of disclinations constructed from the Lagrangian [13, 16] can be formulated by

\[ H = \frac{1}{2} J_1 \mathcal{D}_{ab} k^{ab} k^{bd} \mathcal{D}^d_c + \frac{1}{2} J_2 \mathcal{F}_{ab} g_{ab} g^{bd} \mathcal{F}^d_c, \]

(4)

where \( J_1, J_2 \) are the coupling constants, \( \mathcal{D}_{ab} \), \( \mathcal{F}_{ab} \) are the curvature and field tensors of a 2-form field, \( k^{ab} \), \( g^{ab} \) are components of the strain tensor equal to \( -\partial^{ab} \), these configurations are also contained in the Hamiltonian (4), \( \tilde{\varepsilon} \) is antisymmetric tensor, \( \chi \) is a time dependent characteristic configuration [16].
We can formulate the field for dissipative and total kinetic energy in $\text{U}(1) \sim \text{SO}(2)$ with the dual gauge field $G_{\mu \nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$, where $B_\mu$ is the dual gauge field analogous to electromagnetic field $G_{\mu \nu} = \frac{1}{2} \varepsilon_{\mu \nu \alpha \beta} (\partial_\alpha A_\beta - \partial_\beta A_\alpha)$, where $\varepsilon_{\mu \nu \alpha \beta}$ is the Levi-Civita symbol and $A_\mu$ is usual gauge field, $\lambda_2$ is the self-action coefficient for the scalar field. Disclinations with a core $r_0$ and monopoles in their interactions with a flux tube via a Coulomb potential are identical. So we can apply differential operators to calculate a partition function of interactions between defects.

3. Numerical results and discussions

Composing Hamiltonians together (2) and (4) into a dual lattice Hamiltonian and using the partition function [18]

$$Z = \text{const} \sum_{j \in \mathbb{Z}^D} \exp \left\{ -4\pi^2 \beta (j, \Delta^{-1} j) \right\},$$

we can calculate the energy and disclination currents with lattice Monte Carlo method.

In (5), summation is carried out on $(D - k - 2)$-forms of monopole currents $j$ over the monopole defects of an original lattice, $k$ is a rank of a differential form, $C_k$ is a $k$-dimensional cell of a lattice, $\beta$ is inverse temperature, $\Delta$ is the Laplace operator on a dual lattice. At $k = 0$, $D = 2$, we have 0-dimensional vortices of the $XY$ model, the standard action is $1/T \sum_{x,u} \cos(\phi_x - \phi_{x+u})$, where $x$ are the lattice sites, $\phi_i$ are compact dynamical variables running from $-\pi$ to $\pi$, $i = 1 \ldots 4$ at bypassing plaquette of the dual cube lattice. The dual currents calculated in modulo $2\pi$, are $j = \frac{1}{2\pi} (|\phi_1 - \phi_2|_{2\pi} + |\phi_2 - \phi_3|_{2\pi} + |\phi_3 - \phi_4|_{2\pi} + |\phi_4 - \phi_1|_{2\pi})$.

Fig. 1 shows such thermodynamics at the dual cube lattice with size 96.
In these Monte Carlo calculations, the defect currents are connected with dynamical gauge fields of (2) [13], it is possible to observe the series of BKT-type phase transitions in any active systems: on the substrate [9], on a spherical surfaces [19], membranes and other curved surfaces [19-22] in spite of the fact of SO(2) group symmetry of disclinations.

In the exclusive case of tactoid surfaces of ANs, we need to introduce an additional gauge field in (2), connected with the own polar boojums.

4. Conclusion
In this modelling, we demonstrated that topological defects may induce the mechanisms of active flows, which can have an influence on electrical, mechanical and other properties of the active soft materials. And the gauge field modeling for surface defects can propagated to another types of curved surfaces of active liquid crystals.

Acknowledgements
This event is supported by RFBR, grant No. 19-57-45011 Ind_a.

References
[1] Aranson I S 2019 Uspekhi Fizicheskikh Nauk 189 955
[2] Genkin M M, Sokolov A, Lavrentovich O D, Aranson I S 2017 Phys. Rev. X 7 011029
[3] Sanchez T, Chen D T N, DeCamp S J, Heymann M, and Dogic Z 2012 Nature 491 431
[4] Vicsek T, Czirok A, Ben-Jacob E, Cohen I, Shochet O 1995 Phys. Rev. Lett 75 1226
[5] Toner J, Tu Y 1995 Phys. Rev. Lett 75 4346
[6] Green R, Toner J, Vitelli V 2017 Physical Review Fluids 2 104201
[7] Marchetti M C, Joanny J F, Ramaswamy S, Liverpool T B, Prost J, Madan R, Aditi Simha R 2013 Reviews of Modern Physics Vol. 85 1143
[8] Loewe B, Souslov A, and Goldbart P M 2018 New Journal of Physics 20 013020
[9] Shankar S and Marchetti M C 2019 Phys. Rev. X 9 041047
[10] Ryskin G, Kremenetsky M 1991 Phys. Rev. Lett. 67 1574
[11] Darmon A, Dauchot O, Lopez-Leon T, and Benzaquen M 2016 Phys. Rev. E 94 062701
[12] Duclos G, Adkins R, Banerjee D, Peterso M S E, Varghes M, Kolvin I, Arvind Baskaran, Pelcovits R A, Powers Th R, Baskaran A, Toschi F, Hagen M F, Streichan S J, Vitelli V, Beller D A, Dogic Z 2019 Topological structure and dynamics of three dimensional active nematics Preprint cond-mat/1909.01381v1
[13] Kochtev E A and Osipov V A 1999 J. Phys. A: Math.Gen 32 1961
[14] Kadić A, Edelen D G B 1983 A gauge theory of dislocations and disclinations (Berlin Heidelberg: Springer)
[15] Casiulis M, Tarzia M, Cugliandolo L F, and Dauchot O 2019 J Chem Phys 150 154501
[16] Pudlak M and Osipov V A 2000 Nonlinearity 13 459
[17] Novastyrsky M I 1993 Topology of Gauge Fields and Condensed Matter (New York)
[18] Polikarpov M I 1995 Physics-USpekhi 165 627
[19] Copar S, Aplinc J, Kos Ž, Žumer S, and Ravnik M 2019 Phys. Rev. X 9 031051
[20] Castro-Villarreal P, Sevilla F J 2018 Phys. Rev E 97 052605
[21] Fity Y, Baskaran A, Hagan M F 2016 Active Particles on Curved Surfaces Preprint cond-mat/1601.00324v2
[22] Pearce D J G 2019 Phys. Rev. Lett. 122 227801