How running topological drunkards stay away in nematics

Defect Unbinding in Active Nematics
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Recommended with a Critique by Phanindra Dewan, IISc

Liquid crystals have been studied in equilibrium for a long time. Another direction in which a lot of research has gone into is making the individual components of the liquid crystal active. An interesting thing which happens in nematics is the formation of topological defects, on quenching from disordered to ordered state. A theory of the dynamics of topological defects in active nematics has not been established yet. This paper seeks to provide equations governing the dynamics of active topolgical defects in nematics by viewing them as a mixture of motile particles with interactions.

To do so, a hydrodynamic picture has been used in conjunction with a particle-level picture. The hydrodynamic picture is that of the order parameter $\mathbf{Q}$ and the particle-level picture is the Langevin equation of a single topological defect. The activity has been included in the force balance equation $-\Gamma\mathbf{u} + \nabla \cdot \sigma^{\mathbf{a}} = \mathbf{0}$, in the form of the active stress $\sigma^{\mathbf{a}} = \alpha\mathbf{Q}$.

The dynamical equation for the order parameter can be written as:

$$\partial_t \mathbf{Q} + \mathbf{u} \cdot \nabla \mathbf{Q} - [\mathbf{Q}, \Omega] = \mathbf{L}(\mathbf{Q}, \mathbf{u}) + \frac{1}{\gamma}[a_2 - a_4 \mathrm{tr}(\mathbf{Q}^2)]\mathbf{Q} + \frac{K}{\gamma}\nabla^2 \mathbf{Q} \tag{1}$$

$$\mathbf{L}(\mathbf{Q}, \mathbf{u}) = \lambda_1 \mathbf{D} + \lambda_2 \mathbf{Q}\nabla \cdot \mathbf{u} - \lambda_3 \mathbf{Q}\mathrm{tr}(\mathbf{Q} \cdot \nabla \mathbf{u}) \tag{2}$$

where $2\Omega_{\mu\nu} = \nabla_\mu u_\nu - \nabla_\nu u_\mu$ is the vorticity tensor and $2D_{\mu\nu} = \nabla_\mu u_\nu - \nabla_\nu u_\mu - \delta_{\mu\nu}\nabla \cdot \mathbf{u}$ is the symmetrized and traceless strain rate tensor. Other terms come from the free energy upto the first Frank approximation.

The Langevin equations for the $\pm 1/2$ defects are respectively:

$$\dot{\mathbf{r}}_i^+ = v\mathbf{e}_i - \mu\nabla_i U + \sqrt{2\mu T}\xi_i(t) \tag{3}$$

$$\dot{\mathbf{r}}_i^- = -\mu\nabla_i U + \sqrt{2\mu T}\xi_i(t) \tag{4}$$

$$\tag{5}$$

where $\mathbf{e}_i$ is the $+1/2$ defect, μ is the mobility, ξ is the Gaussian white noise, and $U = -2\pi K \sum_{i \neq j} q_i q_j \ln\left|\frac{\mathbf{r}_i - \mathbf{r}_j}{a}\right|$ is the 2D Coulomb gas interaction potential between defects with charges $q_{i,j}$ with a the size of the defect core. Here v is the nonvanishing flow at the centre of the $+1/2$ defect which makes it propel.

The fact the +1/2 defect has a deterministic velocity means that it runs away from the -1/2 defect, which might lead to unbinding. It is the classic case of someone running away from another.

Using the $\mathbf{Q}$ equation, the equation for the defect polarity dynamics of the +1/2 defect $\mathbf{e}_i = a\nabla \cdot \mathbf{Q}(\mathbf{r}_i^+)$ has been obtained. *Ignoring the noise* and solving the equation for Q *perturbatively* with the quasistatic approximation, the authors derive the dynamical equation for the defect polarity:

$$\dot{\mathbf{e}}_i = -\frac{5\gamma}{8K}[\mathbf{v}_i \cdot (\mathbf{v}_i - v\mathbf{e}_i)]\mathbf{e}_i - \frac{v\gamma}{8K}(\mathbf{v}_i \times \mathbf{e}_i)\epsilon \cdot \mathbf{e}_i \tag{6}$$

It is also seen that the *defect polarization tends to align with the force acting on the defect due to activity*. However, up to this point, the most important part of the dynamics have not been considered - the noise which might play a role in the dynamics of the polarization $\mathbf{e}_i$.

Including both the rotational diffusion and the longitudinal noise, the dynamics of $\mathbf{e}_i$ is shown to be governed by:

$$\dot{\mathbf{e}}_i = \frac{5\mu\gamma}{8K}[\nabla_i U \cdot (v\mathbf{e}_i - \mu\nabla_i U)]\mathbf{e}_i + \frac{v\mu\gamma}{8K}(\nabla_i U \times \mathbf{e}_i)\epsilon \cdot \mathbf{e}_i - \sqrt{2D_R}\epsilon \cdot \mathbf{e}_i\eta_i(t) + \nu_i(t) \tag{7}$$

Once the noise terms have been added, the case changes from that of just runners running around to that of running (topological) drunkards!

The Fokker-Planck equation from the Langevin equations for $\mathbf{r}$, the distance between two defects and that for $\mathbf{e}$, the polaritzation, can be written. From that Fokker-Planck equation the steady state distribution at large distances have been obtained perturbatively in the activity. The result was that the distribution was similar to that seen in equilibrium $\rho_{ss} \propto e^{-U_{\text{eff}}/T}$, with the effective pair potential $U_{\text{eff}} \simeq (\pi K_{\text{eff}}/2)\ln(r/a)$, where

$$K_{\text{eff}}(v) = K - \frac{v^2}{2\mu D_R}\left(1 + \mu\gamma\frac{3T}{4K}\right) + \mathcal{O}(v^4) \tag{8}$$

With this, the BKT transition temperature changes from $T^{eq} = \pi K/8$ to $T_c(v) = \pi K_{\text{eff}}(v)/8$. And we get the phase boundary between disordered state and ordered nematic:

$$\frac{|v_c(T)|}{v_*} = \sqrt{\frac{16\tilde{T}(1-\tilde{T})}{\pi[1 + (3\pi/32)\mu\gamma\tilde{T}]}} \tag{9}$$

where $\tilde{T} = T/T_c^{\text{eq}}$ and $v = \mu T_c^{\text{eq}}/l_R$.

The interpretation of all these results is that at low activity, the rotational diffusion is enough to make the defect motion less persistent and hence unable to lead to defect unbinding. However, as activity is increased, the persistent motion helps to unbind the defects.

Consider the case of two (topological) drunkard friends who drink at the same bar but at the moment they leave the bar, a stray dog starts to chase one of them. It is natural that the one being chased starts to run but will he/she be able to get far away from the other friend? Now consider the case that they are *very* drunk. Then the two of them will not

be able to run far away but will keep moving in random directions. It is very possible that one of them gets bitten by the dog and the other friend eventually has to help the other. This is the case of **binding of defect pairs**. However, if the one running is somehow less drunk and can run very fast, then he/she will eventually outrun the dog, leaving behind the other drunkard alone. This is the case of **unbinding of defects**. Which of the two happens will depend on two factors: how fast the drunkard can run (activity, v), and how drunk the drunkard is (temperature, T). This is exactly what Suraj Shankar *et al.* have derived with rigorous mathematics for the topological defects in active nematics. *A nonequilibrium phase transition can thus be observed from an ordered nematic phase to a phase of unbound defects by increasing the activity above a certain threshold.*

In my opinion, the paper does an excellent job in working out some key results to further our understanding of topological defects in active nematics. There are still some points that the authors have left out. One pertinent question still remains: what about many defect features of the problem such as screening effects which might play a role in the dynamics of these defects? Could we also develop a coarse-grained hydrodynamic theory of defects by considering a fluid of these defects?