On the way of classifying new states of active matter

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Abstract

With ongoing research into the collective behavior of self-propelled particles, new states of active matter are revealed. Some of them are entirely based on the non-equilibrium character and do not have an immediate equilibrium counterpart. In their recent work, Romanczuk et al (2016 New J. Phys. 18 063015) concentrate on the characterization of smectic-like states of active matter. A new type, referred to by the authors as smectic P, is described. In this state, the active particles form stacked layers and self-propel along them. Identifying and classifying states and phases of non-equilibrium matter, including the transitions between them, is an up-to-date effort that will certainly extend for a longer period into the future.

The study of active and self-propelled particles defines a prospering area of research, as witnessed by a thriving number of recent review articles [1–13]. One reason for this development might be the insight that we ourselves are actually representatives of this kind of objects. As we know, dynamics as an individual can already be quite challenging. Yet, when several of such active self-propelled objects act together, the collective dynamics can lead to new and unforeseen behavior.

This assertion becomes apparent already from an early minimal model [14]. Let active point particles constantly self-propel with identical speed. Each direction of self-propulsion is subject to rotational noise. Yet, each particle tends to align its self-propulsion direction with all its neighbors within a delimited environment around itself. In this kind of Vicsek model [14], an isolated particle performs uncoordinated motion. However, simply by increasing the density, a transition to orientationally ordered collective motion can arise.

Over time, several variants of this Vicsek model were studied [5, 15–20], including ‘apolar’ particles randomly reversing their propulsion direction [21, 22], metric-free alignment interactions [23–25], or particle mixtures [26]. The basic phenomenology was observed in several experiments, although details vary [27–37]. Complementary hydrodynamic continuum theories described macroscopic properties on the basis of symmetry arguments [7, 38–44]. Besides orientational ordering, also properties of translationally ordered crystal-like arrangements of self-propelled particles were investigated [45–53].

In their recent article [54], Romanczuk et al extend the analysis of translationally ordered active structures. Using a two-dimensional Vicsek model they observe self-organization of the active particles into stacked high-density layers. Simultaneously, orientational order is maintained. Following the nomenclature of equilibrium liquid crystals [55], the observed structures are referred to as active smectic states [56, 57]. Two ingredients are essential. First, they study relatively high global densities. Second, they include alignment rules for the self-propulsion directions that effectively mimic steric interactions.

The authors address both ‘polar’ and ‘apolar’ types of self-propulsion, the latter randomly reversing its direction. Moreover, apart from isotropic steric interactions that had already been introduced into the Vicsek model before [19, 27, 45, 52, 58–61], also anisotropic steric interactions are allowed for [54]. As a result, a broad range of active smectic states can be observed. In smectic-A-like structures, the self-propulsion directions collectively order normal to the high-density layers, while in smectic-C-like states an oblique configuration prevails. Both arrangements have counterparts in equilibrium [55].
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Central task for the future. We may safely conclude that there are still many accomplishments to be achieved on additional ones, as well as characterizing their non-equilibrium properties on different length scales, will be a task for the future. Identifying these and possibly new state of active matter is observed. We can see that, in general, developing universal concepts of characterizing non-equilibrium phase behavior is a topic of high complexity. On the one hand, explicit analytical solutions could play a significant role. Yet, active self-convection renders their derivation a difficult task.

Most frequently, however, at least within the studied parameter ranges, the authors observe yet another active smectic state. There, the particles form lanes, that is the self-propulsion directions are oriented parallel to the high-density layers. Consequently, the authors term such configurations smectic P, see figure 1. Their observations are backed by the analysis of a symmetry-based hydrodynamic continuum description.

The lanes are roughly separated by the interaction distances prescribed by the Vicsek model. Remarkably, in the polar case, the particles within neighboring lanes propel into the same direction. A related state has been observed before under supporting confinement within a channel geometry, there called undirectional laning. This polar situation is markedly different from previously reported laning scenarios, where the systems self-organize into neighboring lanes of opposite relative migration directions. Altogether, a new state of active matter is observed.

In this context, the work by Romanczuk et al. touches a general but very subtle issue. Assuming a statistical-mechanics point of view, how can we actually classify new states of active matter? In fact, on this basis, how do we identify and how do we distinguish between different phases? Can we adopt established equilibrium concepts? How can we locate phase transitions?

If a non-equilibrium situation can be effectively traced back to an equilibrium picture, the circumstances become familiar. Interestingly, a corresponding example is given by another truly non-equilibrium state of active matter that does not have a direct equilibrium counterpart. It concerns systems in which the self-propelled particles can mutually block their motion via steric interactions. Then, a separation into high-density clusters and a coexisting, surrounding, low-density gas-like environment can occur.

Although this is a truly non-equilibrium transition driven by the self-propulsion of the particles, its phenomenology can be described by an effective free-energy functional. Thus, it can be discussed in terms of equilibrium free-energy concepts, albeit predominantly on coarse length scales.

A converse example is provided by the basic Vicsek model itself. Strongly sensitive to slight variations of the numerical implementation, an actual discontinuity in the described order–disorder transition can be observed. Around the order–disorder transition, traveling high-density bands were detected. Propulsion directions within these bands align, leading to correlated band propagation, while in the surrounding low-density background the particles still show uncorrelated, disordered motion. One point of view is to consider the situation in the spirit of a phase coexistence as typical for first order phase transitions. A slightly extended perception is the picture of an actually microphase-separated state, linking the phenomenology again to the concept of smectic states.

We can see that, in general, developing universal concepts of characterizing non-equilibrium phase behavior is a topic of high complexity. On the one hand, explicit analytical solutions could play a significant role. Yet, active self-convection renders their derivation a difficult task. On the other hand, when we use for analysis continuum equations coarse-grained from particle-based models, we must be aware that approximations typically enter during the coarse-graining process. Moreover, not only the presented symmetry groups, but in principle any symmetry class behind a certain phase in equilibrium could have corresponding manifestations in non-equilibrium. Identifying these and possibly additional ones, as well as characterizing their non-equilibrium properties on different length scales, will be a central task for the future. We may safely conclude that there are still many accomplishments to be achieved on the way of classifying new states of active matter.

Figure 1. In the newly identified smectic-P state of active matter, the self-propelled particles self-organize into stacked layers. Their self-propulsion directions orient parallel to the layers, i.e. the active particles form lanes. The distance between the lanes roughly corresponds to the range of mutual interaction. (a) In the polar smectic-P state, undirectional laning emerges, i.e. particles in neighboring lanes propel into the same direction. (b) An apolar smectic-P state originates when each self-propulsion direction permanently randomly reverses.
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