Phase transition to dynamic vortex arrays in active fluids

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Active matter systems convert internal or external energy into mechanical energy, thus creating perpetual motion. This nonequilibrium nature gives rise to several surprising results, for example, the emergence of global order prohibited in equilibrium systems. A dynamic XY model proposed by Vicsek et al. in 1995 as well as a phenomenological hydrodynamic theory of active matter have been successful in reproducing these phenomena. While such "flocking phases" of active matter have been studied in great detail, relatively little is known about other phases. Several experiments have reported chaotic, turbulence-like dynamics in active fluids. Experiments on sperm cells and microtubule systems have produced well-ordered vortex arrays. Here we study the emergence of quasi-stationary vortex arrays in active fluids through a hydrodynamic theory of "dry" active matter. We solve the hydrodynamic equations of active matter to study the transition from turbulent phase to vortex array. The resulting vortex array phase emerges from a long turbulent transient and differs significantly in properties as compared to classical patterns. For large domain sizes, this "turbulent" vortex array self-organises into large-scale meta-stable superstructures which share surprising analogies to ferromagnetic systems. Like the flocking phase of active matter, we show that the features of vortex array phase transition in active fluids can be understood by using tools from equilibrium thermodynamics.

Theories inspired by equilibrium statistical mechanics have been used with great success to study flocking phases in nonequilibrium active matter [1,2]. General frameworks such as the hydrodynamic theory of active matter by Toner and Tu exist to investigate the phase transition as well as stability of globally ordered flocks. Apart from the flocking state, both living and non-living active matter display a remarkable variety of patterns and disordered phases [3–6]. While several ad hoc models have been used to examine and predict pattern formation in active matter [7,8], a theory from more fundamental considerations is currently lacking. This behoves us to ask whether phase transition to patterns in active matter can be investigated through more universal approaches. Arguably, the Toner-Tu equations themselves would provide an ideal starting ground for such an analysis. While originally introduced to explain global order in active matter, these equations are based on very general considerations and hence is expected to portray a wider class of phases. Though Toner-Tu equations represent a "dry" model of active matter [9], modified versions of these equations have recently been used with success to model phases such as active turbulence where "wet" physics is expected to dominate [10]. Here we investigate pattern formation and phase transition in active matter by using a modified version of the Toner-Tu equations. Motivated by observations of regular vortex arrays in several living systems [3–5], we seek lattice solutions to this model. Our numerical and theoretical analysis reveal the existence of well ordered vortex arrays qualitatively similar to experiments. We analyse the phase transition from turbulence to vortex arrays, which eventually lead to superstructures of ferromagnetic domains (Fig. 1) similar to vortex domains in bacterial suspensions [5].

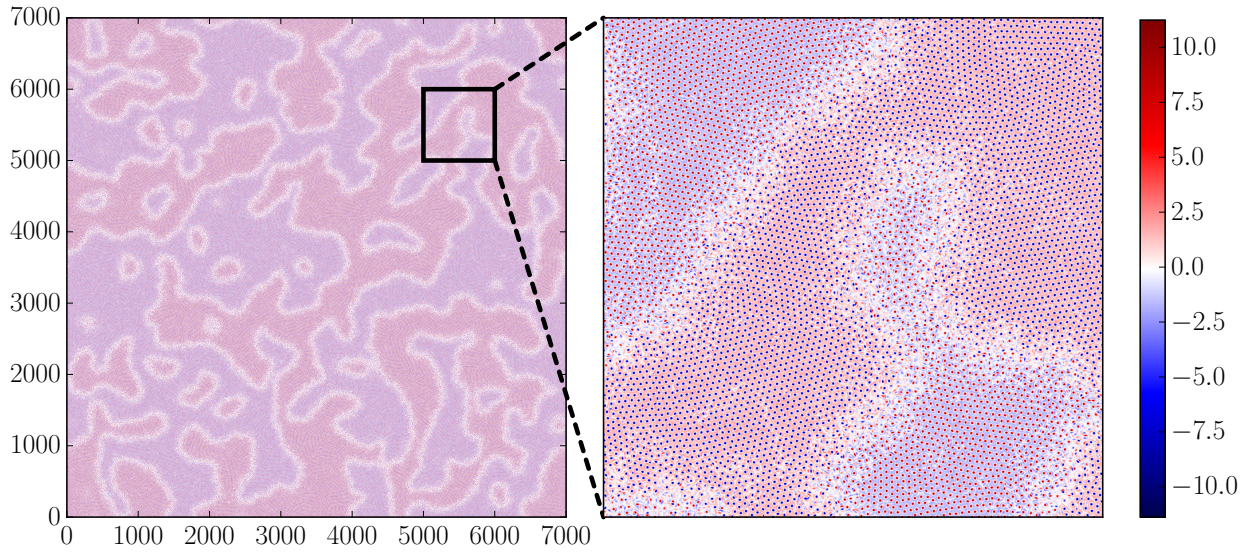


Figure 1: Superstructures of vortex arrays: (left) A snapshot of the vorticity field showing self-organised large-scale vortex domains in active fluid. The right panel shows a zoom-in.

Our starting point is an incompressible version of the Toner-Tu equations as given below.

$$\partial_t \boldsymbol{u} + \lambda \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p - (1+\Delta)^2 \boldsymbol{u} - \alpha \boldsymbol{u} - \beta \boldsymbol{u}^2 \, \boldsymbol{u}. \tag{1}$$

This model was originally introduced to investigate the active turbulence phase in bacterial suspensions [10–12]. Here p is the pressure term and λ and α are free parameters (parameter β can be scaled out). Unlike the Toner-Tu model, Eq. (1) is self driven and has no external noise. This resulting model can thus be thought of as a minimal continuum theory for active fluids [11]. The statistical properties of this theory has been favourably compared to the active turbulence phase. Furthermore, it has been shown that these equations can be derived from microscopic considerations for bacterial systems [13]. The role of the free parameters are as follows; α regulates the energy injection in the system and λ the relative strength of advective to cubic nonlinearity.

Apart from active turbulence, Eq. (1) represents a variety of other phases as a function of α, λ and domain size L. To elucidate these different phases of active matter, we present in Fig. 2 a detailed phase diagram in the $\alpha - \lambda$ plane at a fixed domain size of $L = 100$. The phase diagram demarcates three distinct phases; (a) square lattice, (b) active turbulence and (c) hexagonal vortex arrays as well as the transitions between them. For zero advection, we observe a stationary square lattice which can be analysed theoretically by using classical pattern formation theory [14,15]. This square lattice remains stable for finite, but small values of advection. As advection is increased, the square lattice state becomes unstable resulting in a distorted, but stationary lattice. Further increasing the value of λ leads to the dynamic active turbulence phase. For very strong advection, the hexagonal vortex array state starts to emerge. The marginal stability region between active turbulence and hexagonal vortex array is characterised by temporally intermittent patterns.

The hexagonal vortex array, which becomes stable for strong values of advection, shows significantly different properties as compared to a classical pattern [16]. Supplementary video (1) shows the emergence of this vortex arrays from random initial conditions. As the video illustrates, this pattern does not spontaneously emerge but is preceded by a long turbulent transient. During this turbulent transient, the number of positive and negative vortices remain approximately equal, similar to the turbulent phase. Overtime, a spontaneous symmetry breaking lead to the emergence of the hexagonal vortex array. This vortex array is not stationary but is made dynamic by the presence of continuous turbulent background fluctuations. Interestingly, this turbulent vortex array does not select the fastest growing mode as its dominant wavenumber [16].

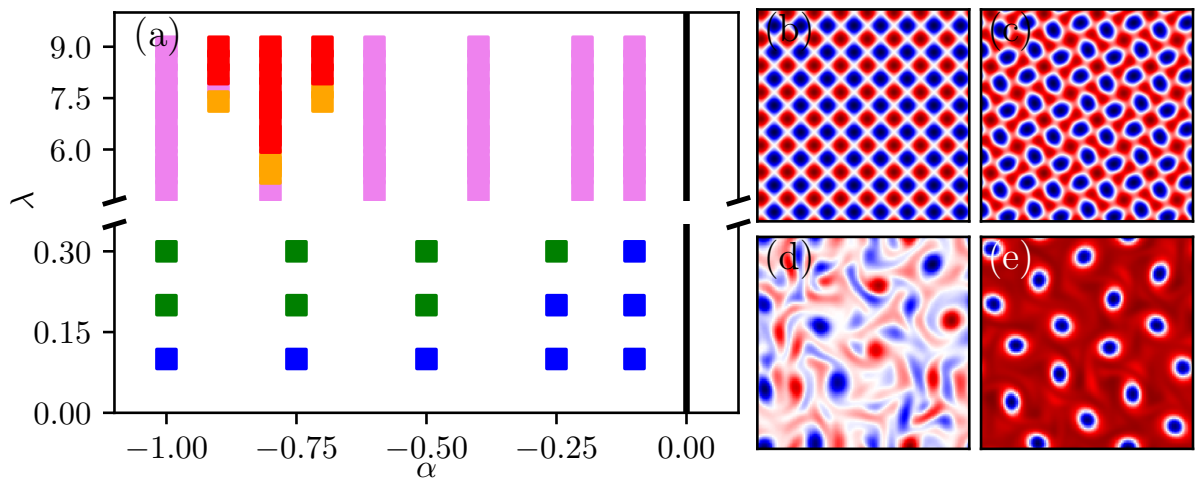


Figure 2: Phase diagram of the active fluids model: (a) Different phases of the active fluids system obtained by numerically solving Eq. (1). Blue, green, magenta and red regions correspond to square lattice (b), distorted square lattice (c), active turbulence (d) and turbulent vortex array (e) respectively. The orange region is the marginal stability region between the active turbulence phase and the hexagonal vortex array.

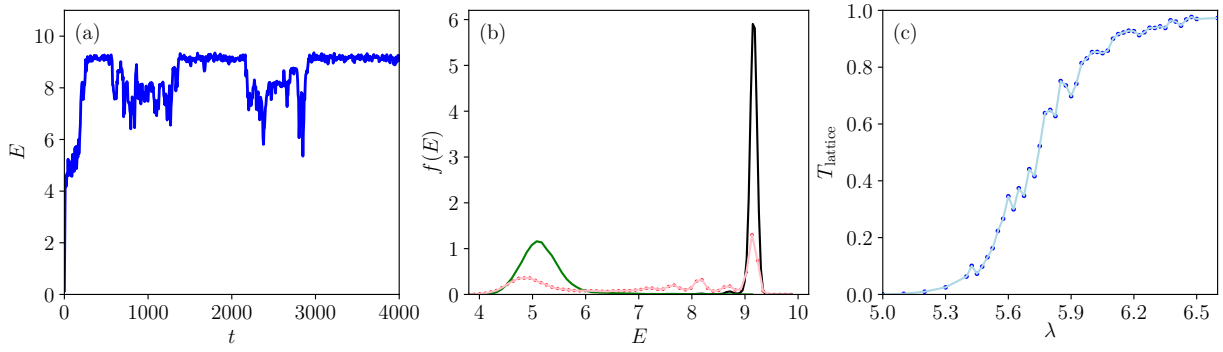


Figure 3: Phase transition: (a) A typical energy time series for a simulation in the marginal stability region. (b) Probability density functions of the energy time series for values of $\lambda = 5$ (green), 5.5 (red) and 6 (black). (c) Phase transition from active turbulence to vortex array as a function of control parameter λ ($\alpha = -0.8$).

To track the phase transition from turbulence to vortex array, we systematically characterised the the marginal stability region. In this region, the vortex array periodically emerges, evolving in to turbulence over time and this process repeats after itself. Supplementary video (2) illustrates this transition phase. This video also shows that the sign of the vortex array may flip during the periodic reversals. The marked difference between the vortex array state and the turbulent state is clearly seen in the time series of the total energy (Fig. 3 (a)). The vortex array state is more dynamic as compared to the turbulent state. Also, the close packing of the vortices allows for a higher concentration of total energy. Consequently the plateaus in Fig. 3 (a) correspond to the vortex array state. The state switching can be analysed by looking at the probability density function (PDF) of the energy time series for different values of advection as shown in Fig. 3 (b). Below the critical value of advection, for $\lambda = 5$, the PDF has only one peak centred at around 5. Above the critical point, in the marginal stability region, a second peak arises close to $E = 9$. For stronger advection, the vortex array state start becoming more likely. Well above the critical point, only one peak, close to $E = 9$, remains. The probability of finding the system in the vortex array state is a natural order parameter that can characterise this transition. We use this order parameter to map out the phase transition (Fig. 3 (c)). The probability continuously increases starting with a value of $\lambda = 5$, eventually saturating for values of λ beyond 6.5. To classify the type of transition, we mapped out the phase transition starting with a vortex array as the initial condition. This did not result in a hysteresis loop thus confirming the continuous nature of the phase transition.

Notable differences in the active matter system become apparent when we increase the domain size. For very large domains the transients are characterised not by a turbulent state but by

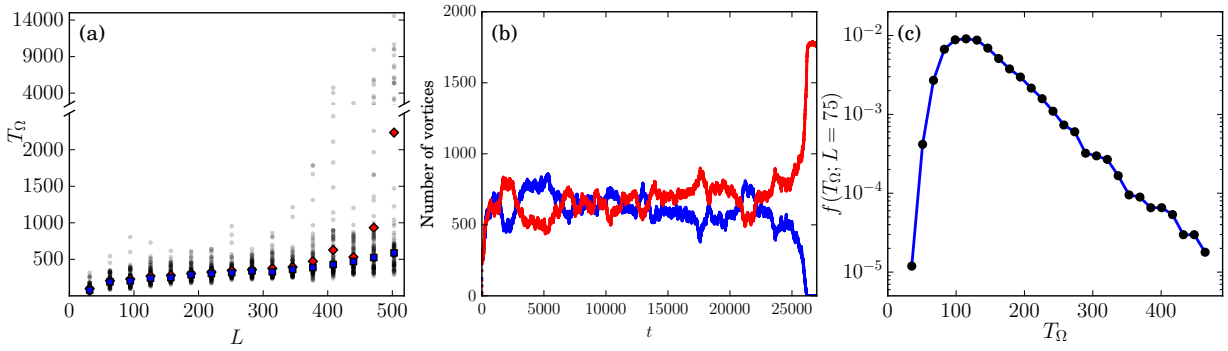


Figure 4: Supertransients: (a) Duration of the transient leading to the dynamic vortex array, T_Ω, as a function of domain size L. The red and blue dots are the mean and median values respectively. The change in slope at 350 mark the domain size where superstructures start to become stable. (b) Time series of the number of positive (blue curve) and negative vortices for a typical simulation with large domain size (L=503). (c) Probability density function of T_Ω.

a metastable superstructure of vortex arrays (Fig. 1 (a)). To study this state, we investigated the evolution of the active matter system as a function of the domain size. Both the mean as well as median duration of the transients T_Ω continuously increase with domain size L (Fig. 4 (a). The mean duration sharply takes off at around $L = 350$, marking the point where superstructures of vortex arrays start to emerge. This divergence of mean transient duration is observed in several dynamical systems and is termed supertransients [17–19]. Supplementary video (4) shows a typical simulation in which the metastable superstructures dominate the dynamics. This can also be analysed by calculating the number of positive and negative vortices (Fig. 4 (b)). As Fig. 4 (a) indicates T_Ω has a wide distribution and for some random initial conditions, even for large domains a vortex array can emerge without going through the supertransient state (supplementary video (4)).

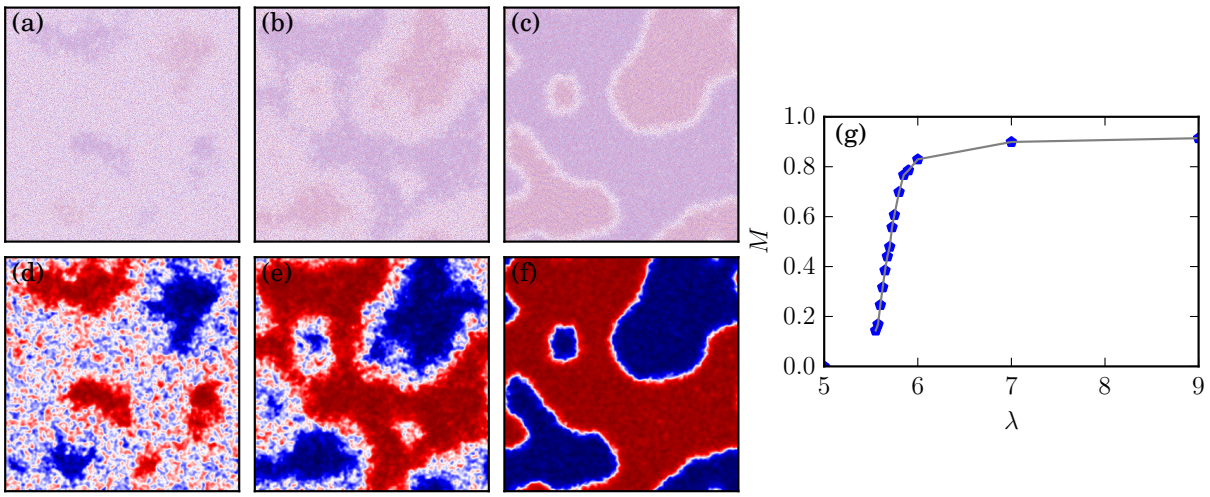


Figure 5: Turbulent boundary layer: (a,b,c) Superstructures of vortex arrays for $\lambda = 5.550, 5.725$ and 7 respectively. (d), (e) and (f) are the corresponding smoothed magnetisation fields. (g) Fraction of magnetic domain to total domain area as a function of λ.

The probability density function of the transient duration T_Ω has a prominent peak closer to shorter durations and then falls off exponentially (Fig. 4 (c)). The form of this distribution can be understood from probabilistic arguments. We start by making the following observations; (a) there is a critical domain size Δ which a single patch of vortex array can cover and (b) the lifetime of a single vortex decays exponentially in the transient state. Then the probability for a single vortex patch to emerge at any part of the domain is exponentially distributed. Let us call the timescale associated with this distribution τ. A complete vortex array emerges when multiple such vortex patches cover the entire domain. Hence the resulting PDF is the probability of maximum of multiple exponentially distributed random variables, i.e. $N(1 - e^{-t/\tau})^{\frac{L^2}{\Delta}} e^{-t/\tau}$, thus verifying the numerical results.

The stability of transient superstructure state increases with domain size. For very large domains, they remain mostly stationary with little dynamics in the large scales (supplementary video (6)). The large-scale dynamics is contrasted with the small-scale dynamics close to the boundaries (supplementary video (5)), which is quite turbulent. The large-scale features evolve so as to minimise the turbulence fraction. Furthermore, the approximate width of the boundary layer remains constant throughout the entire domain.

The superstructures of vortex arrays reported here is analogous to magnetic domains observed in ferromagnetic systems. To make this analogy more quantitative, we looked at how the superstructures evolve as a function of control parameter λ. The role which the parameter λ plays can be thought of as analogous to temperature. For ferromagnetic systems, increasing temperature would lead to a continuous transition from spontaneous magnetisation to zero magnetisation. In magnetic domains this is manifested in the increasing area of the boundary wall as a function of temperature, which diverges at a critical value of temperature. We conducted a similar analysis with the turbulent boundaries between the vortex domains, with λ as control parameter. Starting with same initial conditions we solved the active fluids model for different values of λ. Figure 5 (a), (b) and (c) shows three representative snapshots for increasing values of λ close to the critical point. The fraction of the total area covered by the vortex array increases as the value of the control parameter is increased. Following the analysis detailed in the methods section, we extracted positive and negative vortex arrays as well as the turbulent boundaries as shown in Fig. 5 (d), (e) and (f) where red and blue regions correspond to the positive and negative vortex arrays respectively. This allows for a natural order parameter for the phase of the system: the fraction of the total area

covered in the vortex array state. Figure 5 (g) shows this "magnetisation" plotted as a function of control parameter λ, mapping the phase transition between turbulent or isotropic phase to superstructures of vortex arrays. The superstructures of vortex arrays remain stable for λ greater than 6, but below the critical value of 5.5, the area of the isotropic boundary layer diverges. This phase transition curve, as expected, is similar to the phase transition for smaller domains shown in Fig. 3 (c).

Our study shows that phenomenological modelling of active matter systems based on general considerations can capture several phases potentially relevant to experimental observations. The turbulent vortex arrays reported here is a novel path to pattern formation with several intriguing properties. The emergence of this pattern is preceded by a turbulent transient with non-trivial statistical features, analogous to supertransients in several dynamical systems [17,18]. Our observation of metastable superstructures of vortex arrays in this supertransient state provides an important connection to equilibrium systems. The turbulent boundary layer which demarcates different states in these superstructures shows remarkably complex dynamics as compared to the bulk. The two distinct ways to study the transition between the active turbulence phase and the vortex array phase, i.e. through temporally and spatially intermittent patterns, lead to same results. These observations lent credence to the ergodic nature of the underlying model. While we observe a continuous phase transition in our system, it is interesting to note that a modified version of the model presented here has been used to uncover a first-order phase transition to large-scale ordered structures [20]. Transition to turbulence from unstable vortex arrays have also been numerically studied in active liquid crystal models [21]. Furthermore, formation and melting of vortex arrays have been reported on

several hydrodynamic systems [22,23]. While several experiments have reported on pattern formation including hexagonal vortex arrays in active matter systems, the similarities such observations share with the mechanism described here remains an open question. In some systems, such as confined suspensions of sperm cells, spontaneous emergence of vortex arrays from a turbulent phase have been observed. Large scale vortex arrays can emerge in such systems, provided the parameters are chosen so as to minimise the energy associated with alignment. Such direct comparisons to experiments as well as a complete characterisation of these observations within the larger context of nonequilibrium statistical mechanics provides intriguing opportunities for future research.

Methods

Details of simulations.

Phases in the active fluids model.

Phase transition analysis.

List of supplementary videos

(1) The formation of the "turbulent" vortex array from random initial conditions

(2) A simulation of the active turbulence model in the marginal stability region between the turbulent phase and the vortex array phase

(3) An example of quick emergence of the vortex array in a large domain

(4) An example of metastable superstructures of vortex arrays in large domains. Note that the frame rate of this video is ten times faster as compared to supplementary video (3)

(5) Video showing the closeup of the turbulent boundary layer

(6) The temporal evolution of the superstructure of vortex arrays

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