

# Phase Frustration-Induced Spatial Lattice Symmetry

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## 1 The Model

Particles have a spatial position  $\mathbf{r}_i = (x_i, y_i)$  and an internal phase  $\theta_i$  which evolve according to equations:

$$\dot{\mathbf{r}}_i = v \mathbf{p}(\theta_i) , \quad (1a)$$

$$\dot{\theta}_i = \omega_i + \frac{K}{|A_i|} \sum_{j \in A_i} [\sin(\theta_j - \theta_i + \alpha) - \sin \alpha] , \quad (1b)$$

for  $i = 1, 2, \dots, N$ . Here in Eq. (1a),  $\mathbf{p}(\theta) = (\cos \theta, \sin \theta)$ , which means each particle rotates with a constant speed  $v$  in the direction of its instantaneous phase  $\theta_i(t)$ . The particles are treated as point-like with no direct spatial interactions, consistent with classical models of chiral self-propelled particles [1–3, 7, 8]. As per Eq. (1b), the mean runs over neighbors within a coupling radius  $d_0$  around particle  $i$ :

$$A_i(t) = \{j \mid |\mathbf{r}_i(t) - \mathbf{r}_j(t)| \leq d_0\} , \quad (2)$$

$K (\geq 0)$  is the coupling strength, and  $\{\omega_i\}$  are the natural frequencies distributed according to a given frequency distribution  $g(\omega)$ . This means that a particle will rotate with the angular velocity  $|\omega_i|$  in the absence of mutual coupling ( $K = 0$ ), and the sign of  $\omega_i$  represents the direction of rotation, namely, the tribute of the chirality of the  $i$ -th particle. A positive (negative) chirality ( $\omega$ ) describes the counterclockwise (clockwise) rotations of the particle in space.

Additionally,  $\alpha$  is the phase frustration between two neighboring particles. When  $\alpha_0 = 0$ , the dynamics reduces to the normal chiral model [4]. The counter term  $-\sin \alpha$  is introduced to ensure that frustration only interferes with the phase coupling without changing the sign of effective frequency.

## 2 Phase frustration-induced crystallization

### 2.1 Key properties

1. What does the lattice structure look like?
2. **Done** What is each cell composed of?

3. What is the unit cell structure, and what is the spatial arrangement of the unit cells?
4. What is the internal dynamics within a cell? Besides triangular, what other spatial structures exist?
5. What determines the length (periodicity)? (Interaction distance?) In which regions of frustration does it appear? (And what are the corresponding coupling conditions and natural frequency distributions?)

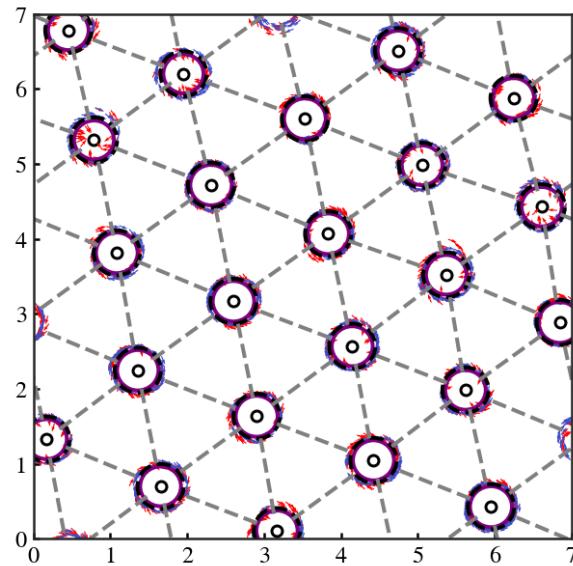


Figure 1: Snapshots of system at  $t = 80$  with  $N = 1000$ ,  $K = 10.5$ ,  $d_0 = 1.07$ ,  $\alpha = 0.6\pi$ ,  $\omega_{\min} = 0$ , and  $\Delta\omega = 1$ .

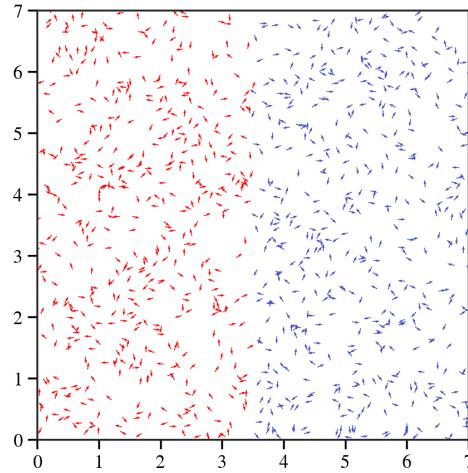


Figure 2: Initial conditions of half on each side.

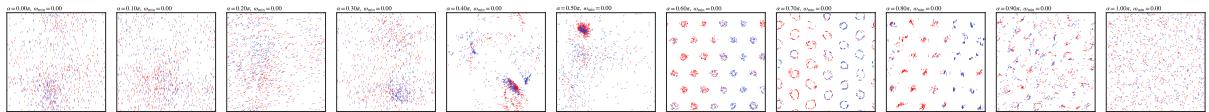


Figure 3: Snapshot of the system at  $t = 80$  with  $N = 1000$ ,  $K = 20$ ,  $\omega_{\min} = 0$ ,  $\Delta\omega = 1$  and initial conditions of half on each side.

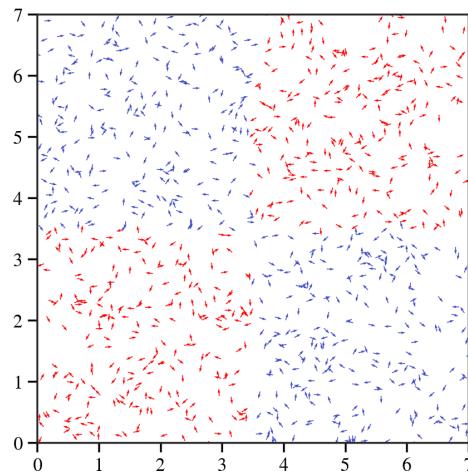


Figure 4: Initial conditions of chessboard pattern.

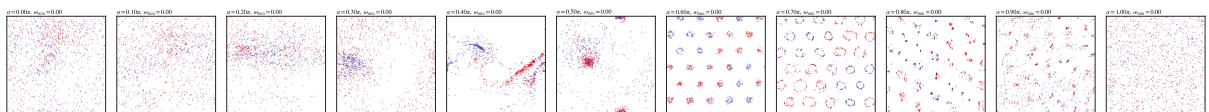


Figure 5: Snapshot of the system at  $t = 80$  with  $N = 1000$ ,  $K = 20$ ,  $\omega_{\min} = 0$ ,  $\Delta\omega = 1$  and initial conditions of chessboard pattern.

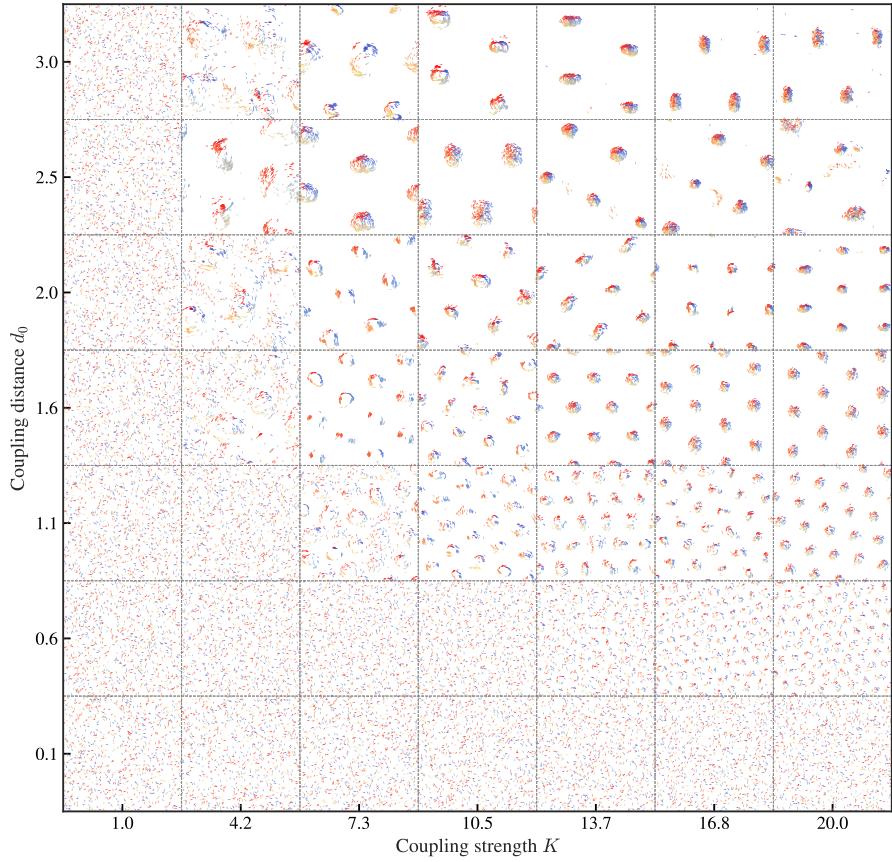


Figure 6: Snapshots of achiral system ( $\omega_{\min} = 0$  and  $\Delta\omega = 0$ ) at different coupling strengths  $K$  and radius  $d_0$  for  $\alpha = 0.6\pi$ . 固定阻挫为  $0.6\pi$ , 不同的耦合强度  $K$  和半径  $d_0$  下的非手性粒子系统快照。粒子颜色根据其瞬时相位  $\theta_i$  着色。随着两个耦合参数的增加, 粒子在空间中逐渐形成三角晶格结构且尺寸和彼此距离不断增加。

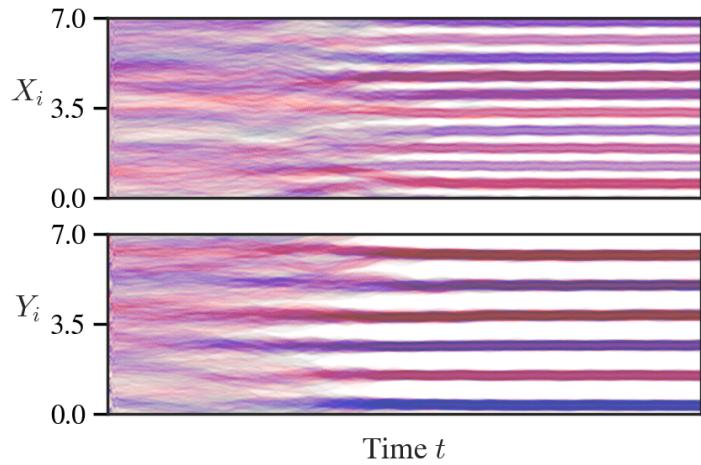


Figure 7: 瞬时旋转中心随时间变化的散点图。其中  $N = 1000$ ,  $K = 20$ ,  $\alpha = 0.6\pi$ ,  $\omega_{\min} = 0.1$ 。随时间演化, 粒子晶格大体呈现红蓝交错分布的趋势。

陆羿辰：从旋转中心的散点图确实能看出一些红蓝交替出现的现象，原因暂时不明（也可能和画散点图时图层的排序有关，可以尝试改变一下图层的顺序）

陆羿辰：调整完图层之后色调发生了改变，目前猜测应该不是类似棋盘格的分布

### 3 Phase Diagram and Mechanism

#### 3.1 Phase Diagram

The phase diagram of the system is constructed by varying the key parameters, including the coupling strength  $K$ , the radius  $d_0$ . The resulting patterns are classified into ordered and lattice states.

The order parameter  $\sigma_\rho(t)$  is defined as the standard deviation of the density, which quantifies the degree of spatial ordering in the system.

$$\sigma_\rho(t) = \sqrt{\frac{1}{L^2} \int [\rho(\mathbf{r}, t) - \langle \rho(\mathbf{r}, t) \rangle]^2 d\mathbf{r}}, \quad (3)$$

where  $\rho(\mathbf{r}, t) = \int_0^{2\pi} f(\mathbf{r}, \theta, t) d\theta$  is the density of particles at position  $\mathbf{r}$  and time  $t$ , and  $\langle \rho(\mathbf{r}, t) \rangle = \frac{1}{L^2} \int \rho(\mathbf{r}, t) d\mathbf{r}$  is the average density over the system.

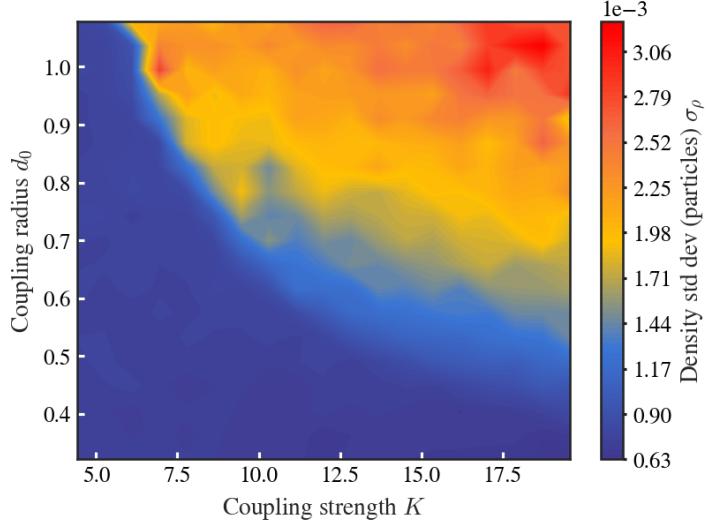


Figure 8: The order parameter  $\sigma_\rho(t)$  as a function of coupling strength  $K$  and radius  $d_0$ . The color indicates the value of the order parameter, with red representing high cohesiveness and blue representing low cohesiveness.

#### 3.2 Hydrodynamics

Here, we develop a continuum theory for the self-propelled particles with phase frustration, following the approach in [2, 3]. We start with the Eqs. (1) but replace the finite range alignment interaction by a pseudopotential (' $\delta$ -interaction), which is justified if the interaction is short ranged enough, such that the shape of the associated interaction potential is irrelevant to the many particle dynamics. Additionally, for simplicity of analysis, we consider achiral systems ( $\omega_i = 0$ ). The

$$\dot{\mathbf{r}}_i = v\mathbf{p}(\theta_i), \quad (4a)$$

$$\dot{\theta}_i = \frac{K}{|A_i|} \sum_{j=1}^N \delta(\mathbf{r}_j - \mathbf{r}_i) [\sin(\theta_j - \theta_i + \alpha) - \sin \alpha]. \quad (4b)$$

In the thermodynamic limit  $N \rightarrow \infty$ , the agent-based model gives rise to the following continuum form:

$$\frac{\partial}{\partial t} f(\mathbf{r}, \theta, t) = -\nabla \cdot (f\mathbf{v}_r) - \frac{\partial}{\partial \theta} (f v_\theta), \quad (5)$$

where  $f(\mathbf{r}, \theta, t)$  is the probability density of particles at position  $\mathbf{r}$  and orientation  $\theta$  at time  $t$ , and  $\mathbf{v}_r$  and  $v_\theta$  are the velocity fields in the position and orientation space, respectively. The velocity fields are given by

$$\mathbf{v}_r(\mathbf{r}, \theta, t) = v\mathbf{p}(\theta) \quad (6a)$$

$$v_\theta(\mathbf{r}, \theta, t) = -\sin \alpha + K \int d\theta' f(\mathbf{r}, \theta', t) \sin(\theta' - \theta + \alpha). \quad (6b)$$

By substituting Eqs. (6) into Eq. (5), we obtain

### 3.3 Abstract phase oscillator model

Let us consider a decoupled phase-oscillator system

$$\dot{\theta}_i = \omega_i - K \sin \alpha + \frac{K}{N} \sum_{j=1}^N \sin(\theta_j - \theta_i + \alpha). \quad (7)$$

To quantify the phase coherence of the system, it is convenient to define the generalized complex-valued order parameters, i.e.,

$$Z(t) = R(t) e^{i\psi(t)} = \frac{1}{N} \sum_{j=1}^N e^{i\theta_j(t)}, \quad (8)$$

where  $n = 1, 2, \dots, N$ , and  $r(t)$ ,  $\psi(t)$  are the amplitudes and arguments of the order parameter. Our starting point is to analyze the critical point for the coherence of the order parameter. In the thermodynamic limit  $N \rightarrow \infty$ , the state of the system in Eq. (7) can be characterized by the single-oscillator distribution  $\rho(\theta, \omega, t)$ , which satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial \theta} = 0, \quad (9)$$

where  $\rho(\theta, \omega, t)$  accounts for the fraction of oscillators with phase  $\theta$  lying in the interval  $(\theta, \theta + d\theta)$  at fixed frequency  $\omega$  and time  $t$ , it satisfies the normalization condition

$$\int_0^{2\pi} \rho(\theta, \omega, t) d\theta = 1. \quad (10)$$

Here,  $v(\theta, \omega, t)$  is the velocity field, given by

$$v(\theta, \omega, t) = K \int_{-\infty}^{+\infty} \int_0^{2\pi} \sin(\theta' - \theta + \alpha) \rho d\theta' d\omega' + \omega - K \sin \alpha. \quad (11)$$

Correspondingly, the order parameter defined in Eq. (8) in the thermodynamic limit reads

$$Z(t) = \int_{-\infty}^{+\infty} g(\omega) d\omega \int_0^{2\pi} e^{i\theta} \rho(\theta, \omega, t) d\theta, \quad (12)$$

then  $v(\theta, \omega, t)$  simplifies to

$$v(\theta, \omega, t) = \omega - K \sin \alpha + \text{Im}[H(t) e^{-i\theta}], \quad (13)$$

with the mean-field being

$$H(t) = K Z(t) e^{i\alpha}. \quad (14)$$

Since the distribution  $\rho(\theta, \omega, t)$  is  $2\pi$ -periodic in  $\theta$ , we can expand it in Fourier series as

$$\rho(\theta, \omega, t) = \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} a_n(\omega, t) e^{in\theta}, \quad (15)$$

where  $a_n(\omega, t)$  is the  $n$ -th Fourier coefficient. In particular, we have  $a_0(\omega, t) \equiv 1$  owing to the normalization condition in Eq. (10) and  $a_{-n}(\omega, t) = a_n^*(\omega, t)$ , where  $*$  denotes the complex conjugate.

According to the Ott-Antonsen ansatz [5, 6], it states that the  $n$ -th Fourier coefficient  $a_n(\omega, t)$  can be expressed in terms of the first-order coefficient, i.e.,  $a_n(\omega, t) = a^n(\omega, t)$ . In this regard, the evolution of  $\rho(\theta, \omega, t)$  degenerates to an invariant manifold, which is

$$\dot{a}(t) = i(K \sin \alpha - \omega) a(t) + \frac{1}{2} [H^*(t) - H(t) a^2(t)] . \quad (16)$$

Consequently, Eq. (16) is closed by the definition of the order parameter in Eq. (12), where

$$\begin{aligned} Z(t) &= \int_{-\infty}^{+\infty} g(\omega) a_{-1}(\omega, t) d\omega , \\ &= \int_{-\infty}^{+\infty} g(\omega) a^*(\omega, t) d\omega . \end{aligned} \quad (17)$$

We stress that Eq. (16) is still infinite dimensional because of the distributed natural frequencies. Thus, we may make a specific choice for the frequency distribution to get around this difficulty, e.g. a Lorentzian distribution  $g(\omega) = \Delta/[\pi(\omega - \mu)^2 + \Delta^2]$  with  $\Delta$  being the width of the distribution and  $\mu$  being the mean frequency. In this setting, the order parameters defined in Eq. (17) can be calculated by using Cauchy's residue theorem with analytical continuation of  $a(\omega, t)$  into the lower half complex plane, which leads to

$$Z(t) = a^*(\mu - i\Delta, t) . \quad (18)$$

As a result, the low-dimensional evolution of the order parameter can be obtained by replacing  $\omega$  with  $\mu - i\Delta$  and by taking into account the complex conjugate, which reads

$$\dot{Z} = -\Delta Z + iZ(\mu - K \sin \alpha) + \frac{1}{2} [KZe^{i\alpha} - KZ^*Z^2e^{-i\alpha}] . \quad (19)$$

Rewrite above equation using polar coordinates  $Z(t) = R(t) e^{i\psi(t)}$ , we have

$$\dot{R} = \frac{R}{2} (K - 2\Delta - KR^2) \cos \alpha , \quad (20a)$$

$$\dot{\psi} = \mu + \frac{K}{2} (R^2 - 1) \sin \alpha . \quad (20b)$$

Obviously, the amplitude  $R(t)$  is decoupled from the mean phase  $\psi(t)$  and Eq. (20a) have a critical coupling strength  $K_c = 2\Delta$  and a pair of critical phase frustration  $|\alpha_c| = \pi/2$ . Let us first consider the simplest case of  $\Delta = 0, \mu = 0$ , which corresponds to the case of achiral particles. In this case, when  $|\alpha_c| > \pi/2$ , the system bifurcates to  $R = 0$ , which corresponds to the incoherent state in phase oscillators and lattice state in self-propelled particles, while for  $|\alpha_c| < \pi/2$ , the system has a unique stable fixed point at  $R = 1$ , which corresponds to the coherent state and swarming state, respectively.

For the incoherent state, the system is totally disordered with the phases distributed uniformly around the unit circle, i.e.,  $\rho(\theta, \omega, t) = g(\omega)/2\pi$ , which implies that the phase velocity of each oscillator/particle becomes

$$\dot{\theta}_i = \omega_i - K \sin \alpha . \quad (21)$$

Correspondingly, the rotational radii of  $i$ -th particle is

$$r_i = \frac{v}{\dot{\theta}_i} = \frac{v}{\omega_i - K \sin \alpha} . \quad (22)$$

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