Notes: Phase Transitions and Partition of Integers

I. MOTIVATION

1. Biology: Molecular motors, microtubules, bacteria.

2. Granular Matter: granular rods and chains.

3. Phase synchronization.

II. THE ROD ALIGNMENT MODEL

In the rod alignment model, introduced by Aranson and Tsimring, there is an infinite number of identical *polar* rods, each with an orientation

$$-\pi \leq \theta \leq \pi. \tag{1}$$

The rod alignment changes via two competing mechanisms:

1. Alignment by Pairwise Interactions: The rods become aligned via irreversible pairwise interactions. As a result of the interaction between two rods with orientations θ_1 and θ_2, both rods acquire the average orientation as follows (see figure 1):

$$(\theta_1, \theta_2) \rightarrow \begin{cases} \left(\frac{\theta_1+\theta_2}{2}, \frac{\theta_1+\theta_2}{2}\right) & |\theta_1 - \theta_2| < \pi \\ \left(\frac{\theta_1+\theta_2+2\pi}{2}, \frac{\theta_1+\theta_2+2\pi}{2}\right) & |\theta_1 - \theta_2| > \pi. \end{cases} \tag{2}$$

Of course, addition and subtraction are implicitly taken modulo 2π.
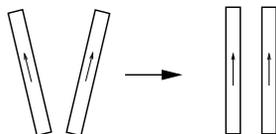
FIG. 1: Illustrating of the alignment process.

2. Diffusive Wiggling: There is also randomness in the form of a white noise: each rod wiggles in a diffusive fashion, and this process is characterized by the diffusion constant D. Specifically, in addition to the alignment process (2), the orientation of a rod is subject to white noise

$$d\theta/dt = \eta \qquad \text{with} \qquad \langle \eta(t)\eta(t') \rangle = 2D\delta(t - t'). \tag{3}$$

III. THE MASTER EQUATION

Let $P(\theta, t)$ be the probability distribution function of rods with orientation θ at time t. It is normalized to one,

$$\int_{-\pi}^{\pi} d\theta \, P(\theta, t) = 1. \tag{4}$$

This distribution function satisfies the integro-differential master equation

$$\frac{\partial P(\theta)}{\partial t} = D \frac{\partial^2 P(\theta)}{\partial \theta^2} + \int_{-\pi}^{\pi} d\phi \, P\left(\theta - \frac{\phi}{2}\right) P\left(\theta + \frac{\phi}{2}\right) - P(\theta). \tag{5}$$

The first term on the right-hand-side describes diffusion. The integral accounts for gain of rods with orientation θ as a result of alignment of two rods with an orientation difference of ϕ, while the negative term accounts for loss due to alignment. Without loss of generality, the alignment rate is set such that the loss rate equals one.

A. Goal: Steady-state distribution

$$0 = D \frac{\partial^2 P(\theta)}{\partial \theta^2} + \int_{-\pi}^{\pi} d\phi \, P\left(\theta - \frac{\phi}{2}\right) P\left(\theta + \frac{\phi}{2}\right) - P(\theta). \tag{6}$$

The disordered state is always a solution of this equation

$$P_{\text{disordered}}(\theta) = \frac{1}{2\pi}. \tag{7}$$

IV. THE FOURIER TRANSFORM

Definition

The governing master equation (6) is nonlinear and nonlocal. Its convolution structure suggests using the Fourier transform

$$P_k = \left\langle e^{-ik\theta} \right\rangle = \int_{-\pi}^{\pi} d\theta \, e^{-ik\theta} \, P(\theta). \tag{8}$$

The zeroth mode equals one, $P_0 = 1$, because of the normalization, and also, $P_k = P_{-k}^*$. The angular distribution can be expressed as a Fourier series

$$P(\theta) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} P_k \, e^{ik\theta}. \tag{9}$$

Rotational Symmetry

Since the alignment process (2) is invariant with respect to an overall rotation

$$\theta \to \theta + \varphi \qquad \text{with} \qquad 0 \le \varphi \le 2\pi.$$

If $P(\theta)$ is solution of (6), so is $P(\theta + \varphi)$. Consequently, if P_k is solution, then so is $P_k e^{ik\varphi}$.

The order parameter

The order parameter

$$R = \left| \langle e^{i\theta} \rangle \right| = |P_{-1}|, \tag{10}$$

with the bounds $0 \le R \le 1$ probes the state of the system. A vanishing order parameter indicates an isotropic, disordered state, while a positive order parameter reflects a nematic, ordered state.

Closed equations for the Fourier transform

We focus on the steady state. Substituting the Fourier series (9) into the master equation (6), and integrating over ϕ, we find that the Fourier transform satisfies a set of coupled nonlinear equations

$$\left(1 + Dk^2\right) P_k = \sum_{i+j=k} A_{i-j} \, P_i \, P_j \tag{11}$$

with

$$A_q = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \, e^{iq\phi/2} = \frac{\sin \frac{\pi q}{2}}{\frac{\pi q}{2}}.$$

The coefficients A_q satisfy

$$A_q = \begin{cases} 1 & q = 0; \\ 0 & q = 2, 4, \ldots; \\ (-1)^{\frac{q-1}{2}} \frac{2}{\pi|q|} & q = 1, 3, \ldots \end{cases} \qquad \text{and} \qquad A_q = A_{-q}. \tag{12}$$

In (11), when $k = 0$, the sum contains only a single term, $P_0 = P_0^2$ and indeed, $P_0 = 1$. Later, we will need to use the following constants

$$A_1 = \frac{2}{\pi}, \qquad A_2 = -\frac{2}{3\pi}. \tag{13}$$

Since $P_0 = 1$ is known, the identical terms $A_{-k} P_0 P_k$ and $A_k P_k P_0$ in the steady-state equation (11) are linear in P_k, and thus, we move them to the left-hand side. Then Eq. (11) becomes

$$\left(1 + Dk^2 - 2A_k\right) P_k = \sum_{\substack{i+j=k \\ i \neq 0, \, j \neq 0}} A_{i-j} \, P_i \, P_j. \tag{14}$$

V.   THE "HOLY GRAIL"

We will work with the following compact nonlinear convolution equation

$$P_k = \sum_{\substack{i+j=k \\ i \neq 0, \, j \neq 0}} G_{i,j} P_i \, P_j. \tag{15}$$

Coupling constants

The kernel $G_{i,j}$ couples the ith and the jth Fourier modes

$$G_{i,j} = \frac{A_{i-j}}{1 + D(i+j)^2 - 2A_{i+j}}. \tag{16}$$

It has the following properties:

$$G_{i,j} = G_{j,i} \tag{17a}$$

$$G_{i,j} = G_{-i,-j} \tag{17b}$$

$$G_{i,j} = 0, \qquad \text{for} \qquad |i - j| = 2, 4, \dots. \tag{17c}$$

The governing equation (15) is nonlinear and moreover, for odd k, the sum contains an infinite number of terms. Despite this, it is still possible to solve this equation analytically!

VI.   EXACT SOLUTION

Repeated iterations

First, we notice that Eq. (15) can be iterated once, leading to a sum of products of three Fourier modes

$$P_k = \sum_{\substack{i+j=k \\ i \neq 0, \, j \neq 0}} \sum_{\substack{l+m=j \\ l \neq 0, \, m \neq 0}} G_{i,j} \, G_{l,m} \, P_i \, P_l \, P_m. \tag{18}$$

Clearly, this procedure can be repeated any number of times, leading to a sum over products of any given number of Fourier modes.

Solution for small k

Let us spell out these equations for the lowest order terms

$$P_2 = G_{1,1}P_1^2 \tag{19a}$$

$$P_3 = 2G_{1,2}P_1P_2 + 2G_{-1,4}P_{-1}P_4 + \cdots \tag{19b}$$

$$P_4 = G_{2,2}P_2^2. \tag{19c}$$

We can solve for P_2 and P_4 in terms of P_1 (equivalent to the order parameter)

$$P_2 = G_{1,1}P_1^2 \tag{20a}$$

$$P_4 = G_{2,2}G_{1,1}^2 P_2^4. \tag{20b}$$

How about P_3? Well, we can simply substitute P_2 and P_4:

$$P_3 = 2G_{1,2}G_{1,1}P_1^3 + 2G_{-1,4}G_{2,2}G_{1,1}^2 P_1^4 P_{-1} + \cdots . \tag{21}$$

Generally, the kth Fourier mode can be written as an infinite series involving terms of the form

$$P_1^{k+n}P_{-1}^n = P_1^k(P_1\,P_{-1})^n = P_1^k R^{2n}$$

with n a positive integer. Recall that $P_1 = R\,e^{i\varphi}$. Without loss of generality, we can set the phase to zero, $\varphi = 0$. In other words, we pick the solution where

$$P_1 = P_1^* = R.$$

Solution for general k

Since $P_1 = R$, the Fourier modes can be written explicitly in terms of the order parameter R

$$P_k = R^k \sum_{n=0}^{\infty} p_{k,n}\, R^{2n}. \tag{22}$$

Of course, $p_{0,n} = p_{\pm 1,n} = \delta_{n,0}$. Since $p_{k,n} = p_{-k,n}$ it suffices to solve for $k > 0$.
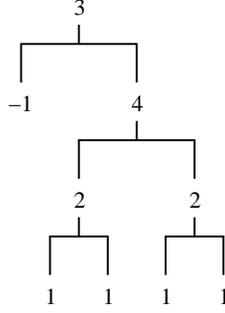
FIG. 2: The iterated integer partitions. Illustrated is the partition corresponding to $p_{3,1} = 2G_{-1,4}G_{2,2}G_{1,1}^2$. Each partition $k = i + j$ with $i \neq 0$ and $j \neq 0$ generates a factor $G_{i,j}$. The factor 2 accounts for the two equivalent partitions.

Relation with iterated integer partitions

The coefficients $p_{k,n}$ represent all iterated partitions of the integer k as follows

$$k = \underbrace{1 + 1 + \cdots + 1 + 1}_{k+n} \underbrace{-1 - \cdots - 1}_{n}. \tag{23}$$

Partition rules

1. $k = i + j$

2. $i \neq 0$ and $j \neq 0$

3. $|k| \neq 1$

4. $G_{i,j} \neq 0$.

The lowest terms ($\leq$ fifth order)

$$p_{2,0} = G_{1,1}, \tag{24a}$$

$$p_{3,0} = 2G_{1,2}G_{1,1}, \tag{24b}$$

$$p_{3,1} = 2G_{-1,4}G_{2,2}G_{1,1}^2, \tag{24c}$$

$$p_{4,0} = G_{2,2}G_{1,1}^2, \tag{24d}$$

$$p_{5,0} = 2G_{1,4}G_{2,2}G_{1,1}^2 + 4G_{2,3}G_{1,2}G_{1,1}^2. \tag{24e}$$

Recursion equation for systematic evaluation

Substituting the series expansion (22) into the steady-state equation (15) and equating the same powers of R, the coefficients $p_{k,n}$ satisfy

$$p_{k,n} = \sum_{l+m=n} \sum_{\substack{i+j=k \\ i\neq 0,\, j\neq 0}} p_{i,l}\, p_{j,m}. \tag{25}$$

Since the indexes l and m are positive, this is now a recursion equation. Starting with $p_{0,0} = p_{1,0} = 1$, and utilizing the symmetry $p_{k,n} = p_{-k,n}$, equation (25) is solved recursively. This provides a systematic method for obtaining the coefficients $p_{k,n}$.

Closed equation for the order parameter

The series (22) expresses all the Fourier modes in terms of the order parameter R. It remains to obtain the order parameter R as a function of the diffusion constant D. By Substituting the Fourier solution (22) into the governing equation (15) and setting $k = 1$, we find that the order parameter itself can be expressed as an infinite series

$$R = \sum_{n=1}^{\infty} r_n R^{2n+1}. \tag{26}$$

The coefficients r_n are given by the very same recursion equation (25)

$$r_n = \sum_{l+m=n} \sum_{\substack{i+j=1 \\ i\neq 0,\, j\neq 0}} p_{i,l}\, p_{j,m}. \tag{27}$$

The coefficient r_n is the counterpart of the coefficients $p_{k,n}$ and it represents iterated partitions of the number 1 as in (23). The partitions may not involve 0's. Except for the very *first* partition, the numbers ± 1 may not be repartitioned (Fig. 2). The first few coefficients are

$$r_1 = 2G_{-1,2}G_{1,1}, \tag{28a}$$

$$r_2 = 4G_{-2,3}G_{1,2}G_{1,1}^2, \tag{28b}$$

$$r_3 = 4(G_{-2,3}G_{-1,4} + G_{-3,4}G_{1,2})G_{2,2}G_{1,1}^3. \tag{28c}$$

The order parameter

In practice, one can calculate the order parameter R as a root of a polynomial of degree N by truncating (26). For $N = 3$, substituting (12) and (16) into (28a) yields

$$r_1 = \frac{4}{3\pi} \frac{1}{\frac{4}{\pi} - 1 - D} \frac{1}{1 + 4D},$$

and using (26) gives the cubic equation for the order parameter

$$R = \frac{4}{3\pi} \frac{1}{D_c - D} \frac{1}{1 + 4D} R^3 \qquad D_c = 2A_1 - 1 = \frac{4}{\pi} - 1. \tag{29}$$

Two regimes:

Supercritical: For $D \geq D_c$, there is only the trivial solution $R = 0$, corresponding to an isotropic state where the rods are randomly aligned: $P_k = \delta_{k,0}$ and $P(\theta) = \frac{1}{2\pi}$.

Subcritical: For $D < D_c$, there is also the nontrivial solution (Fig. 3)

$$R = \sqrt{\frac{3\pi}{4} (1 + 4D)(D_c - D)}. \tag{30}$$

This corresponds to a nematic phase in which the rods are partially aligned. Near the transition point, this alignment is weak, but it becomes stronger and stronger as D decreases. The result of Eq. (30) is approximate—only the cubic term in (26) has been maintained. Close to the transition point, the corrections to the cubic equation (29) are negligible and

$$R \sim C(D_c - D)^\beta \qquad \text{with} \qquad \beta = \frac{1}{2}. \tag{31}$$

As shown in the Appendix, the uniform state is stable for $D > D_c$ but unstable for $D < D_c$.
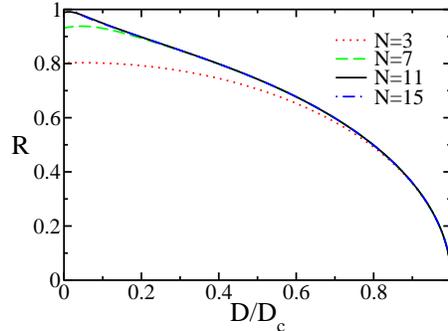
FIG. 3: The order parameter versus the diffusion coefficient. The order parameter was obtained by solving polynomials of increasing order.

The orientation distribution

Well below the critical point, we compute the coefficients $p_{k,n}$ and r_n to higher order from (25) and (27). The order parameter is then obtained by numerically solving (26), truncated at the corresponding order. Since the Fourier modes decay exponentially with the wave number

$$P_k \sim R^k, \tag{32}$$

and since the order parameter obeys $0 \leq R \leq 1$, a moderate number of Fourier modes is sufficient to accurately compute $P(\theta)$. The order parameter rapidly converges with N. For instance, $N = 11$ already provided an accurate value for R (see Fig. 3). We note that at this order, it is still possible to calculate the necessary partitions manually.

Once the order parameter is known, the Fourier modes are obtained from (22). The steady-state distribution (9) becomes

$$P(\theta) = \frac{1}{2\pi} + \frac{1}{\pi} R \cos \theta + \frac{1}{\pi} G_{1,1} R^2 \cos(2\theta) + \frac{2}{\pi} G_{1,2} G_{1,1} R^3 \cos(3\theta) + O(R^4). \tag{33}$$

In the vicinity of the transition point, the lowest mode dominates. As the diffusion coefficient decreases, the angle distribution becomes sharply peaked around $\theta = 0$, reflecting that the rods are strongly aligned (Fig. 4).
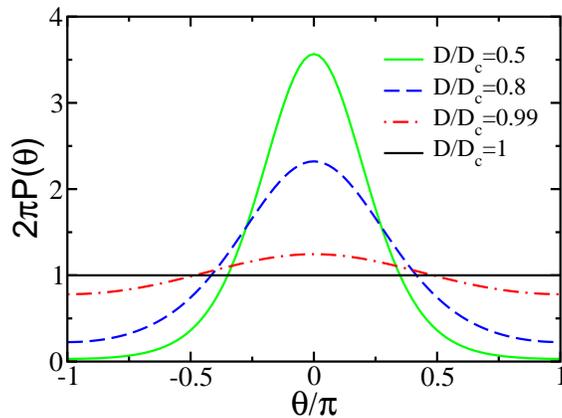
FIG. 4: The angular distribution for various values of D. The angle distribution was obtained from the first 15 Fourier modes.

VII.   GENERAL ALIGNMENT RATES

It is also possible to analyze situations in which the alignment process (2) occurs with arbitrary alignment rate

$$K\left(\theta_1 - \theta_2\right) \qquad K(\phi) = K(-\phi).$$

Without loss of generality, impose the normalization,

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi\, K(\phi) = 1.$$

The master equation becomes

$$0 = D\frac{d^2 P}{d\theta^2} + \int_{-\pi}^{\pi} d\phi\, K(\phi) P\left(\theta - \frac{\phi}{2}\right) P\left(\theta + \frac{\phi}{2}\right) - P(\theta) \int_{-\pi}^{\pi} d\phi\, K(\phi) P(\theta + \phi). \quad (34)$$

The Fourier modes satisfy a generalization of (11)

$$Dk^2 P_k = \frac{1}{2} \sum_{i+j=k} \left(A_{i-j} + A_{j-i} - A_{2i} - A_{2j}\right) P_i P_j. \quad (35)$$

The constant A_q is now

$$A_q = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi\, e^{iq\phi/2} K(\phi).$$

Again $A_0 = 1$ and $A_q = A_{-q}$, but it is not necessarily true that these constants vanish at even indexes as was the case for uniform alignment rates. By excluding the zero modes $i = 0$ and $j = 0$ from the summation in (35), and by following the same steps, we recover the governing steady-state Eq. (15). The generalized coupling constants (16) are

$$G_{i,j} = \frac{1}{2} \frac{A_{i-j} + A_{j-i} - A_{2i} - A_{2j}}{1 + D(i + j)^2 - 2A_{i+j}}. \quad (36)$$

These coupling constants are manifestly symmetric $G_{i,j} = G_{j,i}$. We conclude that the series solutions (22) and (26) hold for arbitrary alignment rates.

Repeating the steps above, the critical diffusivity is

$$D_c = 2A_1 - 1.$$

The condition for having a phase transition is

$$A_1 > \frac{1}{2}.$$

For the hard-sphere rate $K(\phi) = \frac{2}{\pi}|\phi|$, then $A_1 = \frac{4}{\pi^2}(2 - \pi)$, but since $A_1 < 1/2$, the system is always disordered. For the hard-sphere rate $K(\phi) = \frac{2}{\pi}|\phi|$, then $A_1 = \frac{4}{\pi^2}(2 - \pi)$, but since $A_1 < 1/2$, the system is always disordered. For the more realistic hard-rod rate

$$K(\phi) = \frac{\pi}{2}|\sin\phi|, \tag{37}$$

and since $A_1 = \frac{2}{3}$, the system undergoes a phase transition. We conclude that depending on the alignment rate, there may or may not be an ordered phase.

We note that in the kinetic theory of gases, analytic solutions are feasible only for the Maxwell model, where the collision rate is velocity independent, while the general Boltzmann equation is not analytically tractable. Remarkably, the analytic solution presented above does not require a constant rate and for example, the hard-sphere like collision rate $K(\phi) = C|\phi|$ *can* be solved analytically. The discrete nature of the Fourier spectrum enables this.

VIII.   STABILITY OF THE UNIFORM STATE

The uniform state $P(\theta) = \frac{1}{2\pi}$ is always a steady-state of the master equation (6). To check when this state is stable, we write $P(\theta, t) = \frac{1}{2\pi} + p(\theta, t)$. To linear order, the perturbation satisfies

$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial \theta^2} + \int_{-\pi}^{\pi} d\phi \, \frac{p(\theta - \phi/2) + p(\theta + \phi/2)}{2\pi} - p. \tag{38}$$

Let us take a periodic perturbation with wave number k and growth rate λ, that is, $p(\theta, t) \propto e^{ik\theta + \lambda t}$. Substituting this form into Eq. (38) gives the growth rate

$$\lambda_k = 2A_k - 1 - Dk^2. \tag{39}$$

The growth rate is positive only for the lowest mode, $k = 1$, and hence, stability is governed by the smallest wave number $k = 1$ for which $\lambda_1 = D_c - D$. Indeed, the uniform state is unstable below the critical diffusion constant $D_c = \frac{4}{\pi} - 1$.

IX.   CONCLUSIONS

1. Nonequilibrium phase transition.

2. Transition depends sensitively on alignment rates.

3. Boltzmann equation exactly solvable when Fourier spectrum is discrete!