Phase Coupling in Space: A Thermodynamic Approach

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I. INTRODUCTION

Much of the work on coupled oscillators has been carried out by applied mathematicians, who construct proofs of stability and other properties in dynamical systems formulations of the problems. We will summarize relevant findings along the way, but we will complement these by following instead a heuristic approach. Using that mathematicians' hated term "physical intuition," we will make somewhat-cavalier approximations until the system becomes sufficiently simple. These approximations are well-motivated, but issues of convergence will not be discussed in detail. Instead of proving general results, our goal is to construct a qualitative picture where one has not been established by the mathematicians' approach.

II. MEAN-FIELD SYNCHRONIZATION

Steven Strogatz tells the story of swarms of fireflies which all flash in unison and in rhythm (2003). They begin each night flashing at random, and over time, as the swarm coalesces, they synchronize. These fireflies are the prototypical example of a remarkably widespread phenomenon: circadian rhythms, alpha and beta waves in the brain, pendulum clocks that begin to walk in step, and more.

A physical model of such synchronization is the Belousov-Zhabotinsky reaction, in which a chemical model for the Krebs cycle oscillates between colorless and and yellow (Winfree 1984). The original reaction used bromate and citrate, but variants have employed many others. In a traditional equilibrium chemical reaction, reactants and products dissociate and recombine, but due to entropy, the abundance of each stays constant. The Belousov-Zhabotinsky reaction, then, is quite unusual: dissociation and recombination happen in lock-step, and can proceed backwards and forwards many times.

In a solution, mean-field coupling (each oscillator influences every other oscillator equally) is a reasonable approximation. This limit is described by the exactly solvable Kuramoto Model (Kuramoto 1975). In the Kuramoto model, N oscillators θ_i with intrinsic frequency ω_i drawn from a distribution $g(\omega)$ are coupled to one another, leading to dynamical equations

$$\dot{\theta} = \omega_i + K \sum_{j=1}^{N} \sin(\theta_j - \theta_i). \tag{1}$$

This system can be solved explicitly for some frequency distributions g, such as a Lorentzian (Acebrón et al. 2005); in general, it synchronizes for a sufficiently narrow initial distribution.

III. OSCILLATORS IN SPACE

In many cases, oscillators are fixed in place, rather than diffusing in solution, and spatial effects are nontrivial. Professor Emery Brown has observed long-range correlations among oscillations in the brain during general anesthesia (Mukamel et al. 2011). The theory of oscillators with nearest-neighbor interactions is less well-developed, but they have been explored in many experiments. One such model is the Belousov-Zhabotinsky reaction in droplets. Microfluidic tools can be used to create microemulsions, many tiny oscillators, which can couple diffusively through the medium, but much less strongly than they couple to themselves (Torbenson et al. 2017). These systems are often used to model intercell signaling and collective phenomena of multicellular organisms.

We will construct a partition function for an idealized model of a system of Belousov-Zhabotinsky droplets. Although oscillators are not in thermodynamic equilibrium, we can consider them to be in a sort of periodic equilibrium. Consider a system with one continuous dimension and d discrete (lattice) dimensions. Looking for oscillations in d discrete dimensions is equivalent to looking for waves in $d+1$ dimensions, such as in special relativity. We assume coupling between the amplitudes (states) of nearest-neighbor oscillators, and some potential which enforces an intrinsic natural frequency for the oscillators. In systems larger than single molecules, diffusivity is likely a more meaningful control parameter than temperature, because the necessary changes in temperature could destroy biological systems. Nevertheless, we can interpret our coupling K as an inverse temperature, as long as we remember it may not map to temperature in the physical systems.

Notation: We will consider harmonic oscillators i with frequency ω_i, unit amplitude, and phase shift ϕ_i. In our coupled system, we will use d to refer to the spatial dimension only, so that $d = 3$, for example, corresponds

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to Minkowski spacetime. We will always speak of the *wavelength* $1/q$ in the momentum-space representation of statistical fields, and the *frequency* ω_i of individual oscillators, to distinguish these concepts.

The Hamiltonian is

$$\beta\mathcal{H} = \int_0^{2\pi n/\omega_0} dt \frac{K}{2} \sum_{\langle ij \rangle} \left[\cos(\omega_i t + \phi_i) - \cos(\omega_j t + \phi_j)\right]^2 + u \sum_i (\omega_i - \omega_0)^2 \quad (2)$$

where t is integrated over a correlation time over which each oscillator can be assumed to have approximately constant frequency and phase shift. The partition function is then

$$Z = \prod_i \left[\int_0^\infty d\omega_i \int_0^{2\pi} d\phi_i\right] e^{-\beta\mathcal{H}[\omega,\phi]} \quad (3)$$

IV. STATISTICAL FIELD APPROXIMATION

If the frequency and period varies little between neighboring oscillators, we can define continuous fields $\omega(\mathbf{x})$ and $\phi(\mathbf{x})$. Write $\omega_i = \omega(\mathbf{x})$ and $\omega_j = \omega(\mathbf{x} + \delta\mathbf{x}) = \omega(\mathbf{x}) + \delta\omega(\mathbf{x})$, and similarly for ϕ. Integrating over t then gives

$$\begin{aligned}\beta\mathcal{H} = \int d^d\mathbf{x} \Bigg[& \frac{K}{2} \frac{\frac{8\pi n\omega}{\omega_0} + \sin\left(\frac{4\pi n\omega}{\omega_0} + 2\phi\right) - \sin(2\phi)}{4\omega} \\ & + \frac{K}{2} \frac{\sin\left(\frac{4\pi n(\omega+\delta\omega)}{\omega_0} + 2\phi + 2\delta\phi\right) - \sin(2\phi + 2\delta\phi)}{4\omega + 4\delta\omega} \\ & - \frac{K}{2} \frac{\sin\left(\frac{2\pi n(2\omega+\delta\omega)}{\omega_0} + 2\phi + \delta\phi\right) - \sin(2\phi + \delta\phi)}{\delta\omega + 2\omega} \\ & - \frac{K}{2} \frac{\sin\left(\frac{2\pi n\delta\omega}{\omega_0} + \delta\phi\right) - \sin(\delta\phi)}{\delta\omega} + u(\omega - \omega_0)^2 \Bigg] \end{aligned} \quad (4)$$

We will assume a small lattice spacing a. If the vector from i to j is $\mathbf{a}$, then $\delta\omega \approx a^\mu \partial_\mu \omega + \frac{1}{2} a^\mu a^\nu \partial_\mu \partial_\nu \omega$. We will expand in a, systematically keeping terms of order a^2. At this order, interaction terms of order a^0 and a^1 vanish, as do second derivatives of ω and ϕ:

$$\begin{aligned}\beta\mathcal{H} = \int d^d\mathbf{x} \Bigg\{ & \frac{Ka^2}{2} \left[-\frac{\sin\left(\frac{42\pi n\omega}{\omega_0} + 2\phi\right)}{4\omega} + \frac{\pi n}{\omega_0} + \frac{\sin(2\phi)}{4\omega} \right] (\nabla\phi)^2 + \\ & \frac{Ka^2}{2} \left[+ \frac{2\pi^2 n^2}{\omega_0^2} - \frac{\cos\left(\frac{42\pi n\omega}{\omega_0} + 2\phi\right)}{4\omega^2} - \frac{\pi n \sin\left(\frac{42\pi n\omega}{\omega_0} + 2\phi\right)}{\omega_0 \omega} + \frac{\cos(2\phi)}{4\omega^2} \right] \nabla\phi \cdot \nabla\omega \\ & + \frac{Ka^2}{2} \left[\frac{4\pi^3 n^3}{3\omega_0^3} - \frac{\pi^2 n^2 \sin\left(\frac{4\pi n\omega}{\omega_0} + 2\phi\right)}{\omega_0^2 \omega} + \frac{\sin\left(\frac{4\pi n\omega}{\omega_0} + 2\phi\right)}{8\omega^3} \right. \\ & \left. - \frac{\pi n \cos\left(\frac{4\pi n\omega}{\omega_0} + 2\phi\right)}{2\omega_0 \omega^2} - \frac{\sin(2\phi)}{8\omega^3} \right] (\nabla\omega)^2 + u(\omega - \omega_0)^2 \Bigg\} \end{aligned} \quad (5)$$

We have, of course, defined $\nabla\phi$ such that the jump from 2π to 0 is continuous.

To proceed from this model in the continuum case, we note that there is no preferred phase ϕ, so the final Hamiltonian should not depend on ϕ, but only on its derivatives. We assume that these terms are small enough that they can be treated linearly: the errors introduced by bringing the integral inside the exponential, or in the coupling to $\nabla\phi$, are second-order corrections. On these grounds, we integrate the ϕ dependence out of the trigonometric functions: because their mean value over $0 \leq \phi < 2\pi$ is 0, these terms then vanish. This is a drastic approximation, but it makes the model Gaussian:

$$\begin{aligned}\beta\mathcal{H} = \int d^d\mathbf{x} \Bigg\{ & \frac{Ka^2}{2} \frac{\pi n}{\omega_0} (\nabla\phi)^2 + \frac{Ka^2}{2} \frac{2\pi^2 n^2}{\omega_0^2} \nabla\phi \cdot \nabla\omega \\ & + \frac{Ka^2}{2} \frac{4\pi^3 n^3}{3\omega_0^3} (\nabla\omega)^2 + u(\omega - \omega_0)^2 \Bigg\} \end{aligned} \quad (6)$$

In a saddle-point approximation, we can immediately see that the oscillators synchronize and $\omega \to \omega_0$ whenever $u > 0$.

In momentum space, the Hamiltonian becomes

$$\begin{aligned}\beta\mathcal{H} = \int_0^\Lambda \frac{d^d\mathbf{q}}{(2\pi)^d} \Bigg\{ & \frac{Ka^2}{2} \frac{\pi n}{\omega_0} q^2 \left| \tilde{\phi}(\mathbf{q}) + \frac{2\pi n}{\omega_0} \tilde{\omega}(\mathbf{q}) \right|^2 \\ & + \left(\frac{Ka^2}{2} \frac{4\pi^3 n^3}{3\omega_0^3} q^2 + u \right) |\tilde{\omega}(\mathbf{q})|^2 \Bigg\} + 2u\omega_0 \tilde{\omega}(\mathbf{q} = 0) \end{aligned} \quad (7)$$

where we have introduced an explicit ultraviolet cutoff $\Lambda \sim 1/a$. Coarse-graining to remove modes $q > \Lambda/b$, rescaling $\mathbf{q}' = b\mathbf{q}$, and renormalizing $\tilde{\omega}', \tilde{\phi}' = \tilde{\omega}/z, \tilde{\phi}/z$ is trivial. We find two typical recursion relations, and one atypical one:

$$K' = b^{-2-d} z^2 K$$

$$u' = zu$$

$$\left(\frac{K' a^2}{2} \frac{4\pi^3 n^3}{3\omega_0^3} q^2 + u' \right) = \left(\frac{Ka^2}{2} \frac{4\pi^3 n^3}{3\omega_0^3} q^2 b^{-2} + u \right) b^{-d} z^2$$

This last one fixes $z = b^d$, so the renormalization group flow equations and critical exponents are

$$\frac{dK}{dl} = (d-2)K \qquad \Longrightarrow y_K = d - 2$$

$$\frac{du}{dl} = du \qquad \Longrightarrow y_u = d$$

In this Gaussian model, K is relevant for $d > 2$ and u is always relevant. In any dimension, the deviations in ω away from ω_0 get smaller as we coarse-grain and u increases. But in $d < 2$, the phase shifts never fall into line, and the system remains disordered at all finite temperatures. For $d < 2$, this suggests the system does not synchronize. For $d > 2$, the system always tends toward synchronization. For $d = 2$, K is marginal.

V. POSITION-SPACE RENORMALIZATION

In $d = 1$, we can let $\sigma_i' = (\omega_i', \phi_i')$ stand for the frequency and phase shift of the odd-numbered oscillators and $s_i = (w_i, f_i)$ stand for the frequency and phase shift of the even-numbered oscillators. Then the partition function becomes

$$Z = \int d^{N/2}\omega' \, d^{N/2}\phi' \prod_{i=1}^{N/2} \left[\int dw_i \, df_i \, e^{B(\sigma_i', s_i) + B(s_i, \sigma_{i+1}')} \right],$$

$$B(\sigma_i, \sigma_j) = -\frac{u}{2}(\omega_i - \omega_0)^2 - \frac{u}{2}(\omega_j - \omega_0)^2 - \int_0^{2\pi n/\omega_0} dt \frac{K}{2} \left[\cos(\omega_i t + \phi_i) - \cos(\omega_j t + \phi_j)\right]^2 \quad (8)$$

We will decimate the spins s_i, integrating over w_i, f_i. In doing so, it is necessary to make two approximations. First, in expanding B, we find terms such as $\exp[A\sin(f_i)]$, which are well-approximated by $1 + A\sin(f_i) + A^2\sin^2(f_i)/2$ if A does not diverge in the region of interest. This does in fact hold: although there are terms with, e.g., $w_i - \omega_i'$ in the denominator, the numerators vanish as $w_i - \omega_i' \to 0$, so each factor is finite. The f_i integral then becomes a polynomial of trigonometric of functions, which are easily integrated from 0 to 2π.

Second, we perform a saddle-point integral for w_i. For u sufficiently strong, $w_i \approx \omega_0$, so we approximate the integral by replacing w_i with ω_0.

Unlike the $d = 1$ Ising model, the $d = 1$ coupled oscillator system generates higher-order terms under renormalization. However, we can achieve a first-order approximate renormalization group by keeping only the first term, and considering the limit when ω_i' is close to ω_{i+1}' and ϕ_i' to ϕ_{i+1}'. In this limit, we set

$$\int dw_i \, df_i \, e^{B(\sigma_i', s_i) + B(s_i, \sigma_{i+1}')} = e^{B'(\sigma_i', \sigma_{i+1}')},$$

$$B'(\sigma_i', \sigma_{i+1}') = -\frac{u'}{2}(\omega_i' - \omega_0)^2 - \frac{u'}{2}(\omega_{i+1}' - \omega_0)^2 - \int_0^{2\pi n/\omega_0} dt \frac{K'}{2} \left[\cos(\omega_i' t + \phi_i') - \cos(\omega_{i+1}' t + \phi_{i+1}')\right]^2 + \text{higher-order terms}$$

We have decimated half of the spins, so $b = 2$. In this model, with the above approximations, we find that

$$K' = \left(\tfrac{4}{9} + \tfrac{10}{9n^2\pi^2} - \tfrac{5}{4n^4\pi^4}\right)K \approx \tfrac{4}{9}K \implies \quad y_K = -\tfrac{\log(9/4)}{\log 2} \approx -1.17$$

$$u' = u \implies \quad y_u = 0$$

According to the Gaussian model, we should expect $y_K = -1$ and $y_u = 1$. The values for y_K are in good agreement, but the y_u critical exponent is not. This is due to the different simplifications made in the two models. In the decimation model, we treated K and u essentially independently: because the functional forms of their associated terms are quite different, they would not be able to cause corrections to each other that are consistent across the full domain of ω and ϕ. In the Gaussian model, we did just the opposite, simplifying these functional forms until they were of the same type. Both of these are substantial approximations, but this qualitative reasoning suggests that the position-space renormalization group is the more accurate of the two.

VI. TOPOLOGICAL DEFECTS

In $d = 2$, in the limit $u \to \infty$, the system can be mapped onto the XY model, suggesting it too admits topological defects. The elementary vortices are points around which the phase shifts by $2\pi\times$ the winding number. This system admits a Kosterlitz-Thouless transition from long-wavelength fluctuations at high K to a state dominated by defects at low K (Lee 2010).

VII. CONCLUSION

Although it is in principle possible to measure the correlation functions in the experiments discussed here, such a task would require a careful and dedicated setup. Our contribution here is to provide an additional language for describing long-range order of coupled oscillators. Previous models have begun with coupled differential equations; here, we suggest the utility of considering a partition function approach to leverage the thermodynamic discoveries related to lattice models and renormalization.

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