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An integro-differential equation for dynamical systems with diffusion-mediated coupling

Raul P. Aristides · Ricardo L. Viana

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Abstract Many systems of biological interest can be modeled as pointlike oscillators whose coupling is mediated by the diffusion of some substance. This coupling occurs because the dynamics of each oscillator is influenced by the local concentration of a substance which diffuses through the spatial medium. The diffusion equation, on its hand, has a source term which depends on the oscillator dynamics. We derive a mathematical model for such a system and obtain an integro-differential equation. Its solution can be obtained by an approximation scheme for which the unperturbed solution is used to obtain a first-order solution to the coupled oscillators and so on. We present numerical results for the special case of a one-dimensional bounded domain in which the oscillators are randomly placed. Our results show the influence of the coupling parameters on some aspects of the dynamics of the coupled oscillators, like phase and frequency synchronization.

R. P. Aristides · R. L. Viana (✉)
Departamento de Física, Universidade Federal do Paraná, Curitiba, Paraná, Brazil
e-mail: viana@fisica.ufpr.br

R. P. Aristides
e-mail: rparistides@gmail.com

Present Address:
R. P. Aristides
Instituto de Física Teórica, Universidade Estadual Paulista, São Paulo, São Paulo, Brazil

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1 Introduction

The study of collective dynamics exhibited by spatially extended coupled systems like continuous-time flows and discrete-time maps is one of the main topics of contemporary nonlinear dynamics [1]. One of the most widely investigated model consists of phase oscillators with frequencies randomly distributed according to a given probability distribution, which are coupled mutually according to a global (or all-to-all) prescription [2]. This model has been adapted to many different situations so as to describe a variety of effects like complex networks and delay coupling [3]. Synchronization dynamics in complex networks is a subject of intense research [4], especially in the context of propagation of epidemics [5].

There are situations, in particular, where the coupling intensity depends on the relative distance between pairs of oscillators. For example, the coupling among systems can be achieved through releasing of some substance which diffuses through the medium in which the oscillators are embedded. The local dynamics of each system is affected by the local

concentration of this substance. Since the rate of production of this substance depends on the oscillator dynamics, we can say that the coupling is mediated by the diffusion of the substance [6].

Among the various biological applications of this kind of system, there is the assembly of clock cells composing the so-called suprachiasmatic nucleus (SCN), which is supposed to synchronize the circadian rhythms with the external 24-h light–dark cycle [7]. In mammals, there are about ten thousand of clock cells, each one of them having its own frequency [8]. It is necessary that a large amount of these cells synchronize their rhythms so as to yield a collective rhythm that is entrained to the 24-h photic stimulation [9]. This synchronization can be achieved by coupling of the SCN clock cells mediated by the diffusion of neurotransmitter GABA [10]. Other network models of biological interest are discussed in references [11–13].

There are also technological applications for this type of coupled dynamical systems, like chemical reactions occurring in emulsions, where the reactants are in the form of droplets suspended in a liquid or gaseous background (like aerosols). In these systems, nonlinear reactions can occur in spatially localized positions, and there is a diffusion process among those positions [14, 15].

Although models of complex network based on the Kuramoto model have been conceived to describe the synchronization of SCN clock cells [16], it would be desirable to have a model taking into account the physics of neurotransmitter diffusion through the intercell medium. In other words, a self-consistent model for this type of coupling should include also the diffusion equation with a suitable source depending on the oscillator dynamics.

The first model for diffusion-mediated coupling was due to Kuramoto and Nakao, who proposed a system in which the coupling is so fast that the concentration of the diffusing chemical relaxes immediately to its equilibrium value [17, 18]. In this way, a non-local type of coupling was obtained, in which the intensity of the interaction between oscillators decreases exponentially with the spatial distance [19]. The exponentially decaying interaction was thoroughly investigated by Kuramoto and his collaborators [20–23]. The Kuramoto–Nakao model (of diffusion-mediated coupling) has been used to describe frequency synchronization in a system of clock cells in a numerical study of SCN dynamical behavior [24], as well as to investigate bursting synchronization of neurons [25]. The Lyapunov spectrum and the complete synchronization of chaotic systems coupled in the Kuramoto–Nakao model have also been investigated [26].

The Kuramoto–Nakao model can be used in situations where the characteristic diffusion time is negligible with respect to the typical oscillator period. This approximation is valid in many situations of biological interest. For example, in the problem of synchronization of SCN clock cells, the diffusion time is of the order or milliseconds, much shorter than the characteristic 24-h period of circadian rhythms [24]. As a second example, it has been proposed that menstrual rhythms can be synchronized due to the diffusion of pheromones in the atmosphere, the so-called McClintock effect [27]. (The existence of this phenomenon has been questioned by recent studies [28, 29].) Since the menstrual period is about 28 days and the characteristic diffusion time is about a second, the conditions for the Kuramoto-Nakao model to be valid are fulfilled [30].

However, there are examples in which this approximation is not necessarily valid, like neuronal cells exhibit spiking or bursting rhythms with periods in the millisecond range [31]. One of the most important sources of neuron coupling is chemical synapses, in which a neurotransmitter is released by the axon extremities and diffuses through the synaptic cleft, before being absorbed by the post-synaptic dendrites [32]. In this case, the characteristic diffusion time is of the same order of the typical oscillator periods, and there should be used a more general model in which the time dependence of the neurotransmitter concentration has to be taken into account.

In this work, we propose an approach to the latter situation, by tackling the more general problem of coupling the oscillator dynamics, which is a many-dimensional ordinary differential equation system, with the diffusion dynamics, described by a partial differential equation where the source term depends on the oscillator dynamics. We solve the latter using Green function method and obtain an integro-differential equation for the diffusion-mediated coupling when the diffusion time is not negligible with respect to the typical oscillator period.

The resulting integro-differential equation cannot be exactly solved, and we propose a perturbative

scheme akin to the Born approximation used to solve the quantum mechanical integral scattering equation [33]. Using the first-order equation resulting from this perturbative scheme, we consider the coupling among phase oscillators in the general case. We show results of numerical simulations of the coupled dynamics in the simplest one-dimensional case where the oscillators are distributed in a one-dimensional bounded domain with absorbing boundary conditions.

The rest of this paper is organized as follows: In Sect. 2, we develop the model of coupled oscillators with interaction mediated by the diffusion of a substance, so obtaining an integro-differential equation. In Sect. 3, we present some methods of solution of this equation, stressing a perturbative approach. A detailed example is given for a one-dimensional finite domain, where the Green functions allow for an analytical approach of the first-order dynamics. Section 4 considers a example, where the oscillators are embedded in a one-dimensional bounded domain. We perform numerical simulations of the systems of equations for this case and show the effect of the various coupling parameters on the dynamics of the coupled system, specifically phase and frequency synchronization. Our conclusions are left to the final section.

2 Model for coupled oscillators

We consider N pointlike dynamical systems, such as phase oscillators, embedded in a d-dimensional Euclidean space. The position vector of the jth system in such a space is denoted by $\mathbf{r}_j$, where $j = 1, 2, \ldots, N$. The dynamical state of the jth system, on its hand, is described by a vector $\mathbf{X}_j(t)$ in a M-dimensional phase space (Fig. 1). Although we use continuous-time flows in our description, the formalism can be straightforwardly modified to include discrete-time maps also. The time evolution of uncoupled system is described by the following non-autonomous vector field

$$\frac{\mathrm{d}\mathbf{X}_j}{\mathrm{d}t} = \mathbf{F}(\mathbf{X}_j, t), \quad (j = 1, 2, \ldots, N). \tag{1}$$

In this model, the coupling among systems depends on the local concentration of this substance, which is a scalar field denoted by $A(\mathbf{r}, t)$. The coupling function can be represented by a M-dimensional vector field $\mathbf{g}$, in such a way that the coupled systems are described by

$$\frac{\mathrm{d}\mathbf{X}_j}{\mathrm{d}t} = \mathbf{F}(\mathbf{X}_j, t) + \mathbf{g}(A(\mathbf{r}_j, t)). \tag{2}$$

This substance diffuses through the space in which the systems are embedded, according to the following partial differential equation

$$\frac{\partial A}{\partial t} + \eta A - D\nabla^2 A = \mathcal{F}(\mathbf{X}, \mathbf{r}, t), \tag{3}$$

where D is the diffusion coefficient, η is a degradation coefficient and $\mathcal{F}$ is a source function which depends, in general, on the positions and dynamical states of all oscillators. Underlying the existence of this term is the assumption that the systems are capable of producing some substance according to their own dynamics. For example, if the system is a clock cell with some characteristic frequency, we may consider the rate of production of the substance (e.g., a neurotransmitter or a pheromone) as a given function of this frequency [17, 18].

Since the systems are pointwise, we can write the source function as a combination of delta functions at the systems' spatial positions, and whose weights are scalar functions h which generally depend on the dynamical state of the oscillators [17, 18]:

$$\frac{\partial A}{\partial t} + \eta A - D\nabla^2 A = \sum_{k=1}^{N} h(\mathbf{X}_k)\,\delta(\mathbf{r} - \mathbf{r}_k). \tag{4}$$

Once we are able to solve this inhomogeneous diffusion equation, the concentration is substituted at the oscillator positions in Eq. (2) and the coupled system of equations can be solved, at least in principle, to yield the oscillator states at further times. It is

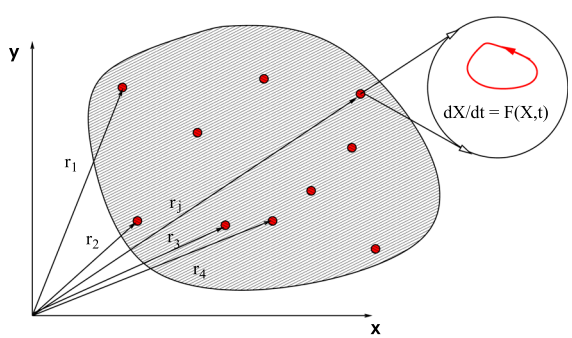

Fig. 1 A system of coupled pointlike oscillators

necessary to specify, when solving Eq. (4), the relevant boundary conditions at some surface $\partial\mathcal{R}$. For simplicity, we shall assume absorbing boundary conditions, i.e., $A(\mathbf{r},t)=0$ for $\mathbf{r}\in\partial\mathcal{R}$. In addition, there should be specified an initial condition $A(\mathbf{r},t=0)$.

The Green function for Eq. (4) is denoted $G(\mathbf{r},t;\mathbf{r}',t')$ and satisfies

$$\frac{\partial G}{\partial t}+\eta\, G-D\,\nabla^2 G=\delta(\mathbf{r}-\mathbf{r}')\,\delta(t-t'), \tag{5}$$

where homogeneous Dirichlet conditions are considered: $G(\mathbf{r},t;\mathbf{r}',t')$ for $\mathbf{r}\in\partial\mathcal{R}$, and the initial condition $G(\mathbf{r},t=0;\mathbf{r}',t')=0$. The Green function can be shown to satisfy the symmetry condition $G(\mathbf{r},t;\mathbf{r}',t')=G(\mathbf{r},-t;\mathbf{r}',t')$.

After Eq. (5) is solved, the resulting Dirichlet Green function can be used to obtain the solution of the inhomogeneous diffusion equation (4):

$$\begin{aligned} A(\mathbf{r},t) \;=\; & \sum_{k=1}^{N}\int_0^{t^+}\mathrm{d}t'\,h(\mathbf{X}_k(t'))\,G(\mathbf{r},t;\mathbf{r}_k,t') \\ & +\int_{\mathcal{R}}\mathrm{d}^d r'\,A(\mathbf{r}',t'=0)\,G(\mathbf{r},t;\mathbf{r}',t'=0) \\ & +D\int_0^{t^+}\mathrm{d}t'\oint_{\partial\mathcal{R}}\mathrm{d}S'\hat{\mathbf{n}}\cdot[\nabla' A(\mathbf{r}',t')G(\mathbf{r},t;\mathbf{r}',t') \\ & -\nabla' G(\mathbf{r},t;\mathbf{r}',t')A(\mathbf{r}',t')], \end{aligned} \tag{6}$$

where $t^+=t+0$ and $\hat{\mathbf{n}}$ is a unit vector pointing outwards the boundary surface $\partial\mathcal{R}$. Considering absorbing boundary conditions in $\partial\mathcal{R}$ and $A(\mathbf{r},t=0)=0$, the solution reduces to

$$A(\mathbf{r},t)=\sum_{k=1}^{N}\int_0^{t^+}\mathrm{d}t'\,h(\mathbf{X}_k(t'))\,G(\mathbf{r},t;\mathbf{r}_k,t'), \tag{7}$$

which, after substitution into Eq. (2), gives an integro-differential equation governing the coupling among systems mediated by the diffusion of a substance

$$\begin{aligned} \frac{\mathrm{d}\mathbf{X}_j}{\mathrm{d}t} =& \mathbf{F}(\mathbf{X}_j,t) \\ &+\mathbf{g}\left(\sum_{k=1}^{N}\int_0^{t^+}\mathrm{d}t'\,h(\mathbf{X}_k(t'))\,G(\mathbf{r}_j,t;\mathbf{r}_k,t')\right). \end{aligned} \tag{8}$$

For the sake of simplicity, we choose a linear coupling function $\mathbf{g}$ which also does not depend on time, in such a way that we rewrite (8) in a simpler form

$$\begin{aligned} \frac{\mathrm{d}\mathbf{X}_j}{\mathrm{d}t} =& \mathbf{F}(\mathbf{X}_j,t) \\ &+\sum_{k=1}^{N}\int_0^{t}\mathrm{d}t'\,\mathbf{H}(\mathbf{X}_k(t'))\,G(\mathbf{r}_j,t;\mathbf{r}_k,t'), \end{aligned} \tag{9}$$

where we have expressed the composition of functions $\mathbf{g}\circ h$ simply as $\mathbf{H}$. The case of future coupling occurs when $\mathbf{H}=\mathbf{F}$, but $\mathbf{H}$ can represent any nonlinear coupling as well.

The Dirichlet Green functions can be obtained by solving (5) in a d-dimensional space with absorbing boundary conditions. Some results of interest in applications are:

1. Free space (i.e., the boundary surface $\partial\mathcal{R}$ goes to infinity, where the Green function itself is expected to vanish):

   (a) $d=1$ dimension

$$\begin{aligned} G(x,t;x',t') \;=\; & \frac{H(t-t')}{\sqrt{4\pi(t-t')}} \\ & \times\exp\left[-\eta\,(t-t')-\frac{(x-x')^2}{4D(t-t')}\right], \end{aligned} \tag{10}$$

   where $H(t-t')$ is the Heaviside unit-step function.

   (b) $d=2$ and 3 dimensions

$$\begin{aligned} G(\mathbf{r},t;\mathbf{r}',t') \;=\; & \frac{H(t-t')}{[4D\pi(t-t')]^{d/2}}\exp \\ & \times\left[-\eta\,(t-t')-\frac{|\mathbf{r}-\mathbf{r}'|^2}{4D(t-t')}\right]. \end{aligned} \tag{11}$$

2. Finite domains

   (a) $d=1$ dimension: interval of finite length $0\le x\le L$

$$\begin{aligned} G(x,t;x',t') =& \frac{2}{L}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x'}{L}\right) \\ & \times\exp\left\{-\left[D\left(\frac{n\pi}{L}\right)^2+\eta\right](t-t')\right\}H(t-t'). \end{aligned} \tag{12}$$

(b) $d = 2$ dimensions: rectangular domain with $0 \le x \le a$ and $0 \le y \le b$

$$G(\mathbf{r}, t; \mathbf{r}', t') = \frac{4}{L}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{n\pi x'}{a}\right) \sin\left(\frac{m\pi y}{b}\right) \times \sin\left(\frac{m\pi y'}{b}\right) H(t-t') \times \exp\left\{-\left[D\left(\frac{n^2}{a^2}+\frac{m^2}{b^2}\right)\pi^2+\eta\right](t-t')\right\}. \tag{13}$$

(c) $d = 2$ dimensions: circular domain $(0 \le r \le a)$

$$G(r, \theta, t; r', \theta', t') = \frac{1}{\pi D}\sum_{m=-\infty}^{\infty}\sum_{n=1}^{\infty} \frac{J_m\left(x_{mn}\frac{r}{a}\right) J_m\left(x_{mn}\frac{r'}{a}\right)}{[J'_m(x_{mn})]^2} \times \cos[m(\theta-\theta')] \exp\left\{-\frac{Dx_{mn}^2}{a^2}(t-t')\right\}, \tag{14}$$

where x_{mn} is the nth positive root of the Bessel function J_m.

(d) $d = 2$ dimensions: complementary circular domain $(a < r < \infty)$

$$G(r, \theta, t; r', \theta', t') = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty}\sum_{n=1}^{\infty} \cos[n(\theta-\theta')] H(t-t') \times \int_0^{\infty} d\alpha \, \exp\left[-D\alpha^2(t-t')\right] \times \frac{\alpha\, U_n(\alpha r)\, U_n(\alpha r')}{J_n^2(\alpha a) + N_n^2(\alpha a)}, \tag{15}$$

where N_n is the Neumann function and we define the special function $U_n(\alpha r) = J_n(\alpha r)N_n(\alpha a) - J_n(\alpha a)N_n(\alpha r)$.

(e) $d = 2$ dimensions: annular domain $a < r < b$,

$$G(r, \theta, t; r', \theta', t') = \frac{\pi}{4}\sum_{m,n} \frac{[J_m(\alpha_{mn} r)]^2 U_m(\alpha_{mn} r) U_m(\alpha_{mn} r')}{[J'_m(\alpha_{mn} a)]^2 - [J'_m(\alpha_{mn} b)]^2} \times \alpha_{mn}^2 \cos[m(\theta-\theta')] H(t-t') \times \exp\left[-D\alpha_{mn}^2(t-t')\right], \tag{16}$$

where $\alpha_{mn} b$ is the nth positive root of U_m.

Analytical expressions for bounded domains in two and three dimensions and also other coordinate systems can be found in the literature on mathematical physics [34]. These expressions reduce, in the limit of very fast diffusion, to the results obtained by Kuramoto and coworkers [17, 19], as explained in "Appendix."

3 Methods of solution

The integro-differential equation (9) is very difficult to solve in the general case, since knowledge of the oscillator state $\mathbf{X}_k(t')$ is required for all values of $0 \le t' \le t$ in order to solve the integral in the right-hand side, for a given time t. A simpler case is when $\mathbf{H}$ does not depend on the oscillator state itself (it can depend on time, though):

$$\frac{d\mathbf{X}_j}{dt} = \mathbf{F}(\mathbf{X}_j, t) + \sum_{k=1}^{N}\int_0^t dt' \, \mathbf{H}(t') \, G(\mathbf{r}_j, t; \mathbf{r}_k, t'). \tag{17}$$

This coupling prescription, however, depends only on the position of the oscillators, not on their dynamics. In the simplest situation, $\mathbf{H}$ is just a constant vector, such that

$$\frac{d\mathbf{X}_j}{dt} = \mathbf{F}(\mathbf{X}_j, t) + \mathbf{H}\sum_{k=1}^{N} \sigma(\mathbf{r}_j, \mathbf{r}_k; t), \tag{18}$$

where we defined the interaction kernel

$$\sigma(\mathbf{r}_j, \mathbf{r}_k; t) = \int_0^t dt' \, G(\mathbf{r}_j, t; \mathbf{r}_k, t'). \tag{19}$$

A possible approach to solve the integro-differential equation (9) is to proceed in an analogous way to the scattering integral equation in quantum mechanics, which is a perturbative procedure. In the first Born

approximation, we insert the zero-order solution, which is a plane wave, in the scattering integral, to get a first-order solution, which turns out to be a spherical wave, and so on [33]. Hence, we may consider the solution of the vector field for the uncoupled oscillators (1) as the zeroth-order solution

$$\frac{\mathrm{d}\mathbf{X}_j^{(0)}}{\mathrm{d}t} = \mathbf{F}\left(\mathbf{X}_j^{(0)}, t\right), \tag{20}$$

and then substitute it into the integral in the right hand side of (9), so as to obtain a first-order solution satisfying

$$\begin{aligned}\frac{\mathrm{d}\mathbf{X}_j^{(1)}}{\mathrm{d}t} &= \mathbf{F}\left(\mathbf{X}_j^{(1)}, t\right) \\ &+ \sum_{k=1}^{N} \int_0^t \mathrm{d}t'\, \mathbf{H}\left(\mathbf{X}_k^{(0)}(t')\right) G\left(\mathbf{r}_j, t; \mathbf{r}_k, t'\right).\end{aligned} \tag{21}$$

This iterative procedure can continue in such a way that a second-order solution is obtained and so on

$$\begin{aligned}\frac{\mathrm{d}\mathbf{X}_j^{(2)}}{\mathrm{d}t} &= \mathbf{F}\left(\mathbf{X}_j^{(2)}, t\right) \\ &+ \sum_{k=1}^{N} \int_0^t \mathrm{d}t'\, \mathbf{H}\left(\mathbf{X}_k^{(1)}(t')\right) G\left(\mathbf{r}_j, t; \mathbf{r}_k, t'\right).\end{aligned} \tag{22}$$

By assuming convergence of the method, one expects to have an acceptable solution after a presumably small number of iterations. However, the key issue here is that the uncoupled (zeroth order) solution $\mathbf{X}_j^{(0)}(t)$ must be known, which is usually difficult, except for very simple dynamical systems.

A such simple system is a phase oscillator, for which $M = 1$ and the system state is described by a single phase $\mathbf{X}_j(t) = \theta_j(t)$, with $0 \le \theta_j < 2\pi$. A uniform oscillator has a constant frequency, which is the vector field $\mathbf{F}(\mathbf{X}_j) = \omega_j$, where the values of ω can be randomly chosen from a given probability distribution function $g(\omega)$, like in the Kuramoto model of globally coupled phase oscillators [2, 3]. The integro-differential equation for coupling (17) becomes in this case

$$\frac{\mathrm{d}\theta_j(t)}{\mathrm{d}t} = \omega_j + \sum_{k=1}^{N} \int_0^t \mathrm{d}t'\, H\left(\theta_j(t')\right) G\left(\mathbf{r}_j, t; \mathbf{r}_k, t'\right), \tag{23}$$

where H is a (nonlinear) coupling function. We can make further contact with the Kuramoto model of phase oscillators by choosing [2, 3]

$$H(\theta_j) = \frac{K}{N} \sin(\theta_k - \theta_j), \tag{24}$$

where $K > 0$ is a coupling strength, for which (23) reads

$$\begin{aligned}\frac{\mathrm{d}\theta_j(t)}{\mathrm{d}t} &= \omega_j \\ &+ \frac{K}{N} \sum_{k=1}^{N} \int_0^t \mathrm{d}t'\, \sin\left(\theta_k(t') - \theta_j(t')\right) G\left(\mathbf{r}_j, t; \mathbf{r}_k, t'\right).\end{aligned} \tag{25}$$

In this case, the zeroth-order solution is simply

$$\theta_j^{(0)}(t) = \omega_j t + \theta_j(0), \tag{26}$$

such that the first-order solution (25) is

$$\begin{aligned}\frac{\mathrm{d}\theta_j^{(1)}(t)}{\mathrm{d}t} &= \omega_j + \frac{K}{N} \sum_{k=1}^{N} \int_0^t \mathrm{d}t'\, \sin\left[(\omega_k - \omega_j)t'\right. \\ &\left. + \theta_k(0) - \theta_j(0)\right] G\left(\mathbf{r}_j, t; \mathbf{r}_k, t'\right).\end{aligned} \tag{27}$$

4 One-dimensional domain

We present in this section numerical results for the model of linearly coupled phase oscillators given by (25) in one spatial dimension, within a finite domain $0 \le x \le L$, for which the Green function with absorbing boundary conditions is given by (12). A straightforward integration gives the following expression for the first-order solution (27):

$$\frac{\mathrm{d}\theta_j^{(1)}(t)}{\mathrm{d}t} = \omega_j + \frac{K}{N} \sum_{k=1}^{N} \mathcal{I}_{jk}(t), \tag{28}$$

where the interaction term in this expression is given by

$$\mathcal{I}_{jk}(t) = \frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi x_j}{L}\right)\sin\left(\frac{n\pi x_k}{L}\right)\left(\alpha_{jk}^2+\gamma_n^2\right)^{-1} \times \left\{\left[\sin\left(\alpha_{jk}t+\beta_{jk}\right)-\alpha_{jk}\cos\left(\alpha_{jk}t+\beta_{jk}\right)\right] - \mathrm{e}^{-\gamma_n t}\left[\sin\beta_{jk}-\alpha_{jk}\cos\beta_{jk}\right]\right\}, \tag{29}$$

and where the following abbreviations have been introduced

$$\alpha_{jk} = \omega_k - \omega_j, \tag{30}$$

$$\beta_{jk} = \theta_k(0) - \theta_j(0), \tag{31}$$

$$\gamma_n = D\left(\frac{n\pi}{L}\right)^2 + \eta. \tag{32}$$

Using the zeroth-order solution, again, we rewrite the interaction term (29) in such a way that the dynamics of the coupled oscillators is governed by the following set of differential equations

$$\frac{\mathrm{d}\theta_j(t)}{\mathrm{d}t} = \omega_j + \frac{K}{N}\sum_{k=1}^{N}\mathcal{I}_{jk}(t), \tag{33}$$

where

$$\mathcal{I}_{jk}(t) = \frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi x_j}{L}\right)\sin\left(\frac{n\pi x_k}{L}\right)\left(\alpha_{jk}^2+\gamma_n^2\right)^{-1} \times \left\{\left[\sin\left(\theta_k(t)-\theta_j(t)\right)-\alpha_{jk}\cos\left(\theta_k(t)-\theta_j(t)\right)\right] - \mathrm{e}^{-\gamma_n t}\left[\sin\beta_{jk}-\alpha_{jk}\cos\beta_{jk}\right]\right\}, \tag{34}$$

where we dropped the superindexes for the sake of notational simplicity.

We consider N pointlike oscillators located at randomly chosen positions within a spatial one-dimensional domain of length L, whose endpoints represent absorbing boundary conditions. We also suppose that the oscillator natural frequencies ω_j are chosen from a Gaussian probability distribution with zero mean $g(\omega)$, such that $g(\omega)\mathrm{d}\omega$ is the probability of finding an oscillator with frequency in the interval from ω to $\omega + \mathrm{d}\omega$, with normalization

$$\int_{-\infty}^{\infty} \mathrm{d}\omega\, g(\omega) = 1. \tag{35}$$

The presence of negative frequencies in this case is not anomalous at all, since we can interpret them as rotations in the opposite sense (e.g., clockwise). The initial phases $\theta_i(0)$ (with $i = 1, 2, \ldots, N$) are randomly chosen according to a uniform distribution in the interval $[0, 2\pi)$. The first-order solution (33)–(34) is numerically integrated using a fourth-order Runge–Kutta method.

Two numerical results of interest are the distribution of phases $\theta_j(t)$ and of perturbed frequencies, defined as

$$\Omega_j = \lim_{t\to\infty}\frac{\theta_j(t+T)-\theta_j(t)}{t}, \quad (j = 1, 2, \ldots, N), \tag{36}$$

where T is chosen in such a way that transients have decayed. The quantities $\Omega_j(t)$ reduce to the natural frequencies ω_j for vanishing coupling. We fix the values of all parameters but three: the coupling constant K, the diffusion coefficient D and the degradation coefficient η.

An example of the phase distribution of coupled oscillators (at a fixed time) is shown in Fig. 2, where a system of $N = 100$ oscillators are coupled with $K = 10.0$ and different values of D and η. Whenever relatively large difference of values among D and η is used as in case of Fig. 2a or Fig. 2b, the phases are incoherently distributed over the domain $[0, 2\pi)$, whereas for smaller values of D and η the phases become almost synchronized, forming a coherent bunch with a few outliers.

In Fig. 3, we show the distribution of perturbed frequencies (at a fixed time), using the distribution of unperturbed frequencies are a label. For both fixed $\eta = 1.0$ and decreasing D-values, and fixed $D = 1.0$ and decreasing η, we see a trend to frequency synchronization. The roles of the diffusion and degradation coefficient are quite similar, suggesting that the decrease of diffusion and the degradation are both factors contributing to synchronization, for a fixed coupling strength K.

Since phase synchronization implies frequency synchronization in this case (although the converse is not always true), we focus on the former. The transition to phase synchronization can be quantified by the complex order parameter introduced by Kuramoto [2]

$$R(t)\,\mathrm{e}^{i\psi(t)} = \frac{1}{N}\sum_{k=1}^{N}\mathrm{e}^{i\theta_k(t)}. \tag{37}$$

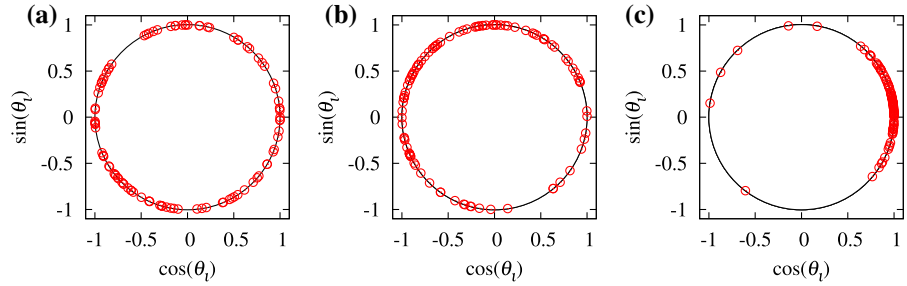

Fig. 2 Phase distribution for the coupled oscillator system described by (33)–(34), with $N = 100$, $K = 10.0$ and **a** $D = 1.0$, $\eta = 12.0$; **b** $D = 4.0$ and $\eta = 1.0$ and **c** $D = \eta = 1.0$

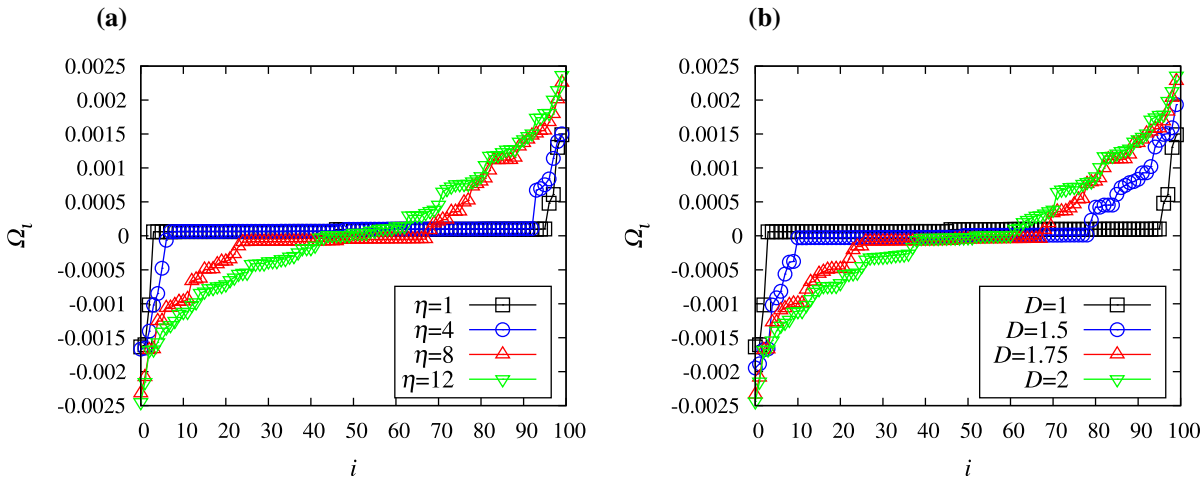

Fig. 3 Perturbed frequency distribution for the coupled oscillator system described by (33)–(34), with $N = 100$, $K = 10.0$ and various values of **a** D, for $\eta = 1.0$ and **b** η, for $D = 1.0$

If $R \approx 0$, the oscillators are completely non-synchronized in phase, whereas if $R \approx 1$, they are completely synchronized. Intermediate values of R characterize partial phase synchronization. Since, for finite N, the order parameter magnitude exhibits size-dependent fluctuations, we compute its mean value over a given time, $\bar{R} = (1/T)\int_0^T R(t)\mathrm{d}t$.

Fixing the values $K = 10.0$ and $D = 1.0$, we compute the values of $\bar{R}$ for increasing D (Fig. 4a) and different number of oscillators. In all cases considered, from $N = 50$ to 400, the order parameter magnitude decreases as D increases, confirming that the effect of a larger diffusion coefficient is to desynchronize the oscillators. The same conclusion comes from varying the degradation coefficient η, for fixed $\eta = 1.0$ (Fig. 4b).

Finally, in Fig. 4c we consider the variation of $\bar{R}$ with increasing coupling constant K, for fixed $\eta = D = 1.0$, where there is a transition to phase synchronization as K increases past a critical value $K \approx 2.5$. The transition is characteristically slow, since for K values as large as 20 we have $\bar{R} \approx 0.9$. Indeed, the coupling constant K actually measures the overall strength of the interaction term (34), similarly to what happens in the classical Kuramoto model (for global coupling). Hence, it is not surprising that the phase synchronization of oscillators increases with increasing K, with a similar transition as that displayed by the Kuramoto model [2].

On the other hand, the decrease of the order parameter magnitude for increasing η and D (Fig. 4a, b, respectively), may seem paradoxical since it is sometimes assumed that the coupling constant is proportional to the diffusion coefficient. In our model, however, the roles of the coupling constant K and diffusion coefficient D are clearly different: The latter enters into the coefficient γ_n which increases with the

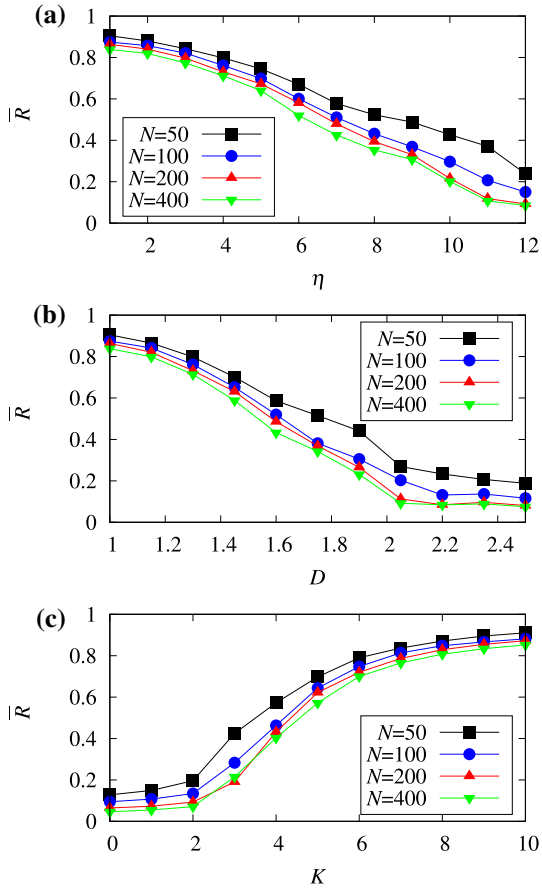

Fig. 4 Order parameter magnitude versus **a** diffusion coefficient D, for $K = 10.0$ and $\eta = 1.0$; **b** degradation coefficient η, for $K = 10.0$ and $D = 1.0$ and **c** coupling constant K, for $\eta = D = 1.0$. Different numbers of oscillators were considered in each case

diffusion coefficient D. In this case, the interaction term (34) decreases its value, such that, for $D \to \infty$, it vanishes. Hence, the coupling effect (in terms of the phase synchronization) actually decreases with increasing D, which is just the result observed in Fig. 4b for the order parameter magnitude.

The degradation parameter η plays a similar role as the diffusion coefficient, since both enter into the interaction term (34) through the coefficient γ_n. As η increases, meaning that the chemical mediating the coupling is becoming scarce, the interaction term decreases its magnitude and the synchronization properties are affected in a way similar to the diffusion coefficient D (Fig. 4a). This explains also why the order parameter magnitude decreases with increasing η, for fixed D and K.

5 Conclusions

We considered in this paper the dynamics of pointlike nonlinear oscillators with coupling mediated by the diffusion of some chemical in the inter-oscillator medium. This coupling occurs because the rate of both secretion and absorption of that chemical depends on the oscillator dynamics. For example, if the phase oscillator has a characteristic frequency, one can assume that the secretion rate is proportional to that frequency and, conversely, that the absorption of the chemical influences the oscillator frequency like a perturbation.

Previous attempts to model this problem have considered the limit in which the diffusion is so fast (compared with the characteristic oscillator timescale, or inverse frequency) that the chemical concentration attains immediately its equilibrium value. If the diffusion timescale is comparable with the oscillator period, however, this approximation is no longer valid and one has to solve a Dirichlet problem for the diffusion equation with pointlike sources. In doing so, we obtained an integro-differential equation which can be approximately solved by using a technique similar to the Born approximation in quantum mechanics: We consider as a zeroth-order approximation the uncoupled motion and use it to solve the integral in the coupling term, obtaining a first-order solution.

If the intensity of the perturbation due to the coupling is not too strong, it is reasonable to assume that this relaxation method converges after a few iterations. In order to use this method, we have to consider a dynamical system sufficiently simple to allow a exact solution in zeroth order. Such a system is found in a uniform phase oscillator, for example, in which each oscillator is endowed with a characteristic frequency randomly chosen according to a given probability distribution. The corresponding first-order solution can be analytically obtained, provided the Green's function of the diffusion equation is known.

The simplest example of an assembly of phase oscillators consists of a bounded one-dimensional domain, where the oscillators are located at random positions. Using the corresponding Green's function, we were able to obtain a closed form for the coupling term, which has some similarity with the classical Kuramoto model. However, in our treatment the coupling term is time dependent and also takes into

account the effect of the spatial distance between pairs of oscillators.

The three basic parameters influencing the coupling properties are the coupling strength, the diffusion coefficient and the degradation coefficient of the chemical mediating the coupling. Phase and frequency synchronization can be observed to depend on these coupling parameters. The dependence on the coupling strength turns to be qualitatively similar to the familiar Kuramoto model of globally coupled oscillators: The order parameter magnitude increases with the coupling strength, displaying a transition from non-synchronized to a partially synchronized regime.

The other two coupling parameters (diffusion and degradation coefficients) play a similar role in the synchronization properties, since they appear in the coupling term in the same foot. The increase of both causes the order parameter to decrease, so destroying a partial phase synchronization. Since the degradation coefficient is related to the loss of the chemical mediating the coupling, it is quite expected that its increase is harmful to synchronization. That the increase of diffusion coefficient provokes the same effect may seem surprising at first, since it is commonly assumed that the coupling strength depends on the diffusion coefficient (for example, see the discussion in Ref. [35], connecting a pulsed reaction–diffusion equation to a locally coupled map lattice). In our model, however, the coupling strength is distinct from the diffusion coefficient, in such a way that the increase in the latter is not related to an enhancement of the coupling term.

The numerical example considered in this paper was limited to the simplest case of a one-dimensional finite domain. Our discussion, however, is not limited to this case, and we provide formulas for other geometries, in two and three dimensions, for which Green's functions are known. The difficulties related to this extension are chiefly of computational effort needed to compute the various terms related to the influence of each and every oscillator, which needs to be updated during the execution time. Moreover, we have used an approximate first-order solution to the integro-differential equation, which limits the application to simple cases where the zeroth-order solution can be analytically obtained. This limits the applications to more complicated non-systems like Rössler, Van der Pol and other systems. In those cases, one will be forced to resort to powerful numerical methods to fully solve the integro-differential equation for the full dynamical problem.

Another interesting, but even more complicated situation, is that of chemotaxis of oscillators, i.e., the possibility of adding the motion of the oscillators to the dynamical system of equations [36]. In this case, we assume that the pointlike oscillators are no longer static but can move through the spatial medium influenced by a chemotactic force which may depend on the local gradient of the chemical mediating the coupling [37]. Due to their motion, the distance among the various oscillators must be likewise updated in each time instant of the numerical solution. The interesting fact here is that the coupling involves three timescales: the oscillator period, the diffusion time and also the timescale characteristic of the motion. Such systems would be important to model the dynamical behavior of moving bacteria and other cell assemblies, with immediate biological applications.

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Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

Appendix: Fast diffusion limit of the interaction kernels

It is instructive to verify that the Green functions we have obtained for the diffusion process reduce to the expressions already obtained by Kuramoto and coworkers in the case of very fast diffusion, for which the concentration of the chemical mediator achieves immediately its stationary state.

From the Green function of the specific geometry in which the system is defined, the corresponding interaction kernel is

$$\sigma(\mathbf{r}_j, \mathbf{r}_k; t) = \int_0^t \mathrm{d}t'\, G\big(\mathbf{r}_j, t; \mathbf{r}_k, t'\big). \tag{38}$$

Using the Green's function of the $d = 1$-dimensional case in free space given by (10), the interaction kernel reads

$$\sigma(x_j, x_k; t) = \int_0^t \mathrm{d}t' \frac{\mathrm{e}^{-\eta(t-t')}}{\sqrt{4\pi D(t-t')}} \exp\left[-\frac{(x_j - x_k)^2}{4D(t-t')}\right], \tag{39}$$

which, after a change of variables, reads

$$\sigma(x_j, x_k; t) = \frac{x_j - x_k}{4D\sqrt{\pi}} \int_{u_1}^{\infty} \frac{\mathrm{d}u}{u^{3/2}} \exp\left(-u - \frac{a_1}{u}\right), \tag{40}$$

where

$$a_1 = \frac{\eta(x_j - x_k)^2}{4D} = \left\{\frac{\gamma(x_j - x_k)}{2}\right\}^2, \quad u_1 = \frac{(x_j - x_k)^2}{4Dt}, \tag{41}$$

and we have defined a coupling length

$$\gamma = \sqrt{\frac{\eta}{D}}. \tag{42}$$

In fast diffusion case is equivalent to take the $t \to \infty$ limit for the interaction kernel, for which $u_1 \to 0$. Taking this limit we have

$$\sigma(x_j, x_k) = \lim_{t\to\infty} \sigma(x_j, x_k; t) = \frac{\gamma}{2\eta} \exp\{-\gamma(x_j - x_k)\}, \tag{43}$$

which coincides with the earlier results of Kuramoto and coworkers [17, 19], in their analysis of the fast-relaxation case.

For the two-dimensional case ($d = 2$) in free space, we use the Green function (11), and the interaction kernel becomes

$$\sigma(\mathbf{r}_j, \mathbf{r}_k; t) = \frac{1}{4\pi D} \int_{u_1}^{\infty} \frac{\mathrm{d}u}{u} \exp\left(-u - \frac{a_2}{u}\right), \tag{44}$$

where

$$a_2 = \frac{\eta[(x_j - x_k)^2 + (y_j - y_k)^2]}{4D} = \left|\frac{\gamma(\mathbf{r}_j - \mathbf{r}_k)}{2}\right|^2, \quad u_1 = \frac{|\mathbf{r}_j - \mathbf{r}_k|^2}{4Dt}, \tag{45}$$

which, in the $t \to \infty$ limit, reduces to the result already found by Nakao [19]:

$$\sigma(\mathbf{r}_j, \mathbf{r}_k) = \lim_{t\to\infty} \sigma(\mathbf{r}_j, \mathbf{r}_k; t) = \frac{1}{2\pi D} K_0(\gamma|\mathbf{r} - \mathbf{r}_k|), \tag{46}$$

where K_0 is the modified Bessel function of the second kind and zeroth order.

Finally, for the three-dimensional free-space case ($d = 3$) we use the Green function (11) to obtain the corresponding the interaction kernel

$$\sigma(\mathbf{r}_j, \mathbf{r}_k; t) = -\frac{1}{4D\pi^{3/2}} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} \times \int_{u_1}^{\infty} \frac{\mathrm{d}u}{\sqrt{u}} \exp\left(-u - \frac{a_3}{u}\right), \tag{47}$$

where

$$a_3 = \frac{\eta}{4D}|\mathbf{r}_j - \mathbf{r}_k|^2, \qquad u_1 = \frac{|\mathbf{r}_j - \mathbf{r}_k|^2}{4Dt}, \tag{48}$$

which, in the limit $t \to \infty$, becomes

$$\sigma(\mathbf{r}_j, \mathbf{r}_k) = \lim_{t\to\infty} \sigma(\mathbf{r}_j, \mathbf{r}_k; t) = \frac{1}{4D\pi} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} \exp\left(-\gamma|\mathbf{r}_j - \mathbf{r}_k|\right), \tag{49}$$

in accordance with the result previously found by Nakao [19].

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