

Lagrangian field theory of reaction-diffusion

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It is commonly accepted that reaction-diffusion equations cannot be obtained by a Lagrangian field theory. Guided by the well known connection between quantum and diffusion equations, we implement here a Lagrangian approach valid for totally general nonlinear reacting-diffusing systems which allows the definition of global conserved observables derived using Nöther's theorem.

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I. INTRODUCTION

The quantitative understanding of growth and form in nature, and in particular in complex living beings, interested scientists dating back to classical Darcy Thompson's monograph [1]. Animal growth (morphogenesis) presents a variety of coat patterns which seem to have typical regularities. Some chemical or hydrodynamical systems too can present complex structured dynamical or stationary regimes [2]. Similar highly regular geometrical patterns appear in different natural contexts, repeated at different spatial scales, suggesting a multiscale behavior. A typical example of this phenomenology is the spherical form, which appears both on a neutron star but also, at much smaller scale, on a water bubble. In the realm of regular patterns, however, the most impressive and mysterious form is the spiral. In space in fact there are many spiral galaxies but also on our planet's surface spirals occur as gaseous eddies. At much smaller scale some biological populations of fungi and amoebae (as the *Dictyostelium Discoideum*) organize themselves in spiraling structures. In the whole heart or in cardiac cell cultures, spiral waves of electrical activity are experimentally observed on the tissue's surface. The motion of the spiral tip or filament (which is the singular organizing center [3] of the spiral/scroll wave regime) seems to be associated with life-threatening arrhythmias. A similar phenomenology is encountered also in the brain and is associated with epilepsy but also retina can support spiral wave patterns [4]. Spiral waves appear spontaneously in growing crystals [5] and in specific chemical reactions such as the classical Zhabotinsky-Belousov one [3]. Finally, in plant morphogenesis such a peculiar pattern can occur in a developmental process which is known as *kinetic phyllotaxis* [6]. From the phenomenology reported, the importance of a quantitative understanding of this complex stringlike [3,7] dynamics is clear. All these nonlinear dynamical systems can be mathematically described successfully by systems of reaction-diffusion (RD) equations [3]. Turing, more than 50 years ago, studied the way in which animals develop formulating an elegant theory for animal coats using RD equations [8]. At the same time Hodgkin and Huxley proposed their model for the electrical activity of nerves whose equations are of reaction-diffusion class. Their article [9] presented the first mathematical model based on experiments quantitatively describing a complex biological system. In the same period

Belousov and later Zhabotinsky posed the experimental basis for the theory of nonlinear chemical oscillators [3]. Some years later, Krinsky proposed a similitude between the spread of excitation in an inhomogeneous chemical medium and the biological cardiac fibrillation [10]. This important conjecture opened the way to modern biophysics of excitable media [11] and computational cardiology [12]. The relevance of reaction-diffusion theory for explaining all these phenomenologies was finally summarized by Prigogine with his pioneering theory on self-organizing complex systems [13]. It is worthwhile to conclude this discussion on the importance of RD systems stressing that even the Navier-Stokes equations of viscous hydrodynamics have the mathematical structure of a system of semilinear reaction-diffusion equations [14]. Reaction-diffusion theory, so manifestly important for many different areas of science, is still lacking, however, of a Lagrangian formulation based on the least action principle and Nöther's theorem [15]. It is remarkable the point of view of Feynman in his *Feynman Lectures on Gravitation* [16] on the importance of least action principle in nature. He stated that: "There is apparently no successful theory which is not derivable from a variational principle which starts from a Lagrangian." In this context, Winfree left in his paper entitled "A prime number of prime questions about vortex dynamics in nonlinear media" a question to be addressed: "Is there any relation to the more recent apparition of linked and knotted vortex rings in Lagrangian field theory?" [17] (recently it has been theoretically proposed an analogy between the motion of the RD vortex lines and those of cosmic strings in a curved universe [18]). In this paper we shall present a general Lagrangian theory for reaction-diffusion. To this aim we shall mix classical and quantum elements of Lagrangian field theory in order to define possible counterparts of quantum conserved quantities for reacting-diffusing systems. More in detail, our analysis is organized as follows. In Sec. II we start studying the nonlinear Schrödinger equation, which at imaginary time (i.e., Wick's rotated) can be shown to describe a reaction-diffusion process. In Sec. III we apply the Lagrangian field theory reviewed in Appendix B on quantum problems while in Sec. IV we frame the RD theory in the least action principle context. For the most interesting two reacting-diffusing variables case (the prototype of any more general RD systems) the total energy, momentum, and angular momentum are derived theoretically via Nöther's theorem in general and confirmed numerically in the specific case of FitzHugh-Nagumo (FHN) [3] theory. We conclude showing

that also Burger's equation of one-dimensional (1D) hydrodynamics, as well as diffusion processes with an advection term, can be obtained by a Lagrangian formulation. Finally, in Sec. V physical implications and future perspectives of our formulation are presented.

II. QUANTUM SYSTEMS AND REACTION-DIFFUSION EQUATIONS

In this section we start our analysis presenting a short review of nonlinear quantum mechanics, establishing then a connection of the imaginary time problem with reaction-diffusion equations.

A. Nonlinear Schrödinger equation

Nonlinear Schrödinger equations (NLSE) appear in many contexts of physics ranging from nonlinear optics to superfluidity and superconductors. While quantum mechanics of many bodies is a complicated theory on phase space, in many physical situations, such as a gas of bosons in the same quantum state as an example, one can use, in a first approximation, a unique self-interacting wave function of physical space (*a mean-field approximation*) [19,20]. In general the nonlinear terms may have complicated functional forms, although usually one considers what is known as "normal form," i.e., a typical polynomial behavior close to a critical point associated with a bifurcation [21]. In this section we shall review specifically equation

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m} (-i\hbar \nabla)^2 \psi + (V + iW)\psi + g|\psi|^2 \psi \quad (1)$$

(∇ is standard gradient operator) which manifests a global U(1) phase invariance. Introducing the real and imaginary parts $\psi = A + iB$, Eq. (1) splits into

$$\begin{aligned} \frac{\partial B}{\partial t} &= + \frac{\hbar}{2m} \nabla^2 A - \frac{1}{\hbar} [VA - WB + gA(A^2 + B^2)], \\ \frac{\partial A}{\partial t} &= - \frac{\hbar}{2m} \nabla^2 B + \frac{1}{\hbar} [VB + WA + gB(A^2 + B^2)], \end{aligned} \quad (2)$$

which is a system of two coupled nonlinear partial differential equations (PDEs). When $g=0$ one obtains standard quantum mechanics with a real potential $V=V(t, \vec{x})$ while the complex one $W=W(t, \vec{x})$ is introduced to take into account the possible creation and destruction of particles in scattering absorption processes of nuclear, atomic, and molecular physics [22]. In this case in particular the Hamiltonian of the problem is non-Hermitian and violates the probability conservation. On the other hand, if $W=0$ but $g \neq 0$ one obtains the Gross-Pitaevskii (GP) equation for the order parameter of a Bose-Einstein condensate (BEC) [23]. More in detail one has $g=(4\pi\hbar^2 a/m)$ where a is the two-body correlation length, m is the single atom mass in the condensate, and for a potential one can choose $V=\frac{1}{2}m\Omega^2|\vec{r}|^2$ with Ω being the angular frequency of the atomic trap [24]. We point out that in general the quantity g could be a function of space and time. In linear Hermitian quantum context, the interpretation

of ψ as a probability density requires $\int |\psi|^2 d^3x = 1$ while in the GP nonlinear case we have $\int |\psi|^2 d^3x = N$, with N being the fixed mean number of boson gas particles [25]. These considerations can still be generalized for $W \neq 0$. An example is represented by the dynamics of bright and dark solitons in BECs with the time-dependent interatomic interaction in an expulsive parabolic and complex potential [26]. If one chooses $W=0$ and $V=\sigma$ (σ being constant) and replaces $-i\hbar \nabla \rightarrow -i\hbar \nabla - e/c\vec{A}$ (where \vec{A} is the vector potential, c is the speed of light, and e is the electric charge), requiring stationarity (time-dependent cases are more delicate to be handled [27]) one gets the standard Ginzburg-Landau theory for superconductivity (again ψ is the complex order parameter) [20,28]. Finally when V, W and g are all complex numbers one obtains the more general complex Ginzburg-Landau theory [29]. We conclude this review stressing that linear and nonlinear Schrödinger equations share a common important feature: they have variational formulations based on Lagrangians or energy functionals [30–32]. It is useful to notice now the well known strict relation between diffusion equation and linear Schrödinger equations when the time parameter is allowed to be imaginary [33] as done in diffusion quantum Monte Carlo methods as an example [34]. The connection with a diffusion equation can be easily obtained by Wick-rotating Schrödinger equation, i.e., replacing $t \rightarrow -i\tau$. A time-dependent analytic example illustrates this useful transformation. Starting in fact from the simplest linear free case of Eq. (1), i.e.,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m} (-i\hbar \nabla)^2 \psi, \quad (3)$$

on the one-dimensional domain $x \in [0, L]$ a possible analytic solution is [35]

$$\psi(t, x) = a \sqrt{\frac{2}{L}} \sum_{n=1}^{+\infty} [\sin(k_n x) e^{-i\omega_n t} e^{-(k_n - K)^2 / 2\sigma^2}], \quad (4)$$

with $k_n = \pi n / L$ and $\omega_n = (\frac{\hbar \pi n}{2mL}) k_n$. Here σ and K are usual constant parameters of Gaussian wave packets while a is computed by normalization condition. Simple manipulations show that the Wick-rotated equation (now a diffusion equation)

$$\hbar \frac{\partial \psi}{\partial \tau} = \frac{\hbar^2}{2m} \nabla^2 \psi \quad (5)$$

admits solution in one dimension [Eq. (4)] replacing t by $-i\tau$. The equation for ψ^* instead describes an antidiffusion process (negative diffusion coefficient associated with a process diffusing backward in time). Solution (4) has a wave behavior bouncing between the ends indefinitely, while its Wick-rotated version, solution of Eq. (5), dies off in time.

B. Reaction-diffusion theory

We extend now to Eq. (1) the Wick rotation procedure obtaining consequently the nonlinear equation

$$\hbar \frac{\partial \psi}{\partial \tau} = \frac{1}{2m} (\hbar \nabla)^2 \psi - (V + iW)\psi - g|\psi|^2 \psi, \quad (6)$$

which will be easily shown to be a reaction-diffusion system whose prototype is presented and discussed in Appendix A. To this aim, posing $\psi = A + iB$ in Eq. (6) and equating to zero separately the real and imaginary parts, respectively, we obtain

$$\begin{aligned} \frac{\partial A}{\partial \tau} &= \frac{\hbar}{2m} \nabla^2 A - \frac{1}{\hbar} [VA - WB + gA(A^2 + B^2)], \\ \frac{\partial B}{\partial \tau} &= \frac{\hbar}{2m} \nabla^2 B - \frac{1}{\hbar} [VB + WA + gB(A^2 + B^2)], \end{aligned} \quad (7)$$

which clearly is a RD system of PDEs of form (A1). We point out that the associated diffusion coefficient $D = \frac{\hbar}{2m}$ is the same for both morphogenes, so Turing instability cannot occur. In general the potentials V and W depend on space and time so that solutions of Eqs. (1) and (A1) can be obtained numerically only, due to the heterogeneities and nonlinearities, although for selected cases (typically one dimensional) one can adopt generation techniques of mathematical physics for nonlinear PDEs in search of exact solutions [36]. We now explore possible Lagrangian links between quantum mechanics and reaction-diffusion theory. To this aim we have given in Appendix B a short review of classical Lagrangian field theory stressing in particular the ‘‘caveats’’ underlying the demonstrations. We apply in the next section these techniques to usual linear and nonlinear quantum mechanics in order to perform then a direct parallel with diffusive problems.

III. LAGRANGIAN QUANTUM MECHANICS

We start from the real Lagrangian density [30,31]

$$\mathcal{L} = -\frac{\hbar^2}{2m} (\nabla \psi^*) (\nabla \psi) - \frac{\hbar}{2i} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) - \psi^* V \psi \quad (8)$$

connected to the action by $L = \int dt \int \mathcal{L} d^3x$. This quantity, once inserted in Euler-Lagrange (EL) equations (B5), assuming $\phi_A = (\psi, \psi^*)$ as an $O(2)$ symmetric set of quantities to be varied independently [15], leads to Schrödinger equation (1) with $W = g = 0$ and to its complex conjugate. We stress here that this operation commonly presented in every quantum textbook is justified only by the fact that the Lagrangian density, only apparently complex, is real instead as simple manipulations performed replacing $\psi = A + iB$ can easily show. While the canonical momenta are $\pi = \partial \mathcal{L} / \partial \dot{\psi} \equiv +i\hbar/2 \psi^*$ and $\pi^* = \partial \mathcal{L} / \partial \dot{\psi}^* \equiv -i\hbar/2 \psi$ (dot here and in the following stands for derivative with respect to time coordinate t), the canonical energy-momentum tensor given by Eq. (B23) is

$$T_{\nu}^{\mu} = \frac{\partial \mathcal{L}}{\partial(\partial \psi / \partial x^{\mu})} \frac{\partial \psi}{\partial x^{\nu}} + \frac{\partial \mathcal{L}}{\partial(\partial \psi^* / \partial x^{\mu})} \frac{\partial \psi^*}{\partial x^{\nu}} - \mathcal{L} \delta_{\nu}^{\mu}. \quad (9)$$

These differential relations must be integrated in space to possibly obtain global conserved physical quantities. If V is

not invariant under time and/or space translations and rotations, then this leads to more general Lagrangian densities in which coordinates are explicitly present. This makes the whole Lagrangian not invariant under translations (or rotations) which requires nontrivial formulations as discussed in Ref. [37], in particular in relation with Nöther’s theorem where certain conservation laws cannot hold anymore. Coming back to Eq. (9), the component $T_0^0 = \mathcal{H} = \hbar^2 / (2m) \nabla \psi^* \nabla \psi + \psi^* V \psi$ is the Hamiltonian density (the energy density), which is independent of time derivatives making the Hamiltonian formulation of Schrödinger Lagrangian relevant in the static case only (or if the field is quantized) [38], so that we shall not adopt a Hamiltonian point of view in this paper (the diffusion problem shall present similar problems). The other components of T_{ν}^{μ} describe the momentum density, i.e., $\mathcal{P}_i \equiv -T_i^0 = \hbar / (2i) (\psi^* \nabla \psi - \psi \nabla \psi^*)$, the energy flux $\mathcal{S}^i \equiv T_i^0 = -\hbar^2 / (2m) (\dot{\psi}^* \nabla \psi + \dot{\psi} \nabla \psi^*)$, and the remaining 3×3 matrix the stress strains. The three-dimensional angular-momentum vector is finally given by Eq. (B28), i.e., $J^m \equiv L^m$ with $\vec{L} = (M_{23}, M_{31}, M_{12})$. Explicitly for the z component (similar relations hold for L_x and L_y) defining $\hat{L}_z = -i\hbar(x\partial_y - y\partial_x)$ we can write

$$L_z^{QM} = \int d^3x \frac{(\psi^* \hat{L}_z \psi - \psi \hat{L}_z \psi^*)}{2} \equiv \int d^3x \operatorname{Re}(\psi^* \hat{L}_z \psi) \quad (10)$$

(here QM stands for quantum mechanics) but the real part notation can be removed because \hat{L}_z is a quantum observable (a Hermitian operator) whose expectation value $\int d^3x (\psi^* \hat{L}_z \psi)$ is real [39]. Regarding the internal symmetries we can easily see that the Lagrangian density in exam is invariant under the global phase field transformation [a $U(1)$ symmetry] and its linearization $\psi' \rightarrow e^{i\varepsilon} \psi \simeq (1 + i\varepsilon)\psi$ and $\psi'^* \rightarrow e^{-i\varepsilon} \psi^* \simeq (1 - i\varepsilon)\psi^*$ which means in Eq. (B29) that $\lambda_{11} = -\lambda_{22} = 1$ while the off-diagonal terms of λ_{AB} vanish. Inserting these relations in Eq. (B31) one easily obtains the integrated probability conservation condition, i.e.,

$$\begin{aligned} \frac{d}{dt} \int d^3x \psi \psi^* &= \frac{i\hbar}{2m} \int_{\mathcal{B}} d^3x \partial_i (\psi^* \partial^i \psi - \psi \partial^i \psi^*) \\ &\equiv \int_{\partial \mathcal{B}} dS_i (\psi^* \partial^i \psi - \psi \partial^i \psi^*). \end{aligned} \quad (11)$$

If the argument in the surface term vanishes on the boundary then the Nöther’s charge $Q = \int d^3x \psi \psi^*$ remains constant in time. Similar arguments on boundary terms on the conservation laws can be applied to the previously defined global quantities in order to ensure their conservation. We can now move to the nonlinear quantum problem: adding to Lagrangian density (8) the interaction term

$$\Delta \mathcal{L} = -i\psi^* W \psi - 1/2g\psi^2(\psi^*)^2 \quad (12)$$

and inserting again in EL equations (B5) one gets exactly Eq. (1). The energy density becomes $T_0^0 = \hbar^2 / (2m) \nabla \psi^* \nabla \psi + \psi^* (V + iW)\psi + 1/2g\psi^2(\psi^*)^2$ while the momentum density

and energy fluxes are unchanged but the stress-strain terms on the other hand do not.

IV. LAGRANGIAN REACTION-DIFFUSION THEORY

It would appear natural now to Wick rotate Eq. (8) obtaining, after addition of the nonlinear term in Eq. (12),

$$\mathcal{L}_W = -\frac{\hbar^2}{2m}(\nabla\psi^*)(\nabla\psi) - \frac{\hbar}{2}\left(\psi^*\frac{\partial\psi}{\partial\tau} - \psi\frac{\partial\psi^*}{\partial\tau}\right) - \psi^*V\psi + \Delta\mathcal{L}. \quad (13)$$

Inserting this relation into Eq. (B5) with t renamed by τ , we immediately obtain a diffusion-type equation (5) once we set $V=0$ and $\Delta\mathcal{L}=0$ together with an antidiffusion one for ψ^* . Unfortunately, such a result appears to be purely accidental. Our variables ψ and ψ^* are complex and substitution $\psi=A+iB$ and $\psi^*=A-iB$ leads to a complex Lagrangian whose space derivatives belong to its real part while the temporal ones to the imaginary [we can stress that the quantum Lagrangian given by Eq. (8) on the other hand is real in terms of A and B functions]. Complex actions are very common in quantum mechanics and especially in quantum field theory where they play a central role in pair creation rates [40], but their presence can pose serious problems of consistency from the point of view of classical field theory. In fact, as pointed out by Weinberg in his Foundations of Quantum Field Theory monograph [41], a complex action for N field variables, once inserted into EL equations, gives a set of $2N$ relations because the real and imaginary parts of EL equations must be equated to zero independently. This overdetermination of the problem in general justifies the use of real Lagrangians only, although in some very specific cases the $2N$ relations could be dependent reducing the problem to N relations. In our case using a little bit of algebra it is clear that the four field equations obtained, in order to be compatible, require $\partial_\tau A=0$ and $\partial_\tau B=0$ (staticity). Similar results can be obtained including nonlinear terms considering Eq. (6). We can conclude then that our relation of NLSE with RD systems is only a fortuitous mathematical correspondence to eventually draw analogies between quantum and chemical systems. Probably this result is intimately related to the fact that in quantum mechanics one has a real Lagrangian and, moreover, that it is usually stated (as we did) that the fields ψ and ψ^* must be treated as independent, which is not completely true because the dynamics of ψ^* is simply obtained computing ψ and operating complex conjugation. On the other hand, the real and imaginary parts of ψ give two independent degrees of freedom which together with the real Lagrangian density make the quantum problem well determined. In any case the Wick's rotated Lagrangian in Eq. (13) is still giving us a strong useful suggestion to reach our final goal of a Lagrangian theory of reaction-diffusion because of its specific mathematical form. It is commonly encountered in the literature in fact the statement that "linear heat diffusion does not admit a Lagrangian density" (see as an example Ref. [42]). While this point of view is correct if one allows a Lagrangian density depending on the diffusing field only, on the other hand, by introducing an auxiliary field and

defining then a Lagrangian similar to Eq. (13), Morse and Feshbach (MF) in their classical monograph on Mathematical Methods for Physics [43] (see also Ref. [44]) obtained a Lagrangian variational version for the linear (only) diffusive problem. Shortly, in that context their variables were two independent *real* fields ψ_1 and ψ_2 [while after Wick's rotation our fields in Eq. (13) remained complex]. Comparing with our Wick-rotated Lagrangian in Eq. (13) one should simply replace $\psi\rightarrow\psi_1$ and $\psi^*\rightarrow\psi_2$ together with $\hbar\rightarrow 1$ and $1/(2m)\rightarrow D$ (D is the diffusion coefficient) in order to obtain the linear diffusion equation following the MF formulation (the original MF notation of a star to denote a real field and not complex conjugation was very unfortunate). After substitution in EL equations (B5), ψ_1 shall satisfy a diffusion equation and the other real field ψ_2 an antidiffusion one, as explicitly shown in detail later in our discussion. MF computed also the physical observables associated with the energy momentum tensor. The energy density results into $\mathcal{H}=D\nabla\psi_1\nabla\psi_2$ and similarly the energy flux vector $\mathcal{S}^i=-(\psi_1\nabla\psi_2+\psi_2\nabla\psi_1)$ together with the momentum density vector $\mathcal{P}_i=1/2(\psi_2\nabla\psi_1-\psi_1\nabla\psi_2)$ (but not the angular momentum) were easily computed. The great problem pointed out by MF was the physical interpretation of the variable ψ_2 which "diffuses backward in time" leading to the apparently "cryptic" statement that one has here a process in which the field ψ_1 loses energy which is gained by the field ψ_2 . Moreover, MF analysis lacked of an important remark: due to the fact that the field ψ_2 has no physical content (it is an auxiliary field not referring to any physical experiment), it should disappear from any measurable quantity. It is clear that in order to proceed toward the definition of physical observables for RD systems we must solve this problem of physical consistency and this task is accomplished in fact in the next pages. We point out, moreover, that unfortunately backward diffusion (or heat) equation leads to an "ill-posed" mathematical problem [45,46] as discussed in detail in Appendix C. On the other hand, the fact that a problem is ill posed is not so dramatic as it could appear at a first glance. Ill-posed diffusion equations arise in a variety of applications including computer vision, population dynamics, and granular flow physics as examples [47]. Diffusive processes which do not respect Fick's law are encountered in biology in chemotaxis, i.e., a process in which diffusion is directed up to points of high concentration (an anti-Fickian behavior in fact). While diffusion is a sort of stabilizing process, chemotaxis is generally destabilizing acting as a negative diffusion [2]. In the retrograde heat problem analyzed in detail in Eq. (C1) of Appendix C, one of the three Hadamard requirements (existence, uniqueness, and stability) required to have a well posed problem is not satisfied: even the constant solution is unstable in fact. Stability here means that, because boundary data are obtained through measurements (so have certain error margins), a small measurement error must not change the solution drastically [48]. If the antidiffusing field, however, does not interact with the physical world (it is an auxiliary variable), there is no reason why one should care about possible measurements error which make the instability growth. So we shall assume that the constant antidiffusing solution is acceptable and shall derive then observable quantities which

will be independent from any antidiffusing fields. To this aim we notice that our nonlinear Wick-rotated Lagrangian in Eq. (13) suggests us the necessity to generalize MF procedure to nonlinear systems of many variables leading naturally to the Lagrangian theory of reaction-diffusion and obtaining the counterparts of the observable quantities previously derived in the quantum case.

A. Linear diffusion problem

Following MF, let us start with Lagrangian density for the two real valued fields ψ_1 and ψ_2 ,

$$\mathcal{L}_{MF} = -D(\nabla\psi_2)(\nabla\psi_1) - \frac{1}{2}\left(\psi_2\frac{\partial\psi_1}{\partial t} - \psi_1\frac{\partial\psi_2}{\partial t}\right) + G(\psi_1, \psi_2). \quad (14)$$

Removing for the sake of simplicity the interaction term $G(\psi_1, \psi_2)$ in Eq. (14) first (which gives the original MF Lagrangian), arranging the variables into a real vector $\phi_A = (\psi_1, \psi_1)$, and inserting into EL equations (B5) we obtain as anticipated the field equations

$$\frac{\partial\psi_1}{\partial t} = D\nabla^2\psi_1, \quad \frac{\partial\psi_2}{\partial t} = -D\nabla^2\psi_2. \quad (15)$$

The canonical momenta are given by $\pi_1 = \partial\mathcal{L}/\partial\dot{\psi}_1 \equiv -1/2\psi_2$ and $\pi_2 = \partial\mathcal{L}/\partial\dot{\psi}_2 \equiv +1/2\psi_1$, similarly to the quantum case previously analyzed (which suggests to us in advance that a time-dependent Hamiltonian formulation of the problem shall not be possible). As anticipated, in order to avoid a physical interpretation of these additional fields diffusing backward in time (and leading to the ill-posed problem previously discussed), we recall that a fundamental requirement must be that the presence of the auxiliary field ψ_2 must not appear in any observable quantity. If we assume that the auxiliary field ψ_2 is a constant C at $t=0$ in entire space domain, imposing constant Dirichlet boundary conditions $\psi_2=C$ for the antidiffusion equation, quantity ψ_2 shall remain constant at any time then: we have found a trivial constant solution of the *ill-posed* retrograde heat problem. In this way we are dealing with the diffusion equation for ψ_1 only. A simple inspection shows that such a constant solution for ψ_2 leads to a vanishing action integral for the stationary problem. One may question on this apparently inconsistent result which does not hold to any problem however. In quantum field theory in fact (and in particular in instanton physics), vacuum is defined as a configuration with vanishing action and typically results in a constant field [15,20,49]. On the other hand, the simple wave equation

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0 \quad (16)$$

derived from the action integral

$$S = \frac{1}{2} \int dt \int dx \left[\left(\frac{\partial u}{\partial t} \right)^2 - \left(\frac{\partial u}{\partial x} \right)^2 \right] \quad (17)$$

following the variational procedure described in Appendix B has plane-wave solutions $u = u_0 \exp(ikx + i\omega t)$ which satisfy

D'Alembert equation if $\omega = k$ and at the same time cause the action to vanish identically. Similar results hold for any solutions of the form $u = f(x+t)$ or $u = g(x-t)$. The fact that the action integral S is zero for such a solution of EL equations is not a pathologic behavior which could invalidate the variational procedure (see as an example the discussion on the value of the action in Ref. [50] on p. 71). We still have to fix the problem of possible observable effects of the constant field ψ_2 on the physical quantities obtained from T_ν^μ and the angular-momentum tensor. The solution here is simple again: the Lagrangian density can be defined up to a constant multiplicative factor K , i.e., $\mathcal{L} \rightarrow \tilde{\mathcal{L}} \equiv K\mathcal{L}$. While the field equations get unchanged in this case, energy momentum tensor T_ν^μ and angular-momentum tensor $\Lambda_{\mu\nu\lambda}$ (see Appendix B) acquire a multiplicative factor K which can be wisely chosen to eliminate the constant quantity ψ_2 from the observables. We shall develop explicitly such a procedure in a more general case of two reacting and diffusing fields in the next sections pointing out that the procedure easily generalizes to more than two species. We can now proceed beyond Morse and Feshbach analysis of the linear diffusion problem considering now the nonlinear term in our Lagrangian density in Eq. (14).

B. Nonlinear diffusion problem

Adopting the *ansatz* $G(\psi_1, \psi_2) = F(\psi_1)(\psi_2 - C)$ in Eq. (14), where C is an arbitrary constant, we obtain from EL equations (B5):

$$\begin{aligned} \frac{\partial\psi_1}{\partial t} &= D\nabla^2\psi_1 + F(\psi_1), \\ \frac{\partial\psi_2}{\partial t} &= -D\nabla^2\psi_2 + \frac{\partial F(\psi_1)}{\partial\psi_1}(C - \psi_2). \end{aligned} \quad (18)$$

Again the choices $\psi_2 \equiv C$ on the entire domain at $t=0$ and Dirichlet boundary condition for ψ_2 everywhere equal to C produce a constant solution $\psi_2 = C$ valid for any time for the antidiffusion equation. As an example, selecting $F = \kappa\psi_1(\psi_1 - a_1)(a_2 - \psi_1)$ where κ , a_1 , and a_2 are constant parameters we obtain the bistable equation [51].

C. Nonlinear two variables reaction-diffusion problem

We pass now to study the case of two diffusing species. Denoting with an odd suffix the physical real field and with an even one the auxiliary ones, we define the following Lagrangian density:

$$\begin{aligned} \mathcal{L} &= -D_1(\nabla\psi_2)(\nabla\psi_1) - D_2(\nabla\psi_4)(\nabla\psi_3) - \frac{1}{2}\left(\psi_2\frac{\partial\psi_1}{\partial t} - \psi_1\frac{\partial\psi_2}{\partial t}\right) \\ &+ S(\psi_1, \psi_3)(\psi_2 - C_1) - \frac{1}{2}\left(\psi_4\frac{\partial\psi_3}{\partial t} - \psi_3\frac{\partial\psi_4}{\partial t}\right) + H(\psi_1, \psi_3) \\ &\times (\psi_4 - C_2). \end{aligned} \quad (19)$$

This quantity, once inserted into EL equations (B5) and defining the real vector $\phi_A = (\psi_1, \psi_2, \psi_3, \psi_4)$, gives

$$\begin{aligned}\frac{\partial \psi_2}{\partial t} &= -D_1 \nabla^2 \psi_2 + \frac{\partial S}{\partial \psi_1} (C_1 - \psi_2) + \frac{\partial H}{\partial \psi_1} (C_2 - \psi_4), \\ \frac{\partial \psi_4}{\partial t} &= -D_2 \nabla^2 \psi_4 + \frac{\partial S}{\partial \psi_3} (C_1 - \psi_2) + \frac{\partial H}{\partial \psi_3} (C_2 - \psi_4), \\ \frac{\partial \psi_1}{\partial t} &= D_1 \nabla^2 \psi_1 + S(\psi_1, \psi_3), \\ \frac{\partial \psi_3}{\partial t} &= D_2 \nabla^2 \psi_3 + H(\psi_1, \psi_3),\end{aligned}\quad (20)$$

where the first two equations are antidiffusion ones, while the remaining ones are the prototype of RD equations of form (A1). As an example, one can apply this machinery to the FHN theory [51] which is a generalization of the bistable equation just discussed given by

$$\begin{aligned}S(\psi_1, \psi_3) &= \kappa \psi_1 (\psi_1 - a_1) (a_2 - \psi_1) - \psi_3, \\ H(\psi_1, \psi_3) &= \eta \psi_1 + \delta \psi_3 + \zeta,\end{aligned}\quad (21)$$

where η , δ , and ζ are real constants. Moreover, one can easily set the diffusion coefficient of one of the two species equal to zero, obtaining also a local dynamics typical of electrophysiological models. We point out that for two RD species, a well known definition of the phase is given by [52] $\tan \Theta(t, \vec{x}) = \psi_3(t, \vec{x}) / \psi_1(t, \vec{x})$ where the singular points are those where ψ_1 and ψ_3 vanish. One can define the index of a curve as the integral $2\pi I = \oint \nabla \Theta \cdot d\vec{l}$: if the curve does not enclose any singular points, then I is zero. Introducing the variable change $\psi_1 = R \cos(\Theta)$ and $\psi_3 = R \sin(\Theta)$ (and similarly for the auxiliary fields) into Lagrangian density (20) one may reformulate the Lagrangian problem in terms of the variables modulus and phase. We leave this analysis to future works [53], however, coming back to our problem (20). As discussed before, we require a constant solution $\psi_2 = \psi_4 = C_1 \equiv C_2$ (on the domain and on the boundaries) and multiply the whole Lagrangian density (19) by a common factor $K = 2/C_1$ leaving the field equations unaltered and eliminating the presence of the auxiliary fields from the observables given by Nöther's theorem.

D. Observables

In this section we shall explicitly derive the Lagrangian observables for the two variable RD system prototype given by Eq. (20), although the one variable case only can be easily obtained setting $\psi_3 \equiv 0$ (we recall that we shall assume constant in space and time solutions ψ_2 and ψ_4). Using the rescaled Lagrangian $\tilde{\mathcal{L}}$ previously discussed, from the energy-momentum density tensor in Eqs. (B22) and (B24) we get

$$\begin{aligned}T_0^0 &= K(D_1 \nabla \psi_1 \nabla \psi_2 + D_2 \nabla \psi_3 \nabla \psi_4) \\ &\quad - K[S(\psi_2 - C_1) + H(\psi_4 - C_2)],\end{aligned}\quad (22)$$

which in our case is identically zero so that, following standard interpretation of the components of the T_ν^μ tensor, one

has a zero total energy $P_0 = E = \int d^3x \mathcal{H} \equiv \int d^3x T_0^0 = 0$. More drastically than in the quantum case, here a Hamiltonian formulation of the problem does not exist at all. Vanishing Hamiltonian densities \mathcal{H} naturally arise in the context of Hamiltonian classical and quantum gravity [54] so that we can analogously say that diffusing systems have zero energy. A simple check shows that the energy flux vector too

$$S^i = -KD_1(\dot{\psi}_1 \nabla \psi_2 + \dot{\psi}_2 \nabla \psi_1) - KD_2(\dot{\psi}_3 \nabla \psi_4 + \dot{\psi}_4 \nabla \psi_3)\quad (23)$$

vanishes which is consistent with the vanishing of the energy density previously demonstrated. This result seems to contrast with standard literature on heat equation however. As anticipated, in thermodynamics it is well known that the heat equation for the temperature T can be derived from balance laws [55] obtaining in the one-dimensional case $\rho c T_t = k \partial_x^2 T$, where in the simplest scenario c is the constant specific heat per unit mass, ρ is the constant material density, and k is the constant thermal conductivity. The internal energy density \tilde{e} in solids is well known to be proportional to the temperature, i.e., $\tilde{e} = \rho c T$ in absence of work done. In dimensionless form the heat equation becomes $u_t = u_{xx}$ which integrated in space, exchanging space integral and time derivative leads to

$$\frac{\partial}{\partial t} \int_{x_1}^{x_2} u dx = \int_{x_1}^{x_2} u_{xx} dx = u_x \Big|_{x_1}^{x_2},\quad (24)$$

which gives a conservation law if the fluxes get balanced on the boundaries. A comparison with the relation for the internal energy density \tilde{e} shows that relation (24) should give a sort of conservation law for the energy. Heat equation, derived using a phenomenological law (Fick's law), seems to lead to a discrepancy with the Lagrangian result (i.e., identically zero energy density). Such a discrepancy is only apparent, however, because we can show immediately that relation (24) does not come from time translational invariance but from an internal symmetry for the linear problem only instead. Let us work with one diffusing species in one dimension only for the sake of brevity (the same arguments directly extend to more diffusing species in higher dimensions). The finite transformations $\psi_1 \rightarrow \exp(i\varepsilon)\psi_1$ and $\psi_2 \rightarrow \exp(-i\varepsilon)\psi_2$ leave unaltered Lagrangian density (14) *only* in absence of self-interacting term $G(\psi_1, \psi_2)$. After linearization close to the identity we get the infinitesimal transformations $\psi_1 \simeq (1+i\varepsilon)\psi_1$ and $\psi_2 \simeq (1-i\varepsilon)\psi_2$ (ε is a constant) and using formulas (B31) we can easily see that $\lambda_{11} = 1$ and $\lambda_{22} = -1$ so that (assuming usual ψ_2 constant solution)

$$-\psi_2 \frac{\partial}{\partial t} \int dx \psi_1 = -D_1 \psi_2 \int_{x_1}^{x_2} dx \frac{\partial(\partial_x \psi_1)}{\partial x} = -D_1 \psi_2 \partial_x \psi_1 \Big|_{x_1}^{x_2},\quad (25)$$

which will be zero, leading to a conserved quantity $\tilde{Q} = \int dx \psi_1$ if the gradient $\partial_x \psi_1$ is the same on the boundaries. Algebraic simplifications together with $D_1 = 1$ give exactly Eq. (24). The addition of the nonlinear terms as anticipated causes a loss of the symmetry of the action integral with respect to the internal transformation just discussed and no

conservation law is expected to hold anymore. Regarding the total momentum instead, we work in the simpler one-dimensional case first obtaining from Eq. (B20) with \mathcal{L} replaced by $\tilde{\mathcal{L}}$ that

$$\begin{aligned} P_x &= \int_{x_1}^{x_2} dx \mathcal{P}_x \\ &\equiv \frac{K}{2} \int_{x_1}^{x_2} dx (\psi_2 \partial_x \psi_1 - \psi_1 \partial_x \psi_2 + \psi_4 \partial_x \psi_3 - \psi_3 \partial_x \psi_4) \\ &\equiv \int_{x_1}^{x_2} dx (\partial_x \psi_1 + \partial_x \psi_3) \\ &\equiv (\psi_1 + \psi_3)|_{x_1}^{x_2}, \end{aligned} \quad (26)$$

which shows that the total momentum is surely constant in time if the functions satisfy constant in time Dirichlet boundary conditions and even vanish if the functions have appropriate values on the boundary. We have still to explore the surface term given by relation (B21) in order to see if our result is consistent. Explicitly we obtain

$$\left(\frac{\partial \tilde{\mathcal{L}}}{\partial (\partial_x \phi_A)} \partial_x \phi_A - \tilde{\mathcal{L}} \right) \Big|_{x_2}^{x_1} \equiv \frac{d}{dt} (\psi_1 + \psi_3) \Big|_{x_2}^{x_1} \quad (27)$$

and one can easily see that this surely vanishes if the fields assume constant in time values on the boundaries (their time derivatives vanish) or if the fields are on the opposite of the other on each point. This is not an unexpected result because in classical Lagrangian field theory (see Appendix B), conservation laws hold if the boundary terms vanished at infinity or on the borders. Coming back to our diffusive problem, the three-dimensional analysis leads to

$$P_i = \int d^3x \mathcal{P}_i \equiv \int d^3x (\partial_i \psi_1 + \partial_i \psi_3) \quad (28)$$

and similar argumentations presented in the 1D case still hold. In Eq. (B24) in fact, considering Lagrangian (19) multiplied by $2/C_1$, for the boundary terms one has $T_n^i \equiv 0$ if Dirichlet boundary conditions constant in time (but not necessarily in space) hold, leading to conservation laws (in two dimensions integrals must be performed with a two-dimensional measure). The only delicate point remains to wisely choose initial data in order to have initial nonvanishing total momentum then. Interestingly if we write the momentum density $\vec{\mathcal{P}} = \vec{\mathcal{P}}_1 + \vec{\mathcal{P}}_3$ with $\vec{\mathcal{P}}_1 = \nabla \psi_1$ and $\vec{\mathcal{P}}_3 = \nabla \psi_3$ we obtain a physical interpretation of the ‘‘mysterious’’ function $\Phi = \max |\nabla \psi_1 \times \nabla \psi_3|$ introduced in Ref. [56] in order to locate spiral’s singular points and filaments. Such a function in fact is peaked exactly on the spiral tip or on the scroll wave filament. Here we see that in terms of cross product of momentum density vectors for the two cross reacting species, i.e., $\max |\vec{\mathcal{P}}_1 \times \vec{\mathcal{P}}_3|$, we have that the singular region is where field momenta density cross product is maximum. Regarding the angular momentum instead from Eq. (B28), with $\tilde{\mathcal{L}}$ instead of \mathcal{L} , we obtain

$$\begin{aligned} L_z &= \frac{K}{2} \int d^3x (\psi_2 \hat{l}_z \psi_1 - \psi_1 \hat{l}_z \psi_2 + \psi_4 \hat{l}_z \psi_3 - \psi_3 \hat{l}_z \psi_4) \\ &\equiv \int d^3x [\hat{l}_z (\psi_1 + \psi_3)], \end{aligned} \quad (29)$$

with $\hat{l}_z = x \partial_y - y \partial_x$ and analogous relations can be worked out for L_x and L_y [so that we can summarize saying that for our diffusive problems the angular-momentum density for the field ψ_A can be written in the more familiar form $\vec{L}_A = \int d^3x (\vec{r} \times \nabla \psi_A)$, which is a result quite different from the quantum case]. Coming back to the L_z component, the associated boundary term in Eq. (B27) is then $-\int dS^i \Lambda_{i12}$. Inserting our Lagrangian density (19) multiplied by $2/C_1$ and performing a little algebra one can easily see that this term surely vanishes if the fields do not depend on time on the boundaries otherwise an angular-momentum variation is expected. It appears clear then that the only delicate point in this case is to find then initial data and boundary conditions with nonvanishing total angular momentum (which is a delicate point in quantum physics too [57]). Using two-dimensional Green’s theorem on a closed domain \mathcal{B} , introducing the vector $\vec{A} = (-yU, xU)$ where $U = U(x, y)$, we can write

$$\int_{\mathcal{B}} (x \partial_y U - y \partial_x U) dx dy \equiv \int_{\mathcal{B}} (\nabla \cdot \vec{A}) dx dy = \oint_{\partial \mathcal{B}} \vec{A} \cdot d\vec{l}. \quad (30)$$

We notice that the vanishing of the total angular momentum is intimately related or with the divergence free nature of the field \vec{A} , or with the behavior of the function U on the boundaries. This is not an unexpected result of classical field theory: in general relativity, as an example, the asymptotic angular momentum of a stationary black hole *in vacuo* is a boundary term too [58]. Clearly in the last step in Eq. (30) the vector field \vec{A} is supposed to be smooth enough and $\partial \mathcal{B}$ to be an oriented piecewise smooth and simple closed curve, in order not to violate Green’s theorem hypotheses. In analogy with L_z , corresponding relations for the x and y angular-momentum components can be easily derived (in two dimensions only the component L_z exists). In chemical active media and electrophysiology usually Neumann zero flux is adopted leading to time-dependent fields on the boundaries: in these cases no angular-momentum conservation laws (nor field momentum) are expected to hold although the nonconserved Lagrangian observables are still physically meaningful. Clearly the Lagrangian procedure here presented can be extended to totally general RD models with more than two variables (Hodgkin-Huxley, Beeler-Reuter, Luo-Rudy [2,51] models and others), but in absence of space-time-dependent heterogeneities in the diffusion tensors and/or in the dynamics. In these more involved cases in fact a Lagrangian formulation with explicit dependence of the Lagrangian density on space and time should be adopted [37], as already discussed in Sec. III in the quantum context. This additional problem, however, will not be investigated here.

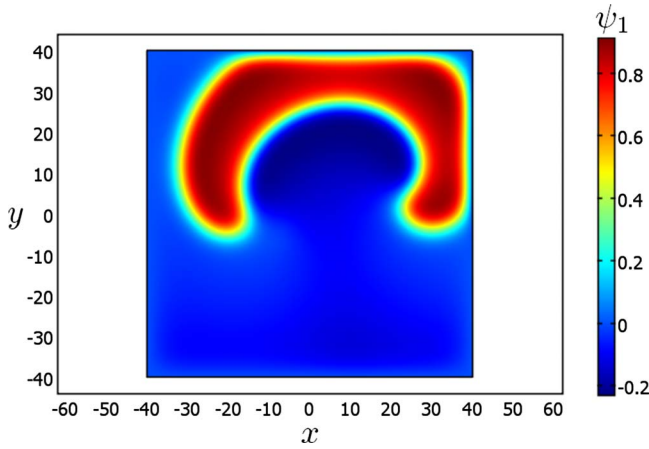


FIG. 1. (Color online) Case A: spiral waves of variable ψ_1 at $t=240$; notice the Dirichlet boundary condition behavior of the spiral to be confronted with case B simulations.

E. Numerical analysis

Our results, derived through analytical methods, have been verified also numerically using the FHN codes described in Refs. [59,60]. In Eqs. (20) and (21) (antidiffusion equations vanish identically) we have adopted the dimensionless parameter's choice: $D_1=1, D_2=0$ together with $\kappa=1, a_1=0.1, a_2=1, \eta=0.005, \delta=0.0125,$ and $\zeta=0$. We have selected then a two-dimensional squared domain centered in the origin with side length of 80 units. Regarding the initial data at $t=0$ we have chosen Gaussian-type functions, i.e.,

$$\psi_1(0, \vec{x}) = \frac{4}{5} \exp \left\{ - \left[\frac{(x-10)^2 + 0.5(y-10)^2}{100} \right] \right\},$$

$$\psi_3(0, \vec{x}) = \frac{1}{20} \exp \left\{ - \left[\frac{(x+10)^2 + 0.5(y+10)^2}{100} \right] \right\} + \frac{1}{10} \exp \left\{ - \left[\frac{(x-15)^2 + 0.5(y+5)^2}{100} \right] \right\}.$$

Two types of boundary conditions have been selected for the simulations: the case A adopts constant in time Dirichlet boundary conditions, where the value of the fields on the border at any time is exactly the value of the initial data computed on the boundaries. The case B instead adopts zero flux Neumann boundary conditions everywhere (i.e., $\hat{n} \cdot \nabla \psi_1 = 0$ and $\hat{n} \cdot \nabla \psi_3 = 0$ where \hat{n} is the unit normal to the boundaries). The numerical technique used is finite elements methods adopting COMSOL MULTIPHYSICS simulation environment (see [59,60] again for more details). The domain has been meshed in 10^4 equal squares of size $\Delta x=0.8$, while quadratic Lagrange elements have been used. A direct parallelized solver (PARDISO) has been adopted to solve the problem with absolute and relative errors thresholds of 10^{-6} . Finally, the software optimized the time steps choice for the integrations. The results of the simulations are the following. For the case A in Fig. 1 we plot the value of the variable ψ_1 at $t=240$ clearly showing spiral waves circulating on the domain. In Fig. 2 we show instead the value of the total angular momentum L_z and of the field momenta P_x and P_y (a two-

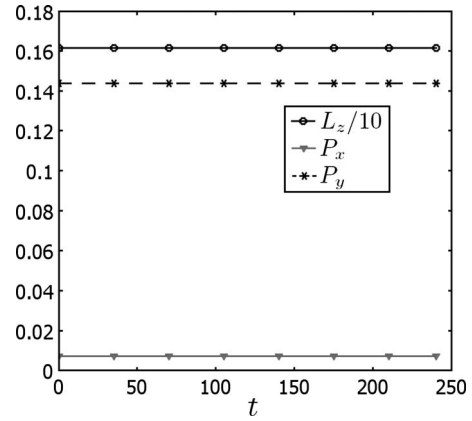


FIG. 2. Case A: total angular momentum L_z and total field momenta P_x and P_y in time; conservation laws hold for all these quantities.

dimensional integration has been performed) in time. As anticipated constant in time Dirichlet boundary conditions lead to conserved quantities. Regarding the case B instead in Fig. 3 we have again a snapshot of ψ_1 at $t=240$ while in Fig. 4 we plot $L_z, P_x,$ and P_y in time. In this case it is evident the lack of conservation laws due to the time dependence of the fields on the boundaries (we recall again that here we have Neumann zero flux conditions). Although these selected numerical studies with particular domains, boundary conditions and initial data have confirmed the conservation laws, a more detailed numerical analysis of the entire problem will be presented in future works [53].

F. Hydrodynamics and advection terms

The variational procedure here exposed can be easily extended to more general reaction-diffusion systems defining for any diffusing variable a companion auxiliary one to be manipulated as in the case just discussed. It is important to notice now that our formulation can describe also semilinear parabolic differential equations [14] typical of hydrodynam-

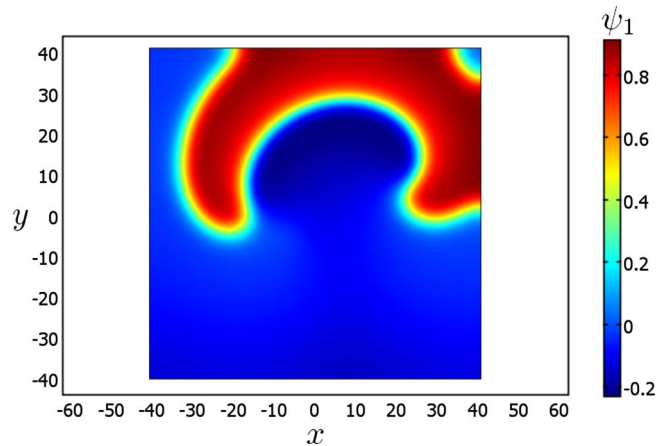


FIG. 3. (Color online) Case B: spiral waves of variable ψ_1 at $t=240$; notice the typical Neumann zero flux boundary condition behavior of the spirals.

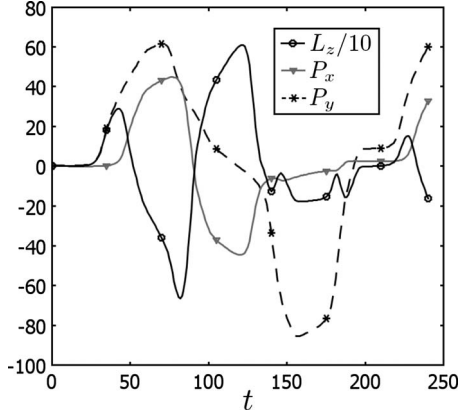


FIG. 4. Case B: total angular momentum L_z and total field momenta P_x and P_y in time; conservation laws do not hold for all these quantities.

ics and gas dynamics. We shall study here a one-dimensional case which shall give us the well known Burger's equation [61] describing the propagation of simple waves in a continuous medium with small dissipation. Starting from the hydrodynamical Lagrangian density

$$\mathcal{L}_H = -D \left(\frac{\partial \psi_2}{\partial x} \right) \left(\frac{\partial \psi_1}{\partial x} \right) - \frac{1}{2} \left(\psi_2 \frac{\partial \psi_1}{\partial t} - \psi_1 \frac{\partial \psi_2}{\partial t} \right) - \psi_1 \psi_2 \left(\frac{\partial \psi_1}{\partial x} \right), \quad (31)$$

we obtain from EL equations (B5) that

$$\begin{aligned} \frac{\partial \psi_1}{\partial t} + \psi_1 \partial_x \psi_1 &= +D \partial_x^2 \psi_1, \\ \frac{\partial \psi_2}{\partial t} + \psi_1 \partial_x \psi_2 &= -D \partial_x^2 \psi_2, \end{aligned} \quad (32)$$

which, requiring the usual constant ψ_2 solution, gives the well known Burger's equation (which is connected to diffusion equation by Hopf-Cole transformation). Although we could develop a Lagrangian theory for higher dimensional hydrodynamics and apply Nöther's theorem in search of conservation laws for Navier-Stokes equations (as well as for Burgers equation), we prefer to continue our discussion of diffusion problem only leaving such a more involved study to a future publication [53]. We point out that in case of diffusion equation with an advection term having (external) constant velocity \tilde{v} , the quantity $-\psi_1 \psi_2 \partial_x \psi_1$ in Eq. (31) should be replaced by $-\psi_2 \tilde{v} \partial_x \psi_1$ and inserted in EL equations leading to the well known advection-diffusion equation [62]. This case too, however, will be explored in detail in a future study.

V. CONCLUSIONS

In this paper we have shown that reaction-diffusion theory can be cast into the Lagrangian field theoretical framework. Our study has been inspired by the Lagrangian formulation

of nonrelativistic quantum mechanics connected with the classical work of Morse and Feshbach on linear diffusion equation. More in detail, we have successfully solved the serious conceptual problems present in the latter analysis and we have implemented then a least action principle procedure for general RD systems, finally applying Nöther's theorem to define total angular momentum, field momentum, and energy. In the discussion presented we have explicitly avoided studying the problem of the heterogeneities in the dynamics and in the diffusion tensor. Although it is well known that in natural systems inhomogeneities and anisotropies are always present (see [63] for an example in cardiac context), we have preferred to postpone this study, which requires the use of Lagrangians depending explicitly on space and eventually on time, to a future work [53]. We conclude this discussion remarking that our analysis has brought reaction-diffusion theory in the framework of fundamental theoretical models, giving perspectives toward a deeper quantitative understanding of organized structures and patterns in a variety of different complex systems of nature.

APPENDIX A: TURING'S REACTION-DIFFUSION THEORY

RD equations are mathematical models describing, in chemistry, the concentration of one or more substances which locally chemical react, being converted into each other, and spatially diffuse. In more general biological contexts they are associated with Turing's theory of animal coat patterns [2] (not necessarily of spiraling form) and with the propagation of electric signals in excitable tissues [3]. The prototype of reaction-diffusion equations with two variables only (the Turing morphogenes) and homogeneous and isotropic diffusion tensors, for the sake of simplicity, is

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_1 \nabla^2 u + f(u, v), \\ \frac{\partial v}{\partial t} &= D_2 \nabla^2 v + h(u, v), \end{aligned} \quad (A1)$$

where f and h typically (but not always) are polynomials of u and v , although in some cases an explicit dependence on time and space may be allowed (heterogeneities). A RD system shows diffusion-driven instability (Turing instability) if the homogeneous state is stable against small perturbations in absence of diffusion but gets unstable if diffusion is present. This mechanism determines the spatial pattern. The necessary conditions for instability obtained using standard perturbation techniques are [2]

$$\begin{aligned} f_u + h_v &< 0, \quad f_u h_v - f_v h_u > 0, \quad df_u + h_v > 0, \\ (df_u + h_v)^2 - 4d(f_u h_v - f_v h_u) &> 0, \end{aligned} \quad (A2)$$

with $d=D_2/D_1$. Here the notation f_u stands for $\partial f/\partial u$ and similarly for the other derivatives with all these quantities are computed at the steady state $(u, v) \equiv (u_0, v_0)$. A well known result of reaction-diffusion theory is that when $D_1=D_2$ (or equivalently $d=1$), the conditions listed above are never sat-

ified and no Turing instability (i.e., steady-state spatially heterogeneous patterns) arises. Suppressing space variations in Eq. (A1), one gets a set of ordinary differential equations whose form depends crucially by f and h . In some cases the medium is “excitable,” i.e., the system locally can make a large excursion in phase space before returning to the resting state or have a direct fast fall on the rest state: this is a natural “analogical” two-state switch of interest in neuroscience [51].

APPENDIX B: A REVIEW OF LAGRANGIAN FIELD THEORY

We present here a short review of classical field theory working explicitly in the simplest case of one space coordinate only and giving then the general formulas for the higher dimensional cases.

1. Euler-Lagrange equations

Let us start considering a scalar field ϕ and work for the sake of simplicity in one space dimension first in order to present to the reader not expert in Lagrangian field theory the necessary procedures to operate with this tool. The action integral is defined as

$$S = \int dt \int dx \mathcal{L}(\phi, \phi_x, \phi_t), \quad (\text{B1})$$

where ϕ_t stands for $\partial_t \phi$ and similarly for the spatial component (an explicit dependence of \mathcal{L} on time and space is here neglected although the extension is clearly possible [37]). Performing a variation of S at fixed boundary (the domain of definition of the fields does not change) we obtain

$$\delta S = \int dt \int dx \left(\frac{\partial \mathcal{L}}{\partial \phi} \delta \phi + \frac{\partial \mathcal{L}}{\partial \phi_x} \delta \phi_x + \frac{\partial \mathcal{L}}{\partial \phi_t} \delta \phi_t \right), \quad (\text{B2})$$

where only if the field $\delta \phi$ and its derivatives vanish sufficiently rapidly on the boundaries [15,31], we can replace $\delta \phi_t \equiv \delta(\partial_t \phi) = \partial_t(\delta \phi)$ and $\delta \phi_x \equiv \delta(\partial_x \phi) = \partial_x(\delta \phi)$. Then integrating by parts we obtain

$$\begin{aligned} \delta S = & \int dt \int dx \left(\frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial \phi_x} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \phi_t} \right) \delta \phi \\ & + \int dt \left(\frac{\partial \mathcal{L}}{\partial \phi_x} \delta \phi \Big|_{x_1}^{x_2} \right) + \int dx \left(\frac{\partial \mathcal{L}}{\partial \phi_t} \delta \phi \Big|_{t_1}^{t_2} \right), \end{aligned} \quad (\text{B3})$$

where the second line terms vanish if the variation in the field $\delta \phi$ is assumed to vanish both at initial and final times and on the boundaries leading to classical EL equations

$$\frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial \phi_x} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \phi_t} = 0. \quad (\text{B4})$$

If the $\delta \phi$ field and its derivatives do not vanish on the boundaries the procedure here presented is not valid anymore and additional terms must be taken into account [64]. The higher

dimensional cases for several n (treated independently) fields, i.e., $\mathcal{L} = \mathcal{L}(\phi_A, \partial_\mu \phi_A)$ with $A = 1 \dots n$, are obtained similarly as in the case just presented. Here and in the following capital Latin letters label the various fields (multiplets). Greek letters, on the other hand, range from 0 to 3 and mean space and time indices. We have adopted here a four-dimensional notation $x^\mu = (x^0, x^i) \equiv (t, \vec{x})$, which incidentally coincides with the relativistic formulation (with speed of light c set equal to 1). On the other hand, lower case Latin letters range from 1 to 3 and stand for purely spatial indices. The general EL equations (both valid in relativistic and non-relativistic contexts) are then [15,31]

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \phi_A} - \frac{\partial}{\partial x^i} \frac{\partial \mathcal{L}}{\partial (\partial \phi_A / \partial x^i)} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\phi}_A} = 0, \quad A = 1 \dots n, \\ i = 1 \dots 3, \end{aligned} \quad (\text{B5})$$

or in four-dimensional more compact notation

$$\frac{\partial \mathcal{L}}{\partial \phi_A} - \frac{\partial}{\partial x^\mu} \frac{\partial \mathcal{L}}{\partial (\partial \phi_A / \partial x^\mu)} = 0, \quad A = 1 \dots n, \quad \mu = 0 \dots 3, \quad (\text{B6})$$

where the quantities ϕ_A may be columns (multiplets) of scalar, spinor, vector, or tensor independent fields. The concept of “independent fields” introduced above requires still a clarification however. In electromagnetism as an example, starting from the Lagrangian density, it can be shown that given a vector potential A^μ the temporal component A^0 is a dependent variable not a dynamical one (in Hamiltonian language this statement is more clear) leading to subtle complications [15,31]. This implies that the geometric characterization of the fields requires specific attention in the manipulation of the variational relations. In this paper we shall study specifically multiplets of real and complex scalar fields only, whose geometric space-time structure is less complicated than the one just described.

2. Conservation laws: Infinitesimal space and time translations

We can now approach the problem of conservation laws for Lagrangian systems. Let us start with infinitesimal space or time coordinate translation (rotations are excluded for the moment) first. We shall start analyzing the 1+1-dimensional field theory. Following Refs. [65,66], we suppose to perform an infinitesimal time translation, i.e., $t \rightarrow t+a$ (a is a constant) such that the field shall transform infinitesimally for a close to zero (notice the appearance of a Lie derivative [67] applied to scalars) as

$$\phi(t, x) \rightarrow \phi(t+a, x) = \phi(t, x) + a \partial_t \phi \equiv \phi + \delta \phi. \quad (\text{B7})$$

As a consequence of this time translation our Lagrangian density varies as

$$\delta \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \phi} \delta \phi + \frac{\partial \mathcal{L}}{\partial (\partial_t \phi)} \delta (\partial_t \phi) + \frac{\partial \mathcal{L}}{\partial (\partial_x \phi)} \delta (\partial_x \phi), \quad (\text{B8})$$

which, using the Euler-Lagrange previously derived Eq. (B4), leads to

$$\begin{aligned}\delta\mathcal{L} &= \left(\frac{\partial}{\partial x} \frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} + \frac{\partial}{\partial t} \frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \right) \delta\phi + \frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \delta(\partial_t\phi) \\ &\quad + \frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \delta(\partial_x\phi) \\ &\equiv \frac{\partial}{\partial t} \left(\frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \delta\phi \right) + \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \delta\phi \right).\end{aligned}\quad (\text{B9})$$

Now $\delta\phi = a\partial_t\phi$, so that we get

$$\delta\mathcal{L} = \left[\frac{\partial}{\partial t} \left(\frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \partial_t\phi \right) + \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_t\phi \right) \right] a. \quad (\text{B10})$$

On the other hand, the Lagrangian is scalar function so that its variation gives

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial t} a. \quad (\text{B11})$$

Equating relations (B10) and (B11) we obtain

$$\frac{\partial\mathcal{L}}{\partial t} a = \left[\frac{\partial}{\partial t} \left(\frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \partial_t\phi \right) + \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_t\phi \right) \right] a, \quad (\text{B12})$$

which trivially gives

$$\frac{\partial}{\partial t} \left[\frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \partial_t\phi - \mathcal{L} \right] + \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_t\phi \right) = 0. \quad (\text{B13})$$

Introducing the energy density [15]

$$\mathcal{H} = \frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \partial_t\phi - \mathcal{L} \quad (\text{B14})$$

our relation (B13) becomes

$$\frac{\partial}{\partial t} \mathcal{H} + \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_t\phi \right) = 0. \quad (\text{B15})$$

Integrating this relation in a space interval $x \in [x_1, x_2]$, exchanging the integral with the derivative, and introducing the total energy $E = \int_{x_1}^{x_2} dx \mathcal{H}$ we get

$$\frac{dE}{dt} = - \int_{x_1}^{x_2} dx \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_t\phi \right) \equiv \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_t\phi \right) \Big|_{x_2}^{x_1}, \quad (\text{B16})$$

which vanishes if the quantity $\Gamma = \frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_t\phi$ is zero on the boundaries. If the field ϕ and its derivatives go to zero on the boundary sufficiently rapidly the Γ term should vanish too (for ‘‘well behaved’’ Lagrangians at least) and if this happens total energy E gets conserved in time. This is the simplest demonstration of Nöther’s theorem: any differentiable symmetry of the action of a physical system is associated with a corresponding conservation law. We stress that if Γ does not satisfy these conditions, conservation law does not hold anymore. In some field theories conservation laws do not descend from a continuous Lagrangian symmetry but come from constraints imposed by topological properties instead (the conserved topological charges) [65]: in our analysis,

however, we do not address these more delicate points (which in quantum field theory are connected with spontaneous symmetry breaking, anomalies, and topological charges), leaving them for future studies [53]. If we would have performed an infinitesimal spatial translation instead of a temporal one, i.e., $x \rightarrow x+b$ (implying $\delta\phi = b\partial_x\phi$) with b being a constant, the corresponding conservation law procedure, working as previously shown with formula (B9) for b close to zero, would have led to

$$\delta\mathcal{L} = \left[\frac{\partial}{\partial t} \left(\frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \partial_x\phi \right) + \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_x\phi \right) \right] b. \quad (\text{B17})$$

This relation together with

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial x} b \quad (\text{B18})$$

finally gives

$$\frac{\partial}{\partial t} \left[\frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \partial_x\phi \right] + \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_x\phi - \mathcal{L} \right) = 0. \quad (\text{B19})$$

Integrating in space, introducing the momentum density [15]

$$\mathcal{P}_x = - \frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} \partial_x\phi \quad (\text{B20})$$

such that the total momentum results in $P_x = \int_{x_1}^{x_2} dx \mathcal{P}_x$ we obtain the balance relation

$$\frac{dP_x}{dt} = \int_{x_1}^{x_2} dx \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_x\phi - \mathcal{L} \right) \equiv \left(\frac{\partial\mathcal{L}}{\partial(\partial_x\phi)} \partial_x\phi - \mathcal{L} \right) \Big|_{x_1}^{x_2}, \quad (\text{B21})$$

which gives a conserved quantity (i.e., P_x) if the right-hand side of the above relation vanishes. The procedure here derived easily generalizes [31] for higher dimensions and n independent fields ϕ_A giving the conservation equations for the energy-momentum tensor $T_{\mu\nu}$ for infinitesimal spatial and temporal translations $x^\mu \rightarrow x^\mu + l^\mu$, i.e.,

$$\frac{\partial}{\partial x_\mu} T_{\mu\nu} = 0, \quad T_{\mu\nu} = \left[\frac{\partial\mathcal{L}}{\partial(\partial\phi_A/\partial x_\mu)} \frac{\partial\phi_A}{\partial x^\nu} - g_{\mu\nu} \mathcal{L} \right], \quad (\text{B22})$$

with $\partial^\mu\phi_A = \partial\phi_A/\partial x_\mu \equiv (\partial\phi_A/\partial t, -\nabla\phi_A)$ and $\partial_\mu\phi_A = \partial\phi_A/\partial x^\mu \equiv (\partial\phi_A/\partial t, \nabla\phi_A)$, while we recall $g_{\mu\nu} = \text{diag}(1, -1, -1, -1)$ is the flat space-time metric tensor used to raise and lower indices. It is useful also to give this expression in mixed form, i.e.,

$$T_\nu^\mu = \frac{\partial\mathcal{L}}{\partial(\partial\phi_A/\partial x^\mu)} \frac{\partial\phi_A}{\partial x^\nu} - \mathcal{L} \delta_\nu^\mu, \quad \partial_\mu T_\nu^\mu = 0, \quad (\text{B23})$$

which contains covariant derivatives only (δ_ν^μ is the Kronecker symbol). The conservation laws just introduced, integrated in space, now read

$$\frac{dP_\nu}{dt} \equiv \frac{\partial}{\partial t} \int_B d^3x T_\nu^0 = - \int_B d^3x \frac{\partial}{\partial x^i} T_\nu^i \equiv - \int_{\partial B} dS_i T_\nu^i, \quad (\text{B24})$$

where divergence theorem has been used and dS_i is intended as the vector equal in magnitude to the area of the surface element, and normal to the element, or in more common form $dS_i = n_i d\Sigma$ where n_i is the normal to the boundary and $d\Sigma$ is the surface element. In three dimensions, if T_ν^i is exactly zero beyond a certain distance (or it goes to zero faster than $1/r^2$ in an infinite space domain) [68], then we can define the conserved total field energy $E = \int d^3x T_0^0$ and momentum $P_i = -\int d^3x T_i^0$. Clearly Eqs. (B14) and (B20) are a particular case of these relations. These are the general expressions of energy and momentum used in our analysis. Before concluding, a comment on the common minus sign in the definition of the field momentum must be given. Although in this paper a Lagrangian theory for a nonrelativistic problem is derived, we have found appropriate to continue to use the relativistic Greiner's monographs notation ([15,31]) i.e., $P_\mu = (E, -\vec{P})$. In fact we can still use the treatment of special relativistic theory even for nonrelativistic actions which do not have the requirements of Lorentz invariance. Unfortunately, the signature's choice with minus signs in the spatial part in nonrelativistic cases leads to a difference in sign between covariant and contravariant spatial vectors and we have to take into account this fact for coherence. Incidentally this choice shall give us for the quantum problem observables in agreement with the conventions of nonrelativistic solid state physics books (see as an example Ref. [69] on p. 167). It is important to conclude remarking, however, that in any case the common sign of energy, momentum, and angular momentum could be arbitrarily chosen due to the possibility to multiply the whole Lagrangian up to a constant factor which does not alter the field equations.

3. Conservation laws: Infinitesimal space and time rotations

One can perform also other types of infinitesimal transformations, i.e., rotations both in time and space (boosts) or in space only (proper rotations). The necessity to have at least two space coordinates forces us to skip the simple x and t scheme previously introduced. The necessary calculations, however, are quite long, so we summarize here all the relevant points referring to Greiner's monograph [15] for all the detailed derivations there performed "step by step." Given the infinitesimal rotation $x^\mu \rightarrow x^\mu + \delta\omega^{\mu\nu} x_\nu$ ($\delta\omega^{\mu\nu}$ is antisymmetric) the n fields transform as $\phi_A \rightarrow \phi_A + \frac{1}{2} \delta\omega_{\mu\nu} (I^{\mu\nu})_{AB} \phi_B$ where in relativistic contexts the I 's are the infinitesimal generators of the Lorentz transformations which are antisymmetric operators. The formulation just presented is valid also for nonrelativistic fields. This is not unexpected: in fact the restricted Lorentz group is generated by ordinary spatial rotations and Lorentz boosts. While we will be interested in the purely spatial rotations (we are studying a nonrelativistic theory), the boosts will not be of interest (every time coordinate is equivalent for the quantum and the diffusive problems analyzed in this paper). The continuity relation, ob-

tained requiring invariance of the action integral again, results in

$$\partial^\mu f_\mu = 0, \quad f_\mu = \frac{1}{2} \delta\omega^{\nu\lambda} \Lambda_{\mu\nu\lambda}, \quad (\text{B25})$$

with

$$\Lambda_{\mu\nu\lambda} = T_{\mu\lambda} x_\nu - T_{\mu\nu} x_\lambda + \frac{\partial \mathcal{L}}{\partial(\partial^\mu \phi_A)} (I_{\nu\lambda})_{AB} \phi_B, \quad (\text{B26})$$

which means that

$$\frac{d}{dt} \mathcal{M}_{0\nu\lambda} \equiv \frac{\partial}{\partial t} \int d^3x \Lambda_{0\nu\lambda} = - \int d^3x \frac{\partial}{\partial x_i} \Lambda_{i\nu\lambda} \equiv - \int dS^i \Lambda_{i\nu\lambda}. \quad (\text{B27})$$

If $\Lambda_{i\nu\lambda}$ vanishes on the boundary as discussed before, six conservation laws arise, three for angular-momentum vectors, i.e., $(\mathcal{M}_{012}, \mathcal{M}_{013}, \mathcal{M}_{023})$ and the remaining three ones $(\mathcal{M}_{010}, \mathcal{M}_{020}, \mathcal{M}_{030})$ for the generalization of the center of mass in relativity (not of interest for us). In order to define angular momenta one must take into account spatial indices only, so that one gets $M_{nl} \equiv \mathcal{M}_{0nl} = L_{nl} + S_{nl}$ where $L_{nl} = \int d^3x [x_n T_{0l} - x_l T_{0n}]$ is the orbital angular-momentum tensor while $S_{nl} = \int d^3x \frac{\partial \mathcal{L}}{\partial(\partial^\mu \phi_A)} (I^{\mu l})_{AB} \phi_B$ is the internal (spin) angular-momentum tensor. For single and multiple scalar fields $(I^{\mu l})_{AB}$ drop out [70] leaving standard angular momentum only. (See Ref. [15] on p. 99 for the explicit example of the charged Klein-Gordon field.) Using Eq. (B22), the quantity $M_{nl} \equiv L_{nl}$ can be rewritten then as

$$M_{nl} = \int d^3x \frac{\partial \mathcal{L}}{\partial(\partial^\mu \phi_A)} \left(x_n \frac{\partial}{\partial x^l} - x_l \frac{\partial}{\partial x^n} \right) \phi_A, \quad (\text{B28})$$

where we recall the notation $x_\mu = (t, -\vec{x})$ (so that x_n give a minus sign in our expression once explicitly expressed in terms of physical coordinates). The three-dimensional angular-momentum vector is finally given by $J^m \equiv L^m = \frac{1}{2} \epsilon^{mnl} M_{nl}$ (ϵ^{mnl} is Levi-Civita alternating symbol [20]) or in components $\vec{L} = (M_{23}, M_{31}, M_{12})$. This is the expression of angular momentum used in this paper.

4. Conservation laws: Infinitesimal internal transformations

Fields ϕ_A can be subject also to transformations which interest the internal index A , so that one usually says that the fields have an internal structure [15,31]. An infinitesimal internal transformation then must mix these indices as follows:

$$\phi_A \rightarrow \phi_A + i\varepsilon \sum_B \lambda_{AB} \phi_B. \quad (\text{B29})$$

If this transformation leaves action S invariant, using the notation $\delta x_\mu = 0$ (no space-time transformation is performed) and $\delta\phi_A = i\varepsilon \sum_B \lambda_{AB} \phi_B$, we can write for the Nöther's current f^μ satisfying $\partial_\mu f^\mu = 0$ that

$$f_\mu = i\varepsilon \sum_A \sum_B \frac{\partial \mathcal{L}}{\partial(\partial^\mu \phi_A)} \lambda_{AB} \phi_B, \quad (\text{B30})$$

which gives the conservation law

$$\begin{aligned}
\frac{dQ}{dt} &\equiv \frac{d}{dt} \int d^3x \sum_A \sum_B \frac{\partial \mathcal{L}}{\partial (\partial^j \phi_A)} \lambda_{AB} \phi_B \\
&= - \int d^3x \frac{\partial}{\partial x_i} \sum_A \sum_B \frac{\partial \mathcal{L}}{\partial (\partial^j \phi_A)} \lambda_{AB} \phi_B \\
&\equiv - \sum_A \sum_B \int dS^i \frac{\partial \mathcal{L}}{\partial (\partial^j \phi_A)} \lambda_{AB} \phi_B. \quad (\text{B31})
\end{aligned}$$

As in the previous cases, charge gets conserved in time if the right-hand side of Eq. (B31) vanishes, i.e., if the argument of the surface integral goes to zero on the boundary.

APPENDIX C: THE RETROGRADE DIFFUSION PROBLEM

Let us suppose [45,46] to have to solve the initial value problem

$$u_t = -u_{xx}, \quad u(0, x) = 1, \quad x \in \mathcal{R}, t > 0. \quad (\text{C1})$$

Obviously $u(t, x) = 1$ is a solution of this problem. On the other hand, the function

$$u_{(n)}(t, x) = 1 + \frac{1}{n} \sin(nx) e^{n^2 t}, \quad n \in \mathcal{N} \quad (\text{C2})$$

is a solution of the initial value problem

$$u_t = -u_{xx}, \quad u(0, x) = 1 + \frac{1}{n} \sin(nx), \quad x \in \mathcal{R}, t > 0. \quad (\text{C3})$$

The initial values of the two problems are different because of the term $\frac{1}{n} \sin(nx)$ which converges to zero uniformly for $n \rightarrow +\infty$. However, the solution $\frac{1}{n} \sin(nx) e^{n^2 t}$ at any fixed value of x (except the values for which the sine vanishes) diverges for $n \rightarrow +\infty$. This means that the constant solution $u(t, x) = 1$ is unstable so that the problem is ill posed. We point out that this result does not depend by the fact that we are considering an infinite space domain. Solving the problem with boundary conditions $u(-\pi, t) = u(\pi, t) = 1$, the solution is again given by Eq. (C2), which is plagued by the same problem. We can conclude this discussion pointing out that the more general problem

$$u_t = u_{xx}, \quad u(0, x) = \phi(x), \quad x \in \mathcal{R}, t < 0 \quad (\text{C4})$$

is ill posed too.

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