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Fick's law and Fokker–Planck equation in inhomogeneous environments

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Abstract

In inhomogeneous environments, the correct expression of the diffusive flux is not always given by the Fick's law $\Gamma = -D\nabla n$. The most general hydrodynamic equation modelling diffusion is indeed the Fokker–Planck equation (FPE). The microscopic dynamics of each specific system may affect the form of the FPE, either establishing connections between the diffusion and the convection term, as well as providing supplementary terms. In particular, the Fick's form for the diffusion equation may arise only in consequence of a specific kind of microscopic dynamics. It is also shown how, in the presence of sharp inhomogeneities, even the hydrodynamic FPE limit may becomes inaccurate and mask some features of the true solution, as computed from the Master equation.

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Introduction. The fluid modelling of the time- and space-evolution of quantities within complex environments, whose dynamics may only be treated on statistical grounds, is made using the diffusion equation (DE) $\partial_t n = D\partial_x^2 n$. This phenomenological equation arises from two more fundamental equations: the continuity equation for n: $\partial_t n = -\partial_x \Gamma$, and the Fick's law (or Fourier's law) [1] $\Gamma = -D\partial_x n$, where x and t are the spatial coordinate and the time, respectively; the diffusivity D is a constant dependent from the medium. A pedagogical overview of Fick's (Fourier's) law and diffusion equation may be found in [2].

The postulate of homogeneity may hold just as a first-order approximation, whereas most systems must ultimately allow for some degree of non-uniformity. Almost unavoidably, therefore, one is faced with the question: how DE has to be generalized to such systems. The exact answer to this question is of relevance for a plethora of problems in practically any branch of natural sciences: from physics, to chemistry, geology, biology, social sciences, ...

Heuristically, the difficulty related to the generalization of DE may be understood as follows: an inhomogeneous environment should make D position-dependent: $D \to D(x)$. There are, however, several choices for Γ that differ when $D = D(x)$, but that collapse to the same identical form when D is constant. Therefore, the problem may be restated as: what is the correct generalization of Fick's law (provided that one exists) in inhomogeneous environments.

This subject appears repeatedly addressed in literature; however, it is difficult to find the explicit exposition of a general solution. In Van Kampen's book [3], it is argued that one cannot decide *a priori* what the correct form for Γ is, which rather depends upon the properties of the problem studied. Landsberg ([4] and references therein), points out that, to some extent, it is a matter of convention, provided that supplementary (convective) terms are added suitably. In other terms, the definition of a diffusive and a convective flux is not univocal, only the total flux is. The Letter providing the clearest intuitive insight and at the same time detailed calculations about what goes on in such situations is probably Schnitzer's [5]. We mention also the papers [6,7], featuring computer experiments and presenting further bibliography about this subject. Papers [8–10] feature analytical and experimental work, demonstrating that the straightforward generalization of Fick's law $\Gamma = -D(x)\partial_x n(x)$ cannot hold in all systems.

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In order to quantitatively address the issue, it is necessary to deal with a reasonably accurate modelling of the dynamics at the microscopic level: transport equations, thus, will emerge at the level of large length scales. The tool we adopt is provided by the Master equation (ME):

$$\frac{\partial n(x,t)}{\partial t} = -\frac{n(x,t)}{\tau(x)} + \int dx'\, p(x-x',x')\frac{n(x',t)}{\tau(x')} \tag{1}$$

ME (1) yields a coarse grained probabilistic description of a microscopic system driven by a Markov process, and can be visualized as the continuity equation for the passive scalar quantity $n(x,t)$ (which, properly speaking, is a probability density) subject to transitions ("jumps") modifying its state from x' to x, with probability $p(x-x',x')$, and at a rate $1/\tau(x)$ (see chapter 1 of [11]). Eq. (1) contains virtually all the solutions of the transport problem, once the functions p and τ are given. On the other hand, it is often unpractical to deal directly with it, particularly in higher-dimensional problems. Therefore, and particularly if a clear-cut separation of scales exists in the problem studied, it is customary to take its long-wavelength limit, which washes out details at the finest scales and turns the integral equation (1) into a famous differential equation: the Fokker–Planck equation (FPE) (see, e.g., chapter 9 of [12]):

$$\frac{\partial n(x,t)}{\partial t} = -\frac{\partial}{\partial x}\big(U(x)n\big) + \frac{\partial^2}{\partial x^2}\big(D(x)n\big). \tag{2}$$

Within the ME formulation, all the physics is built into the functions p and τ. In the passage from ME to FPE, p and τ are packed into the diffusive and convective terms, D, U. Therefore, the analytical expression of D, U, ultimately relies on the constraints that the problem to be solved places on p, τ. Is it possible, basing upon general considerations on the microscopic dynamics, to identify equivalent classes of systems, that is, systems that lead to the same qualitative form of the FPE? As we shall show later, the initial question advanced in this Introduction is related to this point: the Fick's form of the diffusion equation is a particular limiting case of the FPE, that arises when the microscopic dynamics fulfills a given symmetry.

The purpose of this Letter is to provide a discussion about this topic. Furthermore, we will address the broader issue of the validity of the scale separation at the basis of the FPE. We will show that, whenever, this hypothesis is not fulfilled, additional terms to the FPE need to be considered.

From the Master equation to the Fokker–Planck equation. The simplest way to pass from ME to FPE is by expressing the integrand in Eq. (1) in terms of the small parameter $\Delta = x' - x$, which is of order the mean jumping length L_p:

$$\frac{p(x-x',x')}{\tau(x')}n(x') = \frac{p(-\Delta,x+\Delta)}{\tau(x+\Delta)}n(x+\Delta) \tag{3}$$

and expanding around x in powers of Δ (Kramer–Moyal expansion). However, this step is justified provided that p, τ, n, are not strongly varying functions of x over distances of order L_p. If we assume that n is a smooth function of x, we may concentrate on the other quantity: $h = p/\tau$. A branching into two cases is possible: (1) h is a smooth function, or (2) h is not. Although, condition (2) actually contains (1) as a particular case, it turns out convenient to consider them separately, since (1) is easier to deal with.

Finally, we will consider also the case (3), when n itself is not a smooth function.

Case (1): Both n and h are smooth functions. We are allowed to make a Taylor expansion in powers of the function $h \times n$. The result, truncated to second order, yields Eq. (2) with

$$U = \int d\Delta \frac{p(\Delta,x)}{\tau(x)}\Delta, \qquad D = \frac{1}{2}\int d\Delta \frac{p(\Delta,x)}{\tau(x)}\Delta^2. \tag{4}$$

Limiting the truncation to second order is ordinarily justified on the basis of Pawula theorem [13,14].

All the information relevant to our problem is packed into U, D. Two important cases are (A) $U = (dD/dx)$, or (B) $U = 0$. Case (A) recovers Fick's law, while case (B) yields the solution

$$\partial_t n = \partial_x^2\big(D(x)n(x)\big). \tag{5}$$

Both results may be verified by direct substitution into Eq. (2). It turns out that relation (A) arises straightforwardly from ME (1) by postulating the symmetry

$$\frac{p(x'-x,x)}{\tau(x)} = \frac{p(x-x',x')}{\tau(x')} \to \frac{p(\Delta,x)}{\tau(x)} = \frac{p(-\Delta,x+\Delta)}{\tau(x+\Delta)} \tag{6}$$

which ensures the time reversal symmetry of the microscopic dynamics. Indeed, a first-order Taylor expansion of the second argument around x yields, after rearranging,

$$\Delta\frac{dp(-\Delta,x)}{dx} = p(\Delta,x) - p(-\Delta,x) + \Delta p(-\Delta,x)\frac{d\ln\tau}{dx}. \tag{7}$$

Using Eq. (7) into the integrals (4) yields the sought result (A) (For a different derivation, see Prof. Feder's lecture notes [15].)

The solution (B) has some relevance, too, since it corresponds to the choice of a symmetrical kernel: $p(\Delta,x) = p(-\Delta,x)$. Although apparently natural, the range of validity of this condition is actually rather narrow, as it cannot hold under smoothly varying conditions, where $p(\Delta,x) \neq p(-\Delta,x)$; that is, the probability for a particle of jumping rightwards or leftwards cannot be the same. In order to better understand this point, let us consider a system where test particles collide against some scattering centres. Jumps are arcs of ballistic motion between two collisions. If the system is not homogeneous the density n_{sc} of the scattering centres is not uniform. Let us suppose, say, $dn_{sc}/dx < 0$: a test particle at x has a larger probability of striking a scattering centre that is on its left $(x-\delta x)$ rather than on its right $(x+\delta x)$, and therefore of being backscattered in the opposite direction. Hence, there is a larger probability of bouncing back rightwards than the converse.

Having ruled out the case (B) for several inhomogeneous systems, one could wonder how general is condition (A). It turns out that (A) generically holds for a large class of 1-degree-of-freedom Hamiltonian systems [16–18] (see also [19] for another particular case). For more general systems, and especially in systems with more degrees of freedom, the above constraints