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Relation Between Diffusion Equations and Boundary Conditions in Bounded Systems

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Abstract

Differential equations need boundary conditions (BCs) for their solution. It is widely acknowledged that differential equations and BCs are representative of independent physical processes, and no correlations between them are required. Two recent studies by Hilhorst, Chung et al. argue instead that, in the specific case of diffusion equations (DEs) in bounded systems, BCs are uniquely constrained by the form of transport coefficients. In this paper, we revisit how DEs emerge as fluid limits out of a picture of stochastic transport. We point out their limits of validity and argue that, in most physical systems, BCs and DEs are actually uncorrelated by virtue of the failure of diffusive approximation near the system's boundaries. When, instead, the diffusive approximation holds everywhere, we show that the correct chain of reasoning goes in the direction opposite to that conjectured by Hilhorst and Chung: it is the choice of the BCs that determines the form of the DE in the surroundings of the boundary.

Keywords: Fokker–Planck equation; heat equation; master equation; diffusion; boundary conditions

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1. Introduction

Diffusion equations (DEs) are ubiquitous in physics, and they are employed for modeling the behaviour of stochastic or chaotic systems [1]. In this work, we will refer specifically to the two following expressions:

$$\partial_t u = \partial_x(D\,\partial_x u - V\,u). \tag{1}$$

$$\partial_t u = \partial_x(\partial_x(D\,u) - V'\,u). \tag{2}$$

The two expressions above are obviously equivalent and related to each other through $V' = V + \partial_x D$. Historically, they were reached through different paths. Expression (1), with $V = 0$, was first written by Fourier in 1822 to phenomenologically model the propagation of heat and then, in 1855, Fick also included the transport of matter. Expression (2), with the arbitrary V', is the Fokker–Planck Equation (FPE), arising in the context of generic stochastic systems out of a microscopic picture of dynamics. Generally, u represents any scalar quantity that evolves stochastically, D quantifies the level of disorder, and V accounts for any spatial asymmetry.

Just like any differential equation, Equations (1) and (2) need to be supplemented by initial and boundary conditions (BCs) in order to be solved. In physics and engineering,

one attributes different roles and meanings to the transport coefficients D and V from the one side, and the BCs on the other side: transport coefficients express the system's internal dynamics, while BCs represent the effect of external constraints. They are thus expressions of two independent physical mechanisms; hence, no correlation is required to exist between the form of the DE and the kind of BCs that are imposed upon it. Arbitrary combinations of BCs and DEs are routinely employed in practical applications.

This view has been questioned recently by two works [2,3]. These papers examined a "smooth" version of bounded diffusive systems: The boundaries are not infinitely sharp; rather, a transition occurs between the inner region, characterized by finite transport, and the outer region, where transport occurs with arbitrarily small coefficients D and V. The authors of [2,3] argue that once the analytical expression for D and V throughout all spaces is given, only one "natural" kind of BC is consistent with the required boundedness of motion. In particular, these are Neumann BCs with null derivatives for Fick's equation (Equation (1) with $V = 0$) and Dirichlet BCs with null density for the Fokker–Planck equation without convection (Equation (2) with $V' = 0$). Thus, in papers [2,3], DEs and BCs are not independent: The latter ones follow uniquely from the shape of transport coefficients and, therefore, from the DE. These unexpected results call for a thorough re-examination of the subject of diffusive transport: this is the argument of the present paper.

We note, first of all, that the range of validity of DE itself has to be scrutinized: DEs are fluid models for physical processes that, ultimately, possess some sort of granularity. Section 2 is devoted, thus, to a re-examination of the conditions under which diffusion equations arise as appropriate descriptions of physics. We recall that a microscopic picture of stochastic transport can be formulated as an ensemble of random walkers, for which the dynamics is expressed in terms of jump probabilities p from one site to another, and the waiting time τ between successive jumps. The corresponding equation that quantifies the transition rates from different sites is often referred to in the literature as the "Master Equation" (ME). It is commonly argued that DEs arise as long-wavelength limits of the ME: This is the essence of the popular Kramers–Moyal (K-M) expansion. On the other hand, the K-M expansion has been recognized since long to be based upon heuristic and not rigorous arguments. Therefore, we devote Section 3 to a critical review of the arguments that have been advanced along the years to place the K-M result upon firmer grounds, fundamentally basing upon the Central Limit Theorem In Section 4, armed with these results, we return to our main theme: the connection between DEs and BCs. Our conclusions are as follows: (i) in most systems, boundaries are not smooth; rather, the interface between the interior and the exterior of a system is narrower than the average random walkers' step. This introduces a discontinuity: the DE formalism cannot be extended from the core to the boundary, therefore effectively making DEs and BCs independent. (ii) In the presence of smooth boundaries, BCs and DEs may instead be coupled, but in this case, the hypothesis of the independence of the DE fails; rather, we will show that the DE—near the boundaries—must adapt precisely to the BC so as to preserve consistency.

2. DEs as Fluid Limits of Stochastic Dynamics

We write the local rate of change in the scalar quantity u, $\partial_t u(x,t)$, in terms of processes that move u across different points according to some probability [4]:

$$\partial_t u(x,t) = \int \frac{p(x,x')}{\tau(x')} u(x',t) dx' - \frac{u(x,t)}{\tau(x)}. \tag{3}$$

In this expression, a version of a Master Equation (ME), $p(x,x')dx'$, is the probability of the scalar $u(x',t)$ to jump to x. Consistently with most of the literature, we will suppose that p depends on x, x' through the following combination: $p = p(\Delta = x - x'; x')$; i.e.,

it depends on the starting point, and on the relative distance to the arrival point. The integral in Equation (3)—implicitly understood as spanning all spaces—thus becomes a convolution.

Within this simplified picture of dynamics, the time needed for u to move from x' to x is regarded as negligible, but between any two consecutive jumps, there is a waiting time $\tau(x')$—which is assumed to depend upon the starting location x' alone, still adhering to most of the literature. Additional effects may be added to Equation (3). Among them are temporal memory effects, finite traveling times, sources/sinks, etc., but here, we will stick to this barebone picture for stochastic motion. Throughout this work, we will only consider one-dimensional dynamics, but it is clear that Equation (3) may be generalized to higher dimensions and may also be regarded as an effective one-dimensional equation, where the dynamics along the other directions has been averaged out. See [5,6] for further details.

The integro-differential Equation (3) can be turned into a fully differential one under some conditions. The popular Kramers–Moyal (K-M) method [4,6] expands Equation (3) in series with respect to the small parameter Δ, and truncates the expansion after the first two terms. Neither the series's expansion nor the truncation to a finite number of terms is trivially justifiable, and a lot of attention has been devoted to them. We will return to this issue in the next section in order to provide firmer ground for the K-M result.

We arrive, eventually, to the FPE (2), where

$$D = \int d\Delta \frac{\Delta^2}{2} \frac{p(\Delta, x)}{\tau(x)}, \quad V' = \int d\Delta \, \Delta \, \frac{p(\Delta, x)}{\tau(x)}. \tag{4}$$

Important cases correspond to $V' = 0$ and $V' = dD/dx$. In terms of stochastic processes, the condition $V' = 0$ is realized by jumps that are equally probable in both directions: $p(-\Delta, x) = p(\Delta, x)$. The condition $V' = dD/dx$, which—as we have remarked earlier—leads to Fick's form of diffusion, is associated with a more complicated relation:

$$\frac{p(\Delta, x)}{\tau(x)} = \frac{p(-\Delta, x + \Delta)}{\tau(x + \Delta)}. \tag{5}$$

This expression is odd-looking at first sight, but actually, it is just an expression of detailed balance, ensuring that the rate of jumps from x to x' and vice versa is identical [7]. We recall that it was originally argued by Landau that the constraint $V' = dD/dx$ must hold for general 1-degree-of-freedom Hamiltonian dynamics, whereas it vanishes for higher dimensional dynamics [8,9].

3. From the Master Equation to the Diffusion Equation and Back

The mutual relation between the ME and the DE is actually a nontrivial topic that has been—and to some degree still is—debated in the literature.

In the previous section, we have justified the passage from the ME to the DE by employing the popular Kramers–Moyal approach. This amounts to expanding the ME in powers of the jump's length Δ and truncating it after the second-order term. The K-M expansion is implicitly based upon the ansatz that a separation exists between Δ and the slower variation scale of the density u. The lack of a rigorous control parameter, which may provide a justification for the neglect of the higher-order terms, has always been a source of concern. The Pawula theorem [6,10] states that if the number of nonvanishing terms of the series is finite, it must be either one or two in order to avoid unphysical features in the solution, such as negative densities. This is, however, just an *a posteriori* justification of the K-M result.

In order to overcome this lack of rigour, van Kampen [11,12] suggested his system-size expansion in terms of a small parameter Ω^{-1}, where Ω, often (but not necessarily)

identified with the size of the system, is a manifestly large parameter, exceeding all other scales of the system. Van Kampen distinguishes a macroscopic deterministic contribution to the system's trajectory, scaling like Ω, and a fluctuating part, scaling like $\Omega^{1/2}$. Van Kampen's approach is more rigorous than K-M's, but it still contains a dose of arbitrariness, since the relative weight between macroscopic deterministic and fluctuating terms is set ad hoc. Basically, his ansatz is based upon the law of large numbers. Currently, attempts of improving upon van Kampen's approach still appear (see, e.g., [13,14]). However, a convincing analysis was carried out by Ryskin [15], where he recalls how a Markovian process, over times longer than the decorrelation time, fulfills the conditions for the validity of the Central Limit Theorem, and therefore entails the emergence of Gaussian processes. Ryskin's work explains why, even if the higher-order terms in the K-M expansion do not vanish, they nonetheless may be disregarded: The reason is that they do not enter the long-time evolution equation [16]. In conclusion, the DE is a faithful picture of dynamics only over time scales longer than the decorrelation one. Over these time scales, several random steps accumulate. The DE is therefore accurate only over distances that are larger than the jump length: not because of the original Kramers–Moyal scale separation hypothesis but because, over short spatial scales, the conditions for the validity of the Central Limit Theorem cannot be fulfilled.

4. On the Relation Between DEs and BCs

The previous section introduces an important consequence for this work: Transport around sharp structures is not faithfully described by the DE. In the case of neutral fluids bounded by material walls, the interfacial region is provided by the outermost atomic layer of the solid surface, and it is therefore on the atomic scale, which is much smaller that any turbulence scale. In the case of bounded plasmas, there is some ambiguity due to the existence, on the one side, of several physically relevant lengths (Debye sheath and scrape-off layer) over which transport is modified and, on the other side, the existence of several turbulence scales. The ME, on the other hand, does not suffer from the same problem: One is allowed to pick up an arbitrary p and τ provided that they fulfill the coarse-scale constraints dictated by the experiment (this is easily understandable within the framework of the Bayesian approach to statistics); hence, issues of scale are of no concern here: the reader is referred to [7] for the explicit treatment of a case where ME and DE may yield different results.

As long as the boundaries are sharp, the arguments of Hilhorst and Chung therefore do not apply, since there is an interface region where the DE does not hold. This provides an effective discontinuity between the core and the boundary that invalidates their argument.

Now, we show that the alleged inconsistencies invoked by Hilhorst and Chung do not arise even in the presence of a smooth transition between core and boundaries. The BCs encode physical information that is captured in the transport coefficients p and τ of the ME, and then, the information is transmitted to the diffusion coefficients D and V of the DE in a way that must preserve consistency. Let us see how this occurs. For example, let us start with a system whose dynamics, far from the boundaries, is left–right symmetrical, $p(-\Delta, x) = p(\Delta, x)$: $V' = 0$, and the pure FPE (2) holds. When one approaches the boundaries, i.e., when the distance from the boundary is of the order of the average jump length, different scenarios may be envisaged depending upon the boundary conditions holding. Let us start by considering absorbing boundaries: The walker may cross the boundary, but once there, it does not return into the system any longer. This scenario can be modeled with $\tau(x)$ proceeding to infinity when x is outside the boundary, while being finite inside the boundaries. The left–right symmetry properties of p need not be affected; hence, $V' = 0$ still holds everywhere. Let us now consider the case of reflecting boundaries.

Each walker hitting the wall must return back inside the system. This is accomplished provided that the rates of outbound and inbound hops equilibrate: This corresponds to condition (5), which leads to Fick's form of the diffusion equation. In summary, while the DE in the interior of the system may take an arbitrary expression, near the boundaries, it must adapt itself to a form that is consistent with the BCs. The width of this transition layer is likely of the order of the average jump length; hence, it is microscopic and invisible to the experimentalist. For modeling purposes, the "core" expression of the DE is the only one that can be compared with experiments, and the "edge" expression of the DE escapes observations. In practical terms, the edge region remains a zone of discontinuity as long as the diffusive approximation is invoked, just like what occurs in the scenario with sharp interfaces.

To conclude, we mention that—in principle—BCs may incorporate further constraints that cannot be captured into transport properties: for instance, external reservoirs. It is clear that, in this case, the alleged dependence of the BCs from the DE is untenable as well [17].

5. Conclusions

Essentially, our paper aimed to explain how the conclusions drawn in works [2,3] are not physically applicable, since they postulate that one may employ the diffusion equation regardless of any other constraint. We have shown that this is not the case. We have recalled that the DE is a valid picture of the physics of transport only over sufficiently large length scales. When the boundary–system interface's width is smaller than these scales, it acts as an effective discontinuity region, making independent the physics determining the DE, valid in the interior, and that determining the BCs. When the transition region is large enough to make the diffusive approximation valid throughout the whole system, on the other hand, the DE and BCs both arise consistently out of the same model of transport quantified by the ME. This entails that, in the transition region, the DE cannot be specified independently but must instead adapt precisely to the form consistent with the BCs. In both cases, we re-establish the common notion that the BCs do not depend on the DE.

A spin-off of our study—which we regard as valuable for a journal devoted to the foundations of physical theories—is that it compelled us to revisit the historical development that has led to the diffusion equation, highlighting some lesser known results (Ryskin' analysis of the K-M result arising from the Central Limit Theorem) and correcting some misinterpretations (Ryskin' claim of a precedence of the DE equation over the ME).

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16. It is interesting to notice that Ryskin argues, as a corollary, that the DE must be the fundamental equation for describing the evolution of a stochastic system, and the ME only an approximation, differing from the true evolution equation by terms scaling like τ_{coll}. In so doing, he goes against the conventional wisdom of assigning the premacy to the ME–as we have done in this paper. Riskin's argument is flawed, though, since it overlooks that the DE suffers from the same shortcoming that he attributes to the ME. As a matter of fact, Ryskin works out the FPE from the evolution operator of his Equation (17), valid for a Markov process assuming that it is invariant under *arbitrary* rescaling of the time interval; but this conflicts precisely with his original tenet that there is a minimal time scale τ_{corr} under which the statistical picture breaks down. Ryskin's evolution operator should be regarded as valid only for time intervals longer than τ_{coll}. Accordingly, it does not produce the *exact* generator of time displacements A (his Equation (2)), that is valid for arbitrarily small time intervals, but rather the finite-time generator B (his Equation (4)), that differs from A precisely by terms of order τ_{coll}.
17. We thank an anonymous reviewer for pointing out this fact to our attention.

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