

## Fractional generalization of Fick's law: derivation through Continuous-Time Random Walks

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### Introduction

In the study of particle transport in magnetically confined plasmas it is common to construct transport equations based on the Fick law (we assume a one-dimensional system):

$$\Gamma_{F;2}(x,t) = -A_2(x)\partial_x n(x,t), \quad (1)$$

in which the particle flux is proportional to the gradient of the particle density,  $n(x,t)$  (in general, the diffusivity,  $A_2(x)$ , may also depend explicitly on  $t$  and even on other fields). The diffusion equation thus obtained is

$$\partial_t n(x,t) = \partial_x (A_2(x)\partial_x n(x,t)). \quad (2)$$

The validity of Eq. (2) relies on two assumptions:

- Finite characteristic length and time scales exist.
- The microscopic transport process satisfies a certain symmetry [1] which we call *Global Reversibility*: for any  $x$ , the probability (per unit time) of a particle leaving  $x$  equals the probability (per unit time) of a particle arriving at  $x$ .

Numerical simulations and experimental findings seem to suggest that the framework of diffusive transport is too restricted for certain turbulent fusion plasmas [2, 3], in which (particle or energy) transport takes place via correlated avalanches. Transport events in these cases have a maximum size that is only limited by the system size  $L$ , and therefore a characteristic size that diverges with (some power of)  $L$ . The relevance of scale-free transport is by now recognized in many different branches of physics, biology and economics [4].

This work is based on [5] and tries to answer the following question: *how can we construct a scale-free transport equation preserving Global Reversibility?*

### Continuous-Time Random Walk

The Continuous-Time Random Walk (CTRW) provides a suitable framework to derive macroscopic transport equations from the microscopic dynamics. CTRWs are models describing a large number of particles whose motion is defined probabilistically. For Markovian processes, the CTRW is defined in terms of a *step-size* probability distribution function (pdf),  $p(\Delta;x)$ , giving the probability that a particle located at  $x$  jumps to  $x + \Delta$ . Imposing conservation of the number of particles leads to the Generalized Master Equation (GME) governing the time evolution of the density of particles:

$$\partial_t n(x,t) = \int_{-\infty}^{\infty} p(x-x';x') \frac{n(x',t)}{\tau(x')} dx' - \frac{n(x,t)}{\tau(x)}, \quad (3)$$

where  $\tau(x)$  is the mean waiting time at  $x$ .

Denote by  $T(\Delta;x) := p(\Delta;x)/\tau(x)$  the one-particle transition rate. Then, Global Reversibility is easily expressed as

$$\int_{-\infty}^{\infty} T(-\Delta, x+\Delta) d\Delta = \int_{-\infty}^{\infty} T(\Delta, x) d\Delta, \quad \forall x. \quad (4)$$

### Derivation of the classical Fick law from CTRWs

The classical Fick law (2) is obtained from a CTRW under the following hypotheses:

- (i) Global Reversibility is satisfied.
- (ii) All integer moments of  $p(\Delta;x)$  are finite, i.e.  $\langle \Delta^n \rangle < \infty, \forall n \in \mathbb{N}$ .

The usual procedure consists in expanding (3) and (4) in moments of  $p$ , keeping terms up to the second moment, and directly enforcing Global Reversibility. This yields (2), which is called the fluid (or hydrodynamic) limit of the GME.

### Derivation of the fractional Fick law from CTRWs

The family of *Lévy stable distributions* (or simply *Lévy distributions*) are the solutions of the Generalized Central Limit Theorem. They are parameterized by four real numbers  $\alpha \in (0, 2]$ ,  $\beta \in [-1, 1]$ ,  $\sigma > 0$ , and  $\mu \in \mathbb{R}$ . Their characteristic function (i.e. their Fourier transform) is given by:

$$\hat{S}(\alpha, \beta, \sigma, \mu)(k) = \begin{cases} \exp(-\sigma^\alpha |k|^\alpha [1 - i\beta \text{sign}(k) \tan(\frac{\pi\alpha}{2})] + i\mu k) & \alpha \neq 1, \\ \exp(-\sigma |k| [1 + i\beta \frac{2}{\pi} \text{sign}(k) \ln|k|] + i\mu k) & \alpha = 1. \end{cases} \quad (5)$$

The *index of stability*,  $\alpha$ , is related to the asymptotic behaviour of  $S(\alpha, \beta, \sigma, \mu)(x)$  at large  $x$ :

$$S(\alpha, \beta, \sigma, \mu)(x) = \begin{cases} C_\alpha \left(\frac{1-\beta}{2}\right) \sigma^\alpha |x|^{-1-\alpha} & x \rightarrow -\infty, \\ C_\alpha \left(\frac{1+\beta}{2}\right) \sigma^\alpha |x|^{-1-\alpha} & x \rightarrow \infty, \end{cases} \quad (6)$$

for  $\alpha \in (0, 2)$ . For  $\alpha = 2$ ,  $S(2, \beta, \sigma, \mu)$  is a Gaussian distribution.

By *fractional Fick law* we understand the fluid limit of a CTRW under the assumptions:

- (i') Global Reversibility is satisfied.
- (ii') The step-size pdf,  $p(\Delta; x)$ , is a Lévy stable distribution (in  $\Delta$ ) with index<sup>1</sup>  $\alpha$  and  $x$ -dependent  $\sigma, \mu$ .

From (ii'), it follows that a Lévy pdf of order  $\alpha < 2$  does not have finite moments of order equal to or greater than  $\alpha$ . In particular, the second-moment is infinite and the system lacks a characteristic length scale. As a consequence, the calculation of the fluid limit of (3) based on an expansion in moments of  $p$  does not make sense anymore. Now the suitable approach (which coincides with the moment expansion when the latter exists) consists in Fourier transforming (3) and keeping the lowest order terms in  $k$ .

The Fourier transform of the GME (3) with respect to  $x$  yields:

$$\frac{\partial \hat{n}(k, t)}{\partial t} = \int_{-\infty}^{\infty} \frac{n(x', t)}{\tau(x')} (\hat{p}(k; x') - 1) e^{ikx'} dx', \tag{7}$$

where

$$\hat{p}(k; x') = \int_{-\infty}^{\infty} p(\Delta; x') e^{ik\Delta} d\Delta \tag{8}$$

is the characteristic function of  $p(\Delta; x')$ . We introduce now the characteristic exponent,  $\Lambda(k; x')$ , through  $\hat{p}(k; x') \equiv \exp \Lambda(k; x')$ . The fluid limit of the GME is obtained then by performing the small  $k$  approximation  $\hat{p}(k; x') \approx 1 + \Lambda(k; x')$ , which turns Eq. (7) into:

$$\frac{\partial \hat{n}(k, t)}{\partial t} = \int_{-\infty}^{\infty} \frac{n(x', t)}{\tau(x')} \Lambda(k; x') e^{ikx'} dx'. \tag{9}$$

The key point is that, after some straightforward manipulations, the symmetry (4) can be recast into the following, equivalent form:

$$\int_{-\infty}^{\infty} \left[ \frac{\hat{p}(k, x') - 1}{\tau(x')} \right] e^{ikx'} dx' = 0, \quad \forall k. \tag{10}$$

The fluid limit of the symmetry can be expressed in terms of the characteristic exponent:

$$\int_{-\infty}^{\infty} \frac{\Lambda(k, x')}{\tau(x')} e^{ikx'} dx' = 0, \tag{11}$$

which is the small  $k$  approximation of Eq. (10).

Using the explicit form of the characteristic exponent for Lévy distributions (5) we find the relation between  $\sigma(x)$  and  $\mu(x)$  imposed by (11). Inserting the result in (9) and Fourier inverting we obtain the fractional generalization of Fick's law:

$$\partial_t n(x, t) = -\partial_x \Gamma_{F; \alpha}(x, t), \tag{12}$$

<sup>1</sup>We restrict to situations with  $\beta = 0$ .

where the fractional Fick flux is now given by:

$$\Gamma_{F;\alpha} = \left( {}_{-\infty}D_x^{\alpha-1} - {}^{\infty}D_x^{\alpha-1} \right) (A_\alpha n) - \left( \left( {}_{-\infty}D_x^{\alpha-1} - {}^{\infty}D_x^{\alpha-1} \right) A_\alpha \right) n, \quad (13)$$

with

$$A_\alpha(x) := -\frac{1}{2 \cos(\pi\alpha/2)} \frac{\sigma^\alpha(x)}{\tau(x)}. \quad (14)$$

The fractional Fick flux is written in terms of the *Riemann-Liouville fractional derivative operators*:

$$\begin{aligned} {}_{-\infty}D_x^\alpha f &\equiv \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dx^m} \int_{-\infty}^x \frac{f(x')}{(x-x')^{\alpha-m+1}} dx', \\ {}^{\infty}D_x^\alpha f &\equiv \frac{(-1)^m}{\Gamma(m-\alpha)} \frac{d^m}{dx^m} \int_x^{\infty} \frac{f(x')}{(x'-x)^{\alpha-m+1}} dx', \end{aligned}$$

with  $m$  the integer number verifying  $m-1 \leq \alpha < m$ . Observe that the Riemann-Liouville operators extend the notion of differentiation to non-integer  $\alpha$  and reduce to the ordinary derivative operators when  $\alpha$  is an integer. Except for integer  $\alpha$ , they are non-local operators, so that one needs to know  $f$  on the whole space in order to compute its  $\alpha$ -th derivative at a point  $x$ .

### Conclusions and further work

We have derived the appropriate equation on which any description of transport in systems lacking characteristic length scales (e.g. turbulent fusion plasmas) but still satisfying Global Reversibility should be built.

The formalism presented herein also provides the basis for addressing the derivation of the fractional Fick law in three-dimensional inhomogeneous systems. The CTRW construction can be trivially extended to any dimension. However, the formulation in terms of fractional derivative operators requires tackling a number of non-trivial technical details which we plan to study in future work.

### References

- [1] N. G. van Kampen, *Stochastic processes in Physics and Chemistry*, North Holland, New York 1981.
- [2] B. A. Carreras, V. E. Lynch, and G. M. Zaslavsky, *Phys. Plasmas* **8**, 5096 (2001)
- [3] D. del-Castillo-Negrete, B. A. Carreras, and V. E. Lynch, *Phys. Rev. Lett.* **94**, 065003 (2005).
- [4] R. Metzler and J. Klafter, *Phys. Rep.* **339**, 1 (2000).
- [5] I. Calvo, R. Sánchez, B. A. Carreras, and B. Ph. van Milligen, *Phys. Rev. Lett.* **99**, 230603 (2007).