Fractional Diffusion Limit of Non-Classical Transport

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Abstract - We establish an asymptotic fractional diffusion equation limit of non-classical transport in the case of heavy-tail path length distributions. Our analysis uses the Fourier transform. First we introduce the technique by re-deriving the classic diffusion limit, then we apply it to non-classical transport. We introduce a general scaling and identify the scaling that is necessary to produce a meaningful diffusion limit for path length distributions with heavy tails. We conclude with remarks on the diffusion limit of the periodic Lorentz gas equation, which describes transport in a crystal-like medium, and for which the path-length distribution can be computed analytically.

I. INTRODUCTION

Anomalous diffusion, described by a fractional diffusion equation, has gained a lot of interest recently. Among many applications [1], there have been works on radiation transport through clouds (cf. the review [2]). Another interesting application is light transport through Lévy glasses, for which experiments and simulations have been performed [3]. In many other areas, anomalous diffusion has been observed (e.g. plasma physics [4]).

The motivation for this work is to connect the non-classical transport equation proposed by Larsen [5] to anomalous transport. Here we summarize and present in a different language the theoretical mathematical results from [6].

The non-classical transport equation was originally developed to describe measurements of photon path-length in clouds, which could not be explained by classical radiative transfer, cf. [7] or sections 5.1 and 8.3 in the review [2]. Non-classical transport theory has since been extended [8] and has found applications for neutron transport in pebble bed reactors [9] and even computer graphics [10]. The equation is able to model particle transport with given path-length distributions \( p(s) \), \( s \) being the path-length, and \( p \) their probability density function.

In his original paper [5], Larsen has considered the diffusion limit of the non-classical transport equation. However, the classical analysis cannot capture the case when the second moment, i.e. the variance, of the path-length distribution does not exist. The purpose of this paper is to extend the analysis to cover this case. It will turn out that in the case of an infinite variance of the path-length distribution, the limiting equation is a fractional diffusion equation. This paper therefore provides a connection between non-classical transport and anomalous diffusion.

We use a Fourier technique [11] to compute a limit fractional diffusion equation. More specifically, we perform the computation in Fourier space, i.e. we compute the symbol of the fractional diffusion operator.

II. CLASSICAL DIFFUSION LIMIT

To gain intuition for the Fourier analysis technique from the next section, let us first look at the standard diffusion limit for the scaled equation in an infinite (no boundary conditions), homogeneous medium

\[
\epsilon^2 \partial_t \psi + \epsilon \Omega \cdot \nabla \psi = \sigma (\phi - \psi), \quad \psi = \int_{\Omega} \phi d\Omega.
\]

We denote by \( \psi_0 = \psi(t = 0) \) the initial condition. The unknown \( \psi \) has the usual interpretation as the probability density to find a particle at position \( x \in \mathbb{R}^N \), moving into direction \( \Omega \in S^{N-1} \) (unit vector). For later purposes, we will keep the space dimension \( N \) general. For simplicity, we assume that

\[
\int_{S^{N-1}} d\Omega = 1,
\]

i.e. we hide the normalization factor in the integration measure.

To derive the diffusion limit, we apply the Laplace-Fourier transform

\[
\tilde{\psi}(\omega, k, \Omega) = \int_0^{\infty} \int_{\mathbb{R}^N} e^{-\omega t} e^{-ik \cdot x} \psi(t, x, \Omega) dt dx.
\]

to the transport equation and obtain

\[
\epsilon^2 (\omega \tilde{\psi} - \tilde{\psi}_0) + \epsilon ik \cdot \Omega \tilde{\psi} = \sigma (\phi - \tilde{\psi}).
\]

We rearrange

\[
\tilde{\psi} = \frac{\epsilon^2}{\sigma + \epsilon^2 \omega + \epsilon ik \cdot \Omega} \tilde{\psi}_0 + \frac{1}{\sigma + \epsilon^2 \omega + \epsilon ik \cdot \Omega} \sigma \phi
\]

and integrate over \( \Omega \)

\[
\tilde{\phi} = \int_{S^{N-1}} \frac{\epsilon^2 \tilde{\psi}_0}{\sigma + \epsilon^2 \omega + \epsilon ik \cdot \Omega} d\Omega + \sigma \tilde{\phi} \int_{S^{N-1}} \frac{1}{\sigma + \epsilon^2 \omega + \epsilon ik \cdot \Omega} d\Omega.
\]
We reverse the Laplace-Fourier transform and arrive at

$$M$$

Altogether, (1) becomes in the limit $$\psi$$

The imaginary part in the numerator vanishes because it is odd

at position $$x$$.

infinite (no boundary conditions), homogeneous medium as in

III. NON-CLASSICAL DIFFUSION LIMIT

The first steps still follow [5]. We transform (2) by

$$\psi(x, \Omega, s) = \Psi(x, \Omega, s) e^{-\int_0^s \Sigma(s') ds'} \langle s \rangle ,$$

where $$\langle s \rangle$$ denotes a weighted $$s$$-integration. Note that this transformation assumes the existence of the first moment of the path-length distribution. This somewhat limits the analysis, but the physically relevant cases satisfy this assumption. We thus obtain the equivalent of equation (6.6) in [5]

$$\partial_s \Psi(x, \Omega, s) + \epsilon \Omega \cdot \nabla_s \Psi(x, \Omega, s) = 0$$

with initial condition

$$\Psi(x, \Omega, 0) = (1 - \theta(e)(1 - c)) \int_{S^{N-1}} \int_0^\infty \rho(s') \Psi(x, \Omega', s') ds' d\Omega' + \theta(e) \langle s \rangle Q(x).$$
We use the technique developed in [12], and modify certain steps for the situation at hand. First we Fourier-transform in space only
\[
\hat{\Psi}(k, \Omega, s) = \int_{\mathbb{R}^N} e^{-ik \cdot x} \Psi(x, \Omega, s) dx,
\]
and obtain
\[
\partial_t \hat{\Psi}(k, \Omega, s) + \varepsilon ik \cdot \Omega \hat{\Psi}(k, \Omega, s) = 0
\]
with initial condition
\[
\hat{\Psi}(k, \Omega, 0) = (1 - \theta(\varepsilon)(1 - c)) \int_{S^{N-1}} \int_0^\infty p(s') \hat{\Psi}(k, \Omega', s') ds' d\Omega' + \theta(\varepsilon)(s) \hat{Q}(k).
\]
The first equation can be inverted and we get the implicit solution formula
\[
\hat{\Psi}(k, \Omega, s) = e^{-ik \cdot \Omega s} \times \left[ (1 - \theta(\varepsilon)(1 - c)) \int_{S^{N-1}} \int_0^\infty p(s') \hat{\Psi}(k, \Omega', s') ds' d\Omega' + \theta(\varepsilon)(s) \hat{Q}(k) \right].
\]
We define the scalar flux
\[
\hat{\rho}(k) = \int_{S^{N-1}} \int_0^\infty \hat{\Psi}(k, s) ds d\Omega,
\]
and obtain
\[
\hat{\rho}(k) = \int_{S^{N-1}} \int_0^\infty p(s) e^{-ik \cdot \Omega s} (1 - \theta(\varepsilon)(1 - c)) \hat{\rho}(k) ds d\Omega + \int_{S^{N-1}} \int_0^\infty p(s) e^{-ik \cdot \Omega s} \theta(\varepsilon)(s) \hat{Q}(k) ds d\Omega.
\]
We insert a clever 1 = \int \int p(s) ds d\Omega, rearrange terms, divide by \theta(\varepsilon) and arrive at
\[
0 = \hat{\rho}(k) \int_{S^{N-1}} \int_0^\infty \frac{e^{-ik \cdot \Omega s} - 1}{\theta(\varepsilon)} p(s) ds d\Omega + \left( (1 - c) \hat{\rho}(k) + \langle s \rangle \hat{Q}(k) \right) \int_{S^{N-1}} \int_0^\infty e^{-ik \cdot \Omega s} p(s) ds d\Omega.
\]
If \varepsilon \to 0, then the second term has an obvious limit (\varepsilon^p \to 1). The first term needs more work. First we make it real-valued
\[
c^p = \int_{S^{N-1}} \int_0^\infty \frac{e^{-ik \cdot \Omega s} - 1}{\theta(\varepsilon)} p(s) ds d\Omega
\]
and the imaginary part vanishes because it is odd in \Omega. It is not obvious how the integrand behaves when \varepsilon \to 0, because the term is formally \frac{\varepsilon^p}{0^+}, so it requires more detailed analysis.

V. FRACTIONAL DIFFUSION LIMIT

In this section we discuss the singular integral in a way that aims to provide the key understanding as to why a fractional derivative appears for heavy-tail path-length distributions and not for fast-decaying path-length distributions.

We make a growth assumption on \rho, which determines the tail:
\[
\rho(s) = \frac{p_0}{s^{\alpha+1}} \quad \text{for } |s| \geq 1.
\]
For the first moment and the second moment to be finite, we need \alpha > 2. For the first moment to be finite and the second moment to be infinite, we need \alpha > 2. In the following, the borderline case \alpha = 2 will be treated separately. A suitable growth assumption on \rho for |s| \leq 1 will be made later, but is essentially irrelevant.

The \rho-integral is split into \int_0^1 ds + \int_1^\infty ds. We interpret the integral as an \mathbb{R}^N-integral in spherical coordinates. Let \nu = s \Omega (which implies dv = s^{N-1} ds d\Omega). Then
\[
-2 \int_{S^{N-1}} \int_1^\infty \int_0^\infty \sin^2[\varepsilon k \cdot \Omega s]/2 \frac{p_0}{s^{\alpha+1}} ds d\nu = -2 \int_{|w|\leq 1} \sin^2[\varepsilon k \cdot \nu]/2 \frac{p_0}{\nu^{\alpha+1}} |w|^\alpha dw.
\]
Now we make the substitution
\[
\nu = \varepsilon |\nu| v, \quad dv = \varepsilon |\nu|^{\alpha} |v|^\alpha dv
\]
and get
\[
-2 \int_{|w|\leq 1} \sin^2(w_1/2) \frac{p_0}{|w|^{\alpha+1}} |w|^\alpha dw \frac{\varepsilon^{\alpha}}{\theta(\varepsilon)} |w|^\alpha,
\]
where \nu_1 = w \cdot k/|k| is a scalar. From here on, we discuss the convergence (or divergence) of this integral as \varepsilon \to 0. In addition, these arguments give us the necessary scalings. First we observe that the integrand behaves like \nu^{-\alpha-N} for large |\nu|. Thus integration of the tail makes no problem if \alpha > 0. The integral’s behavior is solely determined by the singularity at \nu = 0.

1. THE CASE \alpha > 2

If \alpha > 2, then the integrand behaves like
\[
\frac{\sin^2(w_1/2)}{|w|^{\alpha+N}} \sim \frac{1}{|w|^{\alpha+N-2}} \quad \text{for } |w| \text{ small.}
\]
The integral therefore depends on \varepsilon like
\[
\int_{|w|\leq 1} \frac{\sin^2(w_1/2)}{|w|^{\alpha+N}} |w| d\nu \sim \int_{|w|\leq 1} \frac{1}{|w|^{\alpha+N-2}} |w|^{N-1} d|w| \sim \int_{|w|\leq 1} \frac{1}{|w|^{\alpha-1}} d|w| \sim \varepsilon^{2-\alpha} |k|^{2-\alpha}.
\]
This integral is singular for \varepsilon \to 0. However, together with the other \varepsilon-scale factors, we can balance this singularity. We get
\[
\varepsilon^{2-\alpha} \frac{\varepsilon^p}{\theta(\varepsilon)} = \frac{\varepsilon^2}{\theta(\varepsilon)}.
\]
Thus, in order to control the singularity, it is sufficient to choose

\[ \theta(\varepsilon) = \varepsilon^2, \]

or more precisely so that \( \varepsilon^2 / \theta(\varepsilon) \) well-behaved as \( \varepsilon \to 0 \). The power of \( k \) that appears is

\[ |k|^{2-\alpha}|\rho^\alpha| = |k|^2, \]

which is the symbol of the Laplacian.

Combining the results, (3) becomes in the limit

\[ 0 = -\frac{1}{2} \frac{\langle s^2 \rangle}{N(s)} \Delta \rho + \frac{1 - c}{\langle s \rangle} \rho = Q, \]

which is exactly the diffusion limit in the case of isotropic scattering (compare Eq. (6.12) in [5]). Let us remark that the diffusion coefficient is

\[ D = \frac{1}{2(s)} \int_{\mathbb{R}^N} \frac{v^2}{|v|^{N+1}} p(|v|) dv, \]

where we have used the substitution \( v = s \Omega \), and the fact that \( k \) can be aligned arbitrarily so that instead of \( v \cdot k \) we can write the first component \( v_1 \) of \( v \).

2. The case \( 1 < \alpha < 2 \)

If \( 1 < \alpha < 2 \), then by the growth arguments above, the integral

\[ \int_{\mathbb{R}^N} \frac{\sin^2(w_{1/2})}{|w|^{\alpha+\mu}} dw \]

actually has a finite limit for \( \varepsilon \to 0 \) (there is no singularity in the primitive at \( w = 0 \)). Thus we are left with a scale factor of

\[ \frac{\varepsilon^\alpha}{\theta(\varepsilon)}. \]

To obtain a non-trivial limit for \( \varepsilon \to 0 \), we therefore choose \( \theta(\varepsilon) \) so that the scale factor is well-behaved as \( \varepsilon \to 0 \). For example, we can take

\[ \theta(\varepsilon) = \varepsilon^2. \]

We define

\[ D = \frac{p_0}{\langle s \rangle} \int_{\mathbb{R}^N} 2 \frac{\sin^2(w_{1/2})}{|w|^{\alpha+\mu}} dw \]

(compare this to the classical diffusion coefficient) and obtain in the limit

\[ 0 = -D|k|^2 \rho - \frac{1 - c}{\langle s \rangle} \rho + \bar{Q}. \]

Now \(-|k|^2\rho\) is the symbol of the fractional Laplacian. We reverse the Fourier transform and obtain the strong form

\[ -D(\Delta_\rho)^{\mu/2} \rho + \frac{1 - c}{\langle s \rangle} \rho = Q, \]

i.e. a fractional/anomalous diffusion equation.

3. The case \( \alpha = 2 \)

In the borderline case \( \alpha = 2 \), the integral

\[ \int_{|w|>\varepsilon |k|} \frac{\sin^2(w_{1/2})}{|w|^{\mu+\nu}} dw \]

has a logarithmic singularity. It behaves like

\[ \int_{|w|>\varepsilon |k|} \frac{\sin^2(w_{1/2})}{|w|^{\mu+\nu}} dw \sim \int_{|w|>\varepsilon |k|} \frac{1}{|w|} dw \sim -\log \varepsilon. \]

Again we demand

\[ -\frac{e^\alpha}{\theta(\varepsilon)} \log \varepsilon = \frac{e^2}{\theta(\varepsilon)} \log \varepsilon = 1 \]

to have a non-trivial limit for \( \varepsilon \to 0 \). This means that \( \theta(\varepsilon) \) has to go to zero slightly slower than \( e^2 \)

\[ \theta(\varepsilon) = -e^2 \log \varepsilon. \]

With this scaling, we obtain a classical diffusion equation, i.e. a Laplacian operator, but with a non-standard diffusion coefficient. More precisely, we set

\[ D = \frac{p_0}{6\langle s \rangle} \]

and obtain the limit equation

\[ -D\Delta_\rho + \frac{1 - c}{\langle s \rangle} \rho = Q. \]

VI. THE PERIODIC LORENTZ GAS

The periodic Lorentz gas, as an example of transport in a correlated background medium, has been studied extensively in the recent mathematical literature (cf. [13, 14, 15] and references therein). Contrary to transport in a random background medium, the scattering obstacles are located on a regular grid (cf. Figure 1).

Fig. 1. Transport in a random background medium (left) versus transport in the crystal-like medium of the periodic Lorentz gas (right).

This medium is homogenized (coarse graining or Boltzmann-Grad limit) by simultaneously shrinking the obstacles and increasing their number such that the collision frequency remains constant, cf. Figure 2.
The path-length distribution of the periodic Lorentz gas in the Boltzmann-Grad limit has been computed e.g. in [16] and is given by

$$p(s) = \frac{\Upsilon(s)}{\int_{0}^{\infty} \Upsilon(\tau) d\tau},$$

which is a probability density by construction. The function $\Upsilon$ is given by $\Upsilon(s) = \frac{24}{\pi^2} s^2$ for $s \leq \frac{1}{2}$ and

$$\frac{24}{\pi^2} \left( \frac{1}{2s^2} + 2\left(1 - \frac{1}{2s}\right)^2 \ln(1 - \frac{1}{2s}) - \frac{1}{2} \left(1 - \frac{1}{s}\right)^2 \ln(1 - \frac{1}{s}) \right)$$

for $s > \frac{1}{2}$. It is shown in Figure 3. Note that the orientation of the lattice does not play a role in the limit.

For $s \to \infty$ it is straightforward to see that this expression behaves like

$$\Upsilon(s) \sim \frac{2}{\pi^2} s^2 + O\left(\frac{1}{s^2}\right).$$

This means that this function is exactly on the borderline between classical and anomalous ($\alpha = 2$). We thus expect a classical diffusion equation with a non-classical coefficient in the asymptotic limit.

VII. DISCUSSION

Altogether we have shown that for a path-length distribution with sufficiently slow-decaying tail, in the limit $\varepsilon \to 0$, the non-classical transport equation becomes a fractional diffusion equation for the scalar flux. As a side result, we could compute the known classical diffusion limit for sufficiently decaying path-length distributions by a simple Fourier technique. We have considered isotropic scattering in an infinite (no boundaries), homogeneous medium. In [6] we treat the case of anisotropic scattering.

There are several open topics related to non-classical transport. Among them are the formulation of correct boundary and interface conditions for heterogeneous media. In a companion paper [17], we make an attempt at this. In heterogeneous media, it is also open how a fractional diffusion limit might look like. To study these questions, it will probably be necessary to generalize the classical kinetic theory technique to derive the diffusion limit, namely Hilbert expansion, to the fractional case. A first step has been made in [18], although the decomposition that was used appears to be heavily inspired by the Fourier analysis.

It would also be interesting to understand if a fractional scaling has a deeper physical meaning. Finally, similar techniques could be applied to other fields, where anomalous transport plays a role, especially plasma physics.

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REFERENCES


