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Fractional calculus and Levy flights: modelling spatial epidemic spreading

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Abstract

We investigate fractional derivatives, especially fractional Laplacian operators, leading to Lévy flights. These notions will be applied to epidemic processes, like the stochastic spatially extended SIS process and models with reinfection, as super-diffusion is a more realistic mechanism of spreading epidemics than ordinary diffusion.

Key words: fractional calculus, fractional Laplace operator, Lévy flight, spatial stochastic epidemics, Kolmogorov-Fisher equation

1 Introduction

Classical derivatives of integer order have been generalized historically in various ways to derivatives of fractional order [8, 10] and especially [2] with more reference and results. On important application of such fractional derivatives is the notion of the fractional Laplacian operator in the theory of Lévy flights. This leads to the notion of sub- and super-diffusion, well applicable in reaction-diffusion systems [3]. In epidemiological systems especially the super-diffusion case is of interest as description of more realistic spreading than normal diffusion on regular lattices.

To understand even basic epidemiological processes it is often necessary to investigate well the spatial spreading since all epidemic processes happen on spatially restricted networks [4]. We have previously studied epidemic processes with reinfection on regular lattices [12] as they also appear in the physics literature [7]. A crucial question in such systems is in how far basic notions like finite spreading and phase diagrams hold not only for ordinary diffusion but also in the super-diffusion case [4, 5]. Wider processes with multi strain interaction [11, 1] could be treated similarly. As our prime example here we will investigate the susceptible-infected- susceptible SIS epidemic, which leads in the framework of reaction diffusion processes to the well know Kolmogorov-Fisher equation [9, 6].

2 Historic ways of generalizing derivatives

There are many definitions for the derivative of arbitrary real order μ [2]. The one that we use bellow is based on the fact that the Fourier transform $\mathcal{F}$ of a function satisfies the relation

$$\mathcal{F}\left(\frac{\partial f}{\partial x_\nu}\right) = ik_\nu \mathcal{F}(f).$$

For any constant coefficient partial differential operator

$$P\left(\frac{\partial}{\partial x_1}, ..., \frac{\partial}{\partial x_n}\right),$$

where P is a polynomial in n variables, we thus have

$$\mathcal{F}\left(P\left(\frac{\partial}{\partial x_1}, ..., \frac{\partial}{\partial x_n}\right) f\right) = P(ik_1, ..., ik_n) \cdot \mathcal{F}[f].$$

In particular, when $P(x_1, ..., x_n) = -|x|^2 = -x_1^2 - ... - x_n^2$then

$$P\left(\frac{\partial}{\partial x_1}, ..., \frac{\partial}{\partial x_n}\right) = \Delta$$

is the n dimensional Laplace operator. The Weyl derivative is then defined by

$$\mathbf{D}^\mu f = \mathcal{F}^{-1}\left[|k|^\mu \mathcal{F}[f]\right]$$

with $k = (k_1, ..., k_n)$. Symbolically $\mathbf{D}^\mu = (-\Delta)^{\mu/2}$ is called the fractional power of the Laplacian of exponent $\mu/2$. We will use the definition of the Laplacian via the Fourier representation below. In the following we will investigate ordinary diffusion in more detail and show how to generalize to super-diffusion. As an example for an application we will investigate the so called susceptible-infected-susceptible epidemic process, which leads in approximation neglecting higher correlation to the well known Kolmogorov-Fisher equation. This can easily be extended to other epidemic processes, like the SIR system or such with reinfection [12].

3 Ordinary diffusion

The simple stochastic differential equation

$$\frac{d}{dt}\; x = \varepsilon(t) \tag{1}$$

with a random variable $\varepsilon(t)$ describes a one-dimensional random walk in space. For probability distributions with finite variance and independent random draws at each time step the distribution of the process converges to a Wiener process with Gaussian distribution.

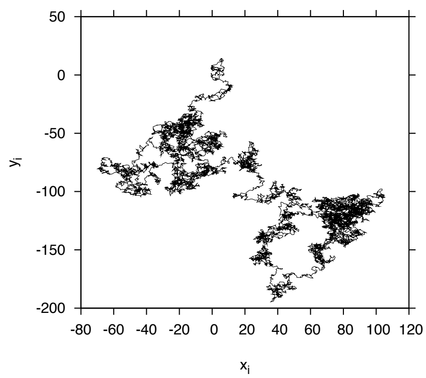

Figure 1: *Random walk with Gaussian distributed steps.*

Hence, for simplicity we can start the process immediately with Gauss normally distributed and stochastically independent random kicks

$$p(\varepsilon) = \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{\varepsilon^2}{2}} \quad . \tag{2}$$

For the Langevin-type equation (1) and independent Gaussian noise, Eq. (2), we obtain for the distribution of the process $p(x,t)$ the Fokker-Planck equation as a simple diffusion equation

$$\frac{\partial}{\partial t} \; p(x,t|x_0,t_0) = \frac{1}{2} \frac{\partial^2}{\partial x^2} \; p(x,t|x_0,t_0) \tag{3}$$

with the solution

$$p(x,t|x_0,t_0) = \frac{1}{\sqrt{2\pi(t-t_0)}} \; e^{-\frac{(x-x_0)^2}{2(t-t_0)}} \tag{4}$$

which is a Gaussian distribution with mean value $\mu = x_0$ and time dependent variance $\sigma^2 = (t-t_0)$. The mean displacement $\sqrt{\langle (x-x_0)^2 \rangle}$ has the famous $\sqrt{t}$ behaviour.

3.1 Simulation of an ordinary diffusion process

To give an impression how processes under ordinary diffusion and under super-diffusion work, we will first simulate a random walker for graphical clarity in two dimensions. Hence the Langevin equations for the x and y components of the vector $\underline{x} = (x,y)^{tr}$ are given by

$$\begin{aligned} \frac{d}{dt}x &= \varepsilon(t) \\ \frac{d}{dt}y &= \eta(t) \end{aligned} \tag{5}$$

with independent noise sources $\varepsilon(t)$ and $\eta(t)$. Or simply given in time discrete form we have

$$\begin{aligned} x_{n+1} &= x_n + \varepsilon_n \\ y_{n+1} &= y_n + \eta_n \end{aligned} \tag{6}$$

The Gaussian distributed random numbers ε_n and η_n can be generated from uniformly distributed random numbers on the unit interval, as given e.g. by the Marsaglia random generator, by the Box-Muller algorithm. Fig. 1 shows a simulation of a Gaussian random walker in two dimensions, starting at the origin, for 10 000 iteration steps. A random walker going with equal probability to one of its four von Neumann neighbouring sites on a regular two dimensional lattice would look on a large scale similar to the Gaussian random walker. The distribution $p(x,t|x_0,t_0)$ of the lattice random walker converges for long times and distances to the distribution of the Gaussian random walker.

3.2 Fourier representation of the ordinary diffusion process

The Fourier transform of the probability $p(x,t) := p(x,t|x_0 = 0, t_0 = 0)$ of the Wiener process, Eq. (4), is simply

$$\tilde{p}(k,t) = e^{-k^2 t} \tag{7}$$

and the Fokker-Planck equation is in Fourier space given by

$$\frac{\partial}{\partial t}\ \tilde{p}(k,t) = -k^2 \cdot \tilde{p}(k,t) \tag{8}$$

which now can be easily generalized to other powers of k than the power of 2 for normal diffusion.

4 Super-diffusion

To describe super-diffusion we generalize the Fourier representation of the diffusion process to $\mu \in (0,2]$ in the solution

$$\tilde{p}(k,t) = e^{-|k|^{\mu} t} \tag{9}$$

which corresponds to

$$\frac{\partial}{\partial t}\ \tilde{p}(k,t) = -|k|^{\mu} \cdot \tilde{p}(k,t) \tag{10}$$

in the Fokker-Planck equation. By inverse Fourier transformation we obtain in real space representation

$$\frac{\partial}{\partial t}\ p(x,t) = -\left(-\Delta_x\right)^{\mu/2} p(x,t) \quad . \tag{11}$$

For $\mu \in (0,1)$ the fractional Laplacian operator $(-\Delta_x)^{\mu/2}$ is given by

$$(-\Delta_x)^{\mu/2}\, p(x,t) = C_\mu \int_{-\infty}^{\infty} \frac{p(x,t) - p(y,t)}{|x-y|^{1+\mu}}\, dy \tag{12}$$

with constant

$$C_\mu = \left(\frac{2^{-\mu}\pi^{3/2}}{\Gamma(1+\frac{\mu}{2})\Gamma(\frac{1+\mu}{2})\sin\left(\frac{\mu\pi}{2}\right)} \right)^{-1} \quad .$$

For $\mu \in [1, 2)$ the fractional Laplacian operator $(-\Delta_x)^{\mu/2}$ is given by

$$(-\Delta_x)^{\mu/2}\, p(x,t) = C_\mu \int_{-\infty}^{\infty} \frac{\triangle_{x-y}\,[p(x,t) - p(y,t)]}{|x-y|^{1+\mu}}\, dy \tag{13}$$

where $\triangle_{x-y}$ is the central-difference operator,

$$\begin{aligned} \triangle_{x-y}\,[p(x,t) - p(y,t)] &= p(y,t) - p(x,t) - (p(y-(y-x)\,,t) - p(x-(y-x)\,,t)) \\ &= p(y,t) - 2p(x,t) + p(2x-y,t) \quad , \end{aligned} \tag{14}$$

with constant

$$C_\mu = \left(\frac{-\left(2^{1-\mu}\right)\pi^{3/2}}{\Gamma(1+\frac{\mu}{2})\Gamma(\frac{1+\mu}{2})\sin\left(\frac{\mu\pi}{2}\right)} \right)^{-1} \quad .$$

Or as master equation it can be written

$$\frac{\partial}{\partial t}\; p(x,t) = \int w_{x|y} p(y,t) - w_{y|x} p(x,t)\; dy \tag{15}$$

with transition rate

$$w_{x|y} = \frac{C_\mu}{|x-y|^{1+\mu}} \tag{16}$$

for $\mu \in (0, 1)$ and

$$w_{x|y} = \frac{C_\mu}{|x-y|^{1+\mu}} \triangle_{x-y} \tag{17}$$

for $\mu \in [1, 2)$. The solution in real space representation for $t > t_0$ is given by

$$p(x,t|x_0,t_0) = \frac{1}{2\pi} \int e^{-ik(x-x_0)-|k|^\mu (t-t_0)}\; dk \tag{18}$$

or with the function

$$G_\mu(z) = \frac{1}{2\pi} \int e^{-ikz-|k|^\mu}\; dk \tag{19}$$

the solution is

$$p(x,t|x_0,t_0) = \frac{1}{(t-t_0)^{1/\mu}}\; G\left(\frac{x-x_0}{(t-t_0)^{1/\mu}} \right) \quad . \tag{20}$$

The function $G_\mu(z)$ has for large argument $|z| >> 1$ a power law tail

$$G_\mu(z) \sim \frac{1}{|z|^{1+\mu}} \tag{21}$$

which however shows up rather slowly, since the series expansion of $G_\mu(z)$ is given by

$$G_\mu(z) = \frac{1}{\pi} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k!}\, \Gamma(1+k\mu) \sin\left(\frac{\pi}{2} k\mu\right) \cdot z^{-(k\mu+1)} \tag{22}$$

hence decreases for $k = 1$ as $|z|^{-(1+\mu)}$, but higher order terms die off only very slowly.

4.1 Cauchy process

For $\mu = 1$ the integral in the function $G_\mu(z)$ can be solved and gives a Cauchy distribution

$$G_{\mu=1}(z) = \frac{1}{\pi(1+z^2)} \tag{23}$$

leading to the Cauchy process as a special case of super-diffusion.

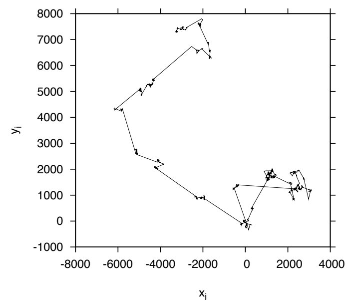

Figure 2: *Lévy flight with Cauchy distributed steps, i.e. Lévy exponent* $\mu = 1$.

4.2 Simulation of super-diffusive Lévy flights

A Cauchy distribution can simply be obtained numerically by dividing two Gauss normally distributed random variables. The simulation of a Cauchy flight in two dimensions is shown in Fig. 2.

For any other Lévy flight exponent μ the generation of random numbers is a bit more involved. We simulate in two dimensions the map

$$\begin{aligned} x_{n+1} &= x_n + r_n \cos(2\pi\varphi_n) \\ y_{n+1} &= y_n + r_n \sin(2\pi\varphi_n) \end{aligned} \tag{24}$$

in random polar coordinates, with φ_n uniformly distributed in the unit interval $[0, 1]$ and r_n random numbers with infinite variance and power law tail $|r|^{-(1+\mu)}$ with Lévy exponent μ.

Since the distribution $G_\mu(z)$ cannot be evaluated analytically, and also no closed invertible cumulative distribution function can be given, we cannot simply draw a random number from this Lévy flight distribution. But we can obtain random numbers r with a power law tail, and have to use an upper cut-off r_0. Such a distribution is

$$p(r) = \frac{\mu}{2} r_0^\mu \quad \cdot \quad \begin{cases} |r|^{-(1+\mu)} & \text{for } r_0 \leq |r| \leq \infty \\ 0 & \text{else} \end{cases} \tag{25}$$

and obtained by using a shot noise distributed random variable s, hence s takes the values -1 and +1 with equal probability, and a uniformly distributed random variable c in the unit interval via

$$r := \frac{r_0 \cdot s}{(1-c)^{1/\mu}} \quad . \tag{26}$$

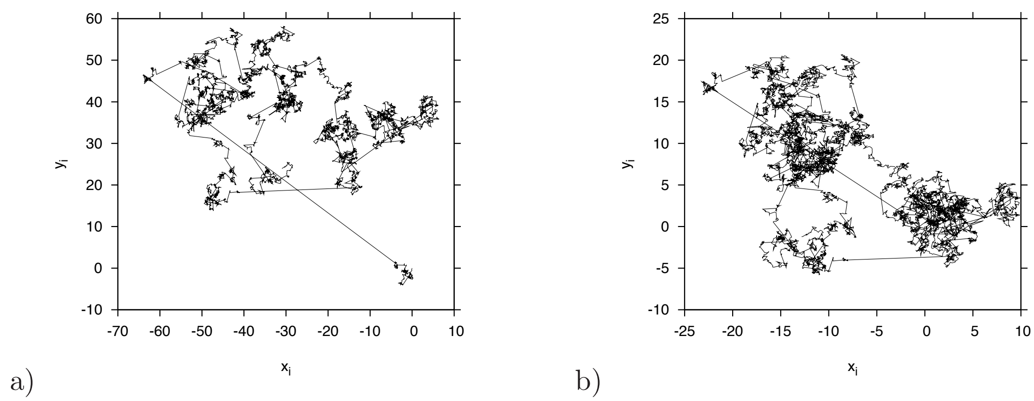

Figure 3: *a) Lévy flight with exponent* $\mu = 1.5$ *and b) with* $\mu = 1.8$.

The distributions of s and c are given by

$$p(s) = \frac{1}{2}\Big(\delta(s+1) + \delta(s-1) \Big) \tag{27}$$

and

$$p(c) = \begin{cases} 1 & \text{for } c \in [0,1] \\ 0 & \text{else} \end{cases} \tag{28}$$

Fig. 3 shows a Lévy flight with exponent $\mu = 1.5$ in two dimensions. As cut-off we use $r_0 = 0.1$. The qualitative differences between ordinary diffusion and super-diffusion with various exponents becomes well visible in the simulations. The Lévy flight type moving pattern of individuals, many local steps but the occasional long distance journey, has consequences for epidemic models of disease spreading in physical space.

4.3 Generalization of fractional Laplacians to higher dimensions

The generalization of the Laplace operator to higher dimensions is straight forward when considering the Fourier representation, hence

$$\mathcal{F}[(-\Delta)^{\mu/2} f](\underline{k}) := |\underline{k}|^{\mu} \cdot \tilde{f}(\underline{k}) \tag{29}$$

for $\underline{k} \in \mathbb{R}^n$. Then in real space via inverse Fourier transform we have the representation, for $\mu \in (0,1)$,

$$\left(-\Delta_{\underline{x}}\right)^{\mu/2} f(\underline{x}) = C_{\mu,n} \int \frac{f(\underline{y}) - f(\underline{x})}{|\underline{x} - \underline{y}|^{n+\mu}} \, d^n y \tag{30}$$

with constant

$$C_{\mu,n} = \frac{2^{-\mu}\pi^{1+n/2}}{\Gamma\left(1+\frac{\mu}{2}\right)\Gamma\left(\frac{n+\mu}{2}\right)\sin\left(\frac{\mu\pi}{2}\right)} \quad .$$

via inverse Fourier transform.

5 From stochastic epidemic models to reaction-diffusion processes

The SIS epidemics is an autocatalytic process given by the reaction scheme

$$\begin{aligned} S + I &\xrightarrow{\beta} I + I \\ I &\xrightarrow{\alpha} S \end{aligned}$$

and can be described via a master equation to capture the population noise of the epidemiological model (see [13] for a more detailed description of the SIS process).

The stochastic spatially extended SIS epidemic process on general lattice or network topologies is given by the following dynamics for the probability p of the state of a network

$$\begin{aligned} \frac{d}{dt} p(I_1, I_2, ..., I_N, t) &= \sum_{i=1}^{N} \beta \left(\sum_{j=1}^{N} J_{ij} I_j \right) I_i \;\; p(I_1, ..., 1 - I_i, ..., I_N, t) \\ &+ \sum_{i=1}^{N} \alpha (1 - I_i) \;\; p(I_1, ..., 1 - I_i, ..., I_N, t) \\ &- \sum_{i=1}^{N} \left[\beta \left(\sum_{j=1}^{N} J_{ij} I_j \right) (1 - I_i) + \alpha I_i \right] \;\; p(I_1, ..., I_i, ..., I_N, t) \end{aligned} \tag{31}$$

for variables $I_i \in \{0, 1\}$ and adjacency matrix (J_{ij}). Local quantities like the expectation value of infected at a single lattice point, which in reaction diffusion systems corresponds to the local density $u(x, t)$ are given by

$$\langle I_i \rangle (t) := \sum_{I_1=0}^{1} \sum_{I_2=0}^{1} ... \sum_{I_N=0}^{1} \;\; I_i \; p(I_1, I_2, ..., I_N, t) \quad . \tag{32}$$

For such quantities dynamics can be derived using the original dynamics of the stochastic process description for $p(I_1, I_2, ..., I_N, t)$. In such dynamics for local quantities there appears the discretized diffusion operator in the case of lattice models

$$\Delta \langle I_i \rangle := \sum_{j=1}^{N} \; J_{ij} (\langle I_j \rangle - \langle I_i \rangle) \tag{33}$$

and defines a generalized Laplace-operators for other network topologies, coded in the adjacency matrix (J_{ij}). Considering the local quantity $\langle I_i \rangle (t)$, which in a countinuous space model corresponds to the local density $u(x, t)$ with spatial variable x corresponding to i and lattice spacing a from our lattice model going to zero, we obtain

$$\frac{d}{dt} \langle I_i \rangle = \beta \sum_{j=1}^{N} \; J_{ij} \langle (1 - I_i) I_j \rangle - \alpha \langle I_i \rangle \quad . \tag{34}$$

Hence

$$\frac{d}{dt}\langle I_i\rangle = \beta\sum_{j=1}^{N} J_{ij}(\langle I_j\rangle - \langle I_i\rangle) + \beta\sum_{j=1}^{N} J_{ij}\langle I_i\rangle - \beta\sum_{j=1}^{N} J_{ij}\langle I_i I_j\rangle - \alpha\langle I_i\rangle \quad (35)$$

where we now use the discrete version of the diffusion operator $\Delta\langle I_i\rangle = \sum_{j=1}^{N} J_{ij}(\langle I_j\rangle - \langle I_i\rangle)$ for the first term of the sum on the right hand side of the equation. Further, in the term $-\beta\sum_{j=1}^{N} J_{ij}\langle I_i I_j\rangle$ we apply a local mean field assumption in the sense that local correlations can be neglected and coarse grained hence $\langle I_i I_j\rangle - \langle I_i\rangle\langle I_j\rangle \approx 0$ and $\langle I_i\rangle\langle I_j\rangle \approx \langle I_i\rangle\langle I_i\rangle$. Furthermore, we use $Q_i = \sum_{j=1}^{N} J_{ij}$ for the total number of neighbours of lattice site i, and in regular lattices $Q_i = Q$ as a single constant for the number of neighbours of any lattice site. Hence we finally obtain

$$\frac{d}{dt}\langle I_i\rangle = \beta Q\langle I_i\rangle\Big(1 - \langle I_i\rangle\Big) - \alpha\langle I_i\rangle + \beta\Delta\langle I_i\rangle \quad . \quad (36)$$

This is for lattice spacing going to zero, hence $u(x,t) = \langle I_i\rangle$ nothing but the Kolmogorov-Fisher equation in the form

$$\frac{\partial}{\partial t}\, u = r\, u\left(1 - \frac{u}{k}\right) + \chi\Delta u \quad (37)$$

where we identify the growth rate $r = \beta Q - \alpha$, the carrying capacity $k = \left(1 - \frac{\alpha}{\beta Q}\right)$ and diffusion constant $\chi = \beta$. Often the carrying capacity is simply set to unity, as well as the diffusion constant.

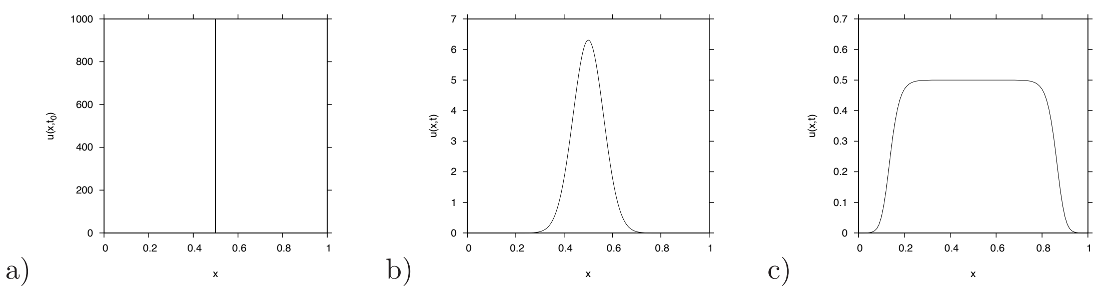

Figure 4: *Integration over the unit interval of ordinary diffusion. a) Initial state of our simulation is a delta function. b) Integration over the unit interval of ordinary diffusion. The final state after some integration time is a Gaussian. c) Same for the Kolmogorov-Fisher equation.*

5.1 First numeric results for reaction diffusion type spatial epidemics

For ordinary diffusion we use the usual discretization for the second derivative in space, hence

$$u_i(t+\Delta t) = u_i(t) + \Delta t\cdot\left(\chi\cdot\frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2}\right) \quad (38)$$

with diffusion constant $\chi = 0.1$. For Fig. 4 we use $\Delta x = 1000$, integration time $t_{max} = 0.02$ and resolution $r_t = 10000$, hence $\Delta t = 0.00002$. The initial δ-peak, Fig. 4 a), is given by zero on the whole unit interval and $1/\Delta x$ at the middle. Then the resulting Gaussian curve, Fig. 4 b), for the final state is invariant under changes of resolution in time and space. The Kolmogorov-Fisher equation shows for slow diffusion, $\chi = 0.0001$, a rapid convergence to the stationary state $u^* = 1 - \frac{\alpha}{\beta Q} = 0.5$, here for $\alpha = 1$ and $\beta Q = 2$ around the center, and a slowly moving diffusion front towards the boundaries. Integration time is $t_{max} = 20$. We then test the program numerically with the representation using the adjacency matrix J_{ij} as discribed in the epidemiological models, hence the Laplacian becomes

$$\frac{\partial^2}{\partial x^2} u_j = \sum_{\ell=1}^{N} J_{j\ell} \frac{1}{\left| \frac{\ell}{N} - \frac{j}{N} \right|^2} (u_\ell - u_j) \tag{39}$$

which gives the same analytics and numerics as the previously used form Eq. (38).

We now use the Fourier representation of a function $u(x,t)$ on the unit interval in discretized form with N discretization points, hence for $u_j(t)$

$$u_j = \sum_{f=1}^{N} \hat{u}_k \cdot e^{2\pi i \frac{j}{N} k} \tag{40}$$

with the Fourier transform

$$\hat{u}_k = \frac{1}{N} \sum_{j=1}^{N} u_j \cdot e^{-2\pi i \frac{j}{N} k} \tag{41}$$

where we have as relations between continuous and discretized version $x = \frac{j}{N}$ and $\Delta x = \frac{1}{N}$. Here Δx just is the difference in x, not to confuse with the Laplace operator Δu which is $\Delta u = \partial^2 u / \partial x^2$ in one dimension. As exact result we obtain using Fourier transformation and back transformation

$$\begin{aligned} \frac{\partial^2}{\partial x^2} u_j &:= \frac{1}{\Delta x^2} (u_{j-1} - 2u_j + u_{j+1}) \\ &= \sum_{\ell=1}^{N} u_\ell \, \frac{1}{N} \sum_{k=1}^{N} e^{2\pi i \frac{j-\ell}{N} k} \, \frac{1}{\Delta x^2} \cdot 2 \left(cos \left(2\pi \frac{k}{N} \right) - 1 \right) \end{aligned} \tag{42}$$

hence the form

$$\frac{\partial^2}{\partial x^2} u_j = \sum_{\ell=1}^{N} w_{j\ell} \cdot u_\ell \tag{43}$$

with $w_{j\ell}$ as specified above through the Fourier transform. We observe that due to 2π periodicity we have

$$2 \left(cos \left(2\pi \frac{k}{N} \right) - 1 \right) = 2 \left(cos \left(2\pi \frac{N-k}{N} \right) - 1 \right) \tag{44}$$

and for the left hand side of Eq. (44) the approximation

$$2\left(cos\left(2\pi\frac{k}{N}\right)-1\right)\approx-\left(2\pi\frac{k}{N}\right)^2 \tag{45}$$

for small values of k and

$$2\left(cos\left(2\pi\frac{N-k}{N}\right)-1\right)\approx-\left(2\pi\frac{N-k}{N}\right)^2 \tag{46}$$

for small $N-k$, hence large k. The power of 2 in Eqs. (42) to (46) gives the handel to generalize to other powers $\mu<2$ for the superdiffusive case.

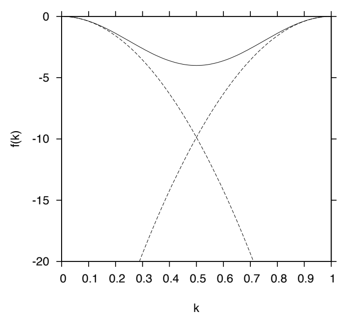

Figure 5: *Expression* $2\left(cos\left(2\pi\frac{k}{N}\right)-1\right)$ *and its quadratic approximations Eqs. (45) and (46).*

The exact result Eq. (42) gives good numerical results compared with Eq. (38), whereas the approximation using Eqs. (45) and (46) shows for moderate step size numerical instabilities due to the not well approximated intermediate part of the k spectrum, see Fig. 5. However, first numerical tests have shown that the exact result, Eq. (42), can be perturbed away from the quadratic power without large numerical errors. For larger perturbations $u(x,t)$ becomes slightly negative at the tails. Further analysis has to be performed on this topic. The description of the Laplacian in form Eq. (43) is in complete analogy to Eq. (39) and can be used to describe the epidemic process we investigate for extensions away from the ordinary diffusion case towards super-diffusion.

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