The modified Bessel K functions and the Fourier Transform of q-Gaussians

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Abstract –Here we show that the Fourier transform of the q-exponential Tsallis functions (also known as q-Gaussians) are generating time correlation functions based on the modified Bessel functions of the second kind. For the q parameter ranging from 2 to 1, we pass from a correlation which is an exponential decaying with time to a Gaussian-like behavior.

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The q-Gaussians, also known as "Tsallis functions", are probability distributions derived from the Tsallis statistics (Tsallis, 1988, 1995, Hanel et al., 2009). The q-Gaussians are based on a generalized form of the exponential function (see discussion in Sparavigna, 2022), characterized by a continuous parameter q in the range 1 < q < 3. As given by Umarov et al., 2008, the q-Gaussian is based on function $f(x) = Ce_q(-\beta x^2)$, where $e_q(.)$ is the q-exponential function and C a constant. The q-exponential has expression: $exp_q(u) = [1 + (1 - q)u]^{1/(1-q)}$. The function $f(x)$ possesses a bell-shaped profile, and, in the case that we have the peak at position x_o, the q-Gaussian is given as:

$$\text{q-Gaussian} = Cexp_q(-\beta(x - x_o)^2) = C[1 - (1 - q)\beta(x - x_o)^2]^{1/(1-q)} \quad (1)$$

Here we will consider (1) in the following form, with dimensionless variable w about $w_o = 0$:

$$\text{q-Gaussian} = Cexp_q(-w^2) = C[1 - (1 - q)w^2]^{1/(1-q)} \quad (2)$$

For q equal to 2, the q-Gaussian is the Cauchy-Lorentzian distribution (Naudts, 2009). For q close to 1, the q-Gaussian is a Gaussian. Consequently, for the q-parameter between 1 and 2, the shape of the q-Gaussian function is intermediate between the Gaussian and the Lorentzian profiles. Due to this feature, the q-Gaussians turn out to be suitable for being used as line shape in the Raman spectroscopy (see Sparavigna, 2023; for instance ChemRxiv1, ChemRxiv2, ChemRxiv3, ChemRxiv4, SSRN). In Zenodo, in discussing the time correlation functions related to Raman line profiles, we started using the Fourier transform of the q-Gaussians. Let us remember that the Fourier transform of a Lorentzian lineshape is producing a time correlation function which is an exponential decaying with time. In the case of the Gaussian lineshape, we have a correlation with is a Gaussian function of time. Being the q-Gaussian a lineshape which is intermediate between Lorentzian and Gaussian profiles, the related time correlation function must be intermediate between exponential and Gaussian functions.

Rodrigues and Giraldi, 2015, have considered in detail the Fourier transform of the q-Gaussian functions. Here we use a more phenomenological approach. Let us start from the link between the q-Gaussians and the Bessel functions.

In Wikipedia it is told that the "Bessel functions can be described as Fourier transforms of powers of quadratic functions". Function K_ν is a modified Bessel function of the second kind, order ν. For instance:

$$2\,K_0(\omega) = \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\sqrt{t^2+1}}\,dt.$$

To have further cases, we can use the on-line Fourier transform calculator, at https://www.wolframalpha.com . Following the notation in Wikipedia, we can find, for instance:

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}(1+(At)^2)^{-1/2}\,e^{iwt}dt = \frac{1}{\sqrt{A^2}}\cdot\sqrt{\frac{2}{\pi}}\cdot K_0\left(\frac{|w|}{\sqrt{A^2}}\right)$$

Note that, in this example, we can see evidenced the time/frequency scaling.

Here, in the following, let us consider some cases of Fourier transform (WolframAlpha) with exponent $-1/(q-1)$, that is $1/(1-q)$ as in (2). Let us consider the Fourier transform from the frequency domain *w* to the time domain *t* (dimensionless variables):

$$F_w\left[(1+w^2)^{-1/(q-1)}\right](t) = \frac{1}{\Gamma\left(\frac{1}{q-1}\right)}\cdot 2^{\frac{q-2}{q-1}}\cdot|t|^{\frac{1}{q-1}-\frac{1}{2}}\cdot K_{\frac{1}{q-1}-\frac{1}{2}}\big(t\,\mathrm{sgn}(t)\big)$$

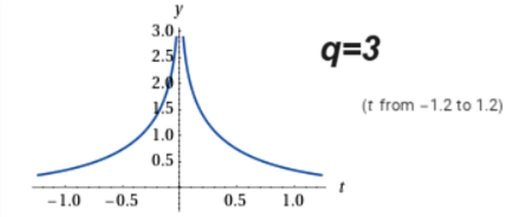
Posing $\xi = 1/(q-1)$:

$$F_w\left[(1+w^2)^{-\xi}\right](t) = \frac{1}{\Gamma(\xi)}\cdot 2^{(q-2)\xi}\cdot|t|^{\xi-\frac{1}{2}}\cdot K_{\xi-\frac{1}{2}}\big(t\,\mathrm{sgn}(t)\big)$$

To illustrate the behavior of the Fourier transform, let us consider different values of q, starting from q=3, including q=2 (Lorentzian), to find the corresponding time correlations (see Zenodo for discussion about time correlation in Raman spectroscopy). From WolframAlpha, we have:

$$F_w\left[(1+w^2)^{-1/(3-1)}\right](t) = \sqrt{\frac{2}{\pi}}K_0\big(t\,\mathrm{sgn}(t)\big)$$

By the way, the q-Gaussian is defined for q ranging from 1 to 3.



Fourier transform in the case q=3

$$F_w\left[(1+w^2)^{-1/(2.5-1)}\right](t) = 0.930437\cdot|t|^{0.166667}\cdot K_{0.166667}(t\,\mathrm{sgn}t) \quad \text{(b)}$$

$$F_w\left[(1+w^2)^{-1/(2-1)}\right](t) = \sqrt{\frac{\pi}{2}}e^{-|t|} \quad \text{(a) (Fourier transform of the Lorentzian function)}$$

$$F_w\left[(1+w^2)^{-1/(1.9999-1)}\right](t) = 0.999988\cdot|t|^{0.5001}\cdot K_{0.5001}(t\,\mathrm{sgn}t) \quad \text{(a')}$$

We can deduce that the exponential is equal to a K Bessel function multiplied by a square root, so that:$K_{0.5}(t\text{sgn}t) = \sqrt{\frac{\pi}{2}} \frac{1}{\sqrt{|t|}} e^{-|t|}$.

$F_w\left[(1+w^2)^{-1/(1.9-1)}\right](t) = 0.977728 \cdot |t|^{0.611111} \cdot K_{0.611111}(t\,\text{sgn}t)$ (b)

$F_w\left[(1+w^2)^{-1/(1.7-1)}\right](t) = 0.838525 \cdot |t|^{0.928571} \cdot K_{0.928571}(t\,\text{sgn}t)$ (c)

$F_w\left[(1+w^2)^{-1/(1.5-1)}\right](t) = \frac{0.626657}{t^2} \cdot e^{-|t|} \cdot |t|^2 \cdot (|t|+1) = 0.626657 \cdot e^{-|t|} \cdot (|t|+1)$ (d)

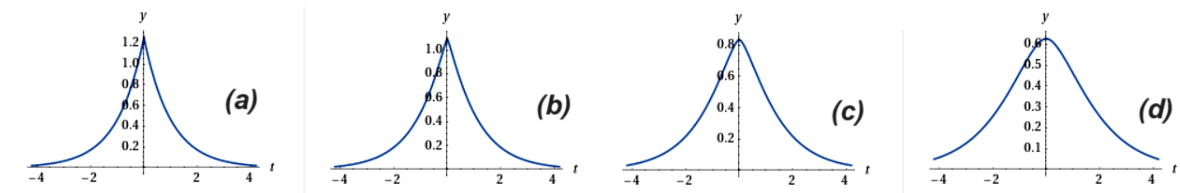
$F_w\left[(1+w^2)^{-1/(1.4999-1)}\right](t) = 0.499777 \cdot |t|^{1.5} \cdot K_{1.5}(t\,\text{sgn}t)$

We have, as given by WoframAlpha, that: $K_{1.5}(t) = \frac{1.253314137}{\sqrt{t}} \cdot e^{(-t)} \cdot \left(\frac{1}{t}+1\right)$, and therefore (d).

$F_w\left[(1+w^2)^{-1/(1.4-1)}\right](t) = 0.265962 \cdot |t|^2 \cdot K_2(t\,\text{sgn}t)$

$F_w\left[(1+w^2)^{-1/(1.3-1)}\right](t) = 0.0714233 \cdot |t|^{2.83333} \cdot K_{2.83333}(t\,\text{sgn}t)$

$F_w\left[(1+w^2)^{-1/(1.15-1)}\right](t) = 0.000050 \cdot |t|^{6.16667} \cdot K_{6.16667}(t\,\text{sgn}t)$



Fourier transforms of four cases given above.

Let us add some further screenshots.

$$\mathcal{F}_w\left[(1+w^2)^{-1/(1.25-1)}\right](t) = \frac{1}{t^4\,\text{sgn}(t)^4} |t|^{3.5} e^{-t\,\text{sgn}(t)} \sqrt{t\,\text{sgn}(t)} \left(0.0261107\,t^3\,\text{sgn}(t)^3 + 0.156664\,t^2\,\text{sgn}(t)^2 + 0.391661\,t\,\text{sgn}(t) + 0.391661\right)$$

$$\mathcal{F}_w\left[(1+w^2)^{-1/(1.2-1)}\right](t) = \frac{1}{t^5\,\text{sgn}(t)^5} |t|^{4.5} e^{-t\,\text{sgn}(t)} \sqrt{t\,\text{sgn}(t)} \left(0.00326384\,t^4\,\text{sgn}(t)^4 + 0.0326384\,t^3\,\text{sgn}(t)^3 + 0.146873\,t^2\,\text{sgn}(t)^2 + 0.342703\,t\,\text{sgn}(t) + 0.342703\right)$$

$$\mathcal{F}_w\left[(1+w^2)^{-1/(1.125-1)}\right](t) = \frac{1}{t^8\,\text{sgn}(t)^8} |t|^{7.5} e^{-t\,\text{sgn}(t)} \sqrt{t\,\text{sgn}(t)} \left(1.94276\times 10^{-6}\,t^7\,\text{sgn}(t)^7 + 0.0000543973\,t^6\,\text{sgn}(t)^6 + 0.000734364\,t^5\,\text{sgn}(t)^5 + 0.0061197\,t^4\,\text{sgn}(t)^4 + 0.0336583\,t^3\,\text{sgn}(t)^3 + 0.12117\,t^2\,\text{sgn}(t)^2 + 0.262535\,t\,\text{sgn}(t) + 0.262535\right)$$

Using the results given above and considering the scaling $(q-1)w^2$ into $t/\sqrt{(q-1)}$, we can plot some time correlations as in the Figure 1 and Figure 2 (semi logarithmic scale).

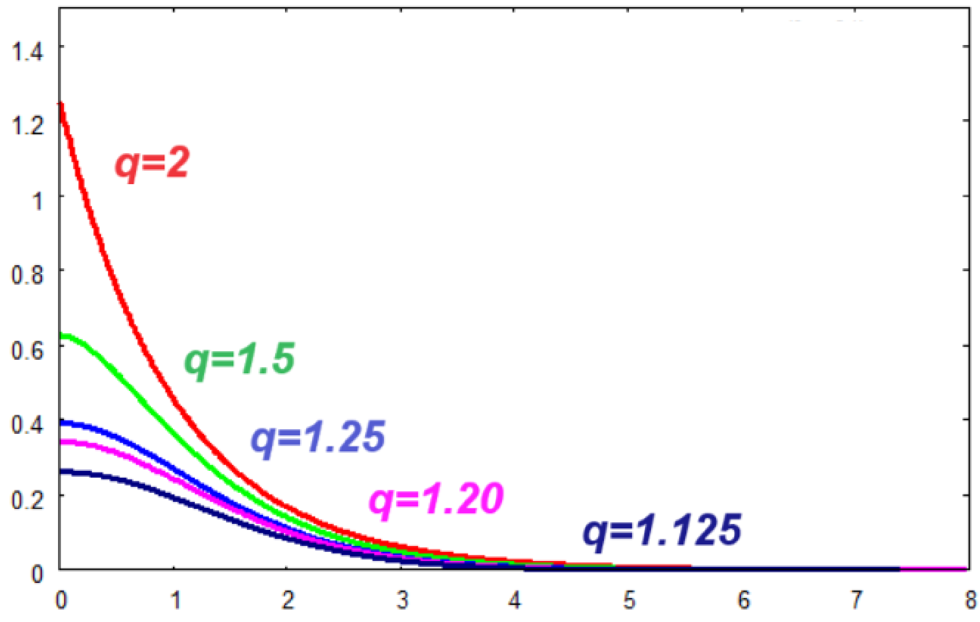


Figure 1: Fourier transforms of some q-Gaussians as given by WolframAlpha, for some values of the q parameter.

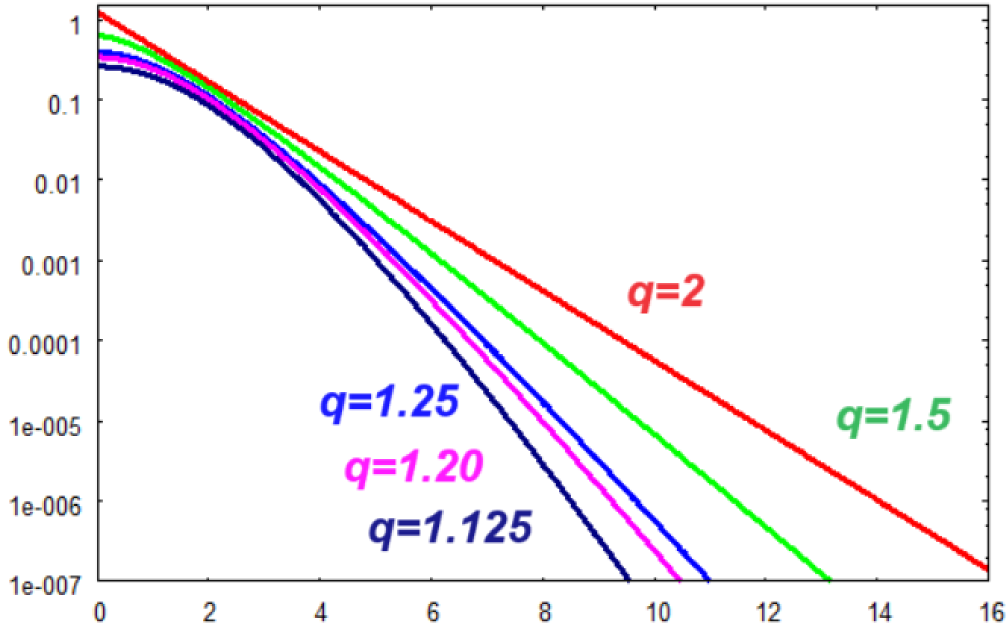


Figure 2: The same as in the Figure 1, in semi-logarithmic scale. For q=2, we have a correlation which is an exponential function (straight red line). For q closer to 1, the curve is Gaussian-like (parabolic behavior in the semi-log plot).

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