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Non-extensive diffusion as nonlinear response

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Abstract. – The porous-media equation has been proposed as a phenomenological "non-extensive" generalization of classical diffusion. Here, we show that a very similar equation can be derived, in a systematic manner, for a classical fluid by assuming nonlinear response, *i.e.* that the diffusive flux depends on gradients of a power of the concentration. The present equation distinguishes from the porous-media equation in that it describes *generalized classical* diffusion, *i.e.* with $r/\sqrt{Dt}$ scaling, but with a generalized Einstein relation, and with power-law probability distributions typical of non-extensive statistical mechanics.

One of the characteristic features of the non-extensive thermodynamics introduced by Tsallis is the appearance of non-exponential distribution functions with power law tails [1, 2]. There has been considerable interest recently in the question of how such non-exponential distributions might arise from first-principle considerations [3–6]. In this paper, we show that it is possible to obtain, in a generic manner, power law distributions for the diffusion of a tracer particle in a liquid by assuming a simple generalization of the usual linear-response arguments.

In classical diffusion, the probability to find the diffuser at point $\overrightarrow{r}$ at time t given that it starts at point $\overrightarrow{r}_0$ at time 0 obeys the diffusion equation

$$\frac{\partial}{\partial t}P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)=-\frac{\partial}{\partial\overrightarrow{r}}\cdot\overrightarrow{u}\left(\overrightarrow{r},t\right)P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)+\frac{\partial}{\partial\overrightarrow{r}}\cdot\overleftrightarrow{D}\cdot\frac{\partial}{\partial\overrightarrow{r}}P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)\,, \quad (1)$$

where $\overrightarrow{u}(\overrightarrow{r},t)$ is the drift and $\overleftrightarrow{D}$ the diffusion tensor, see, *e.g.*, [7]. Note that, in general, we could, instead of probabilities, speak of the concentration of a diffusing species or the density of a single-component system undergoing self-diffusion just as well. There are currently two widely explored generalizations of this classical diffusion equation. The first involves the appearance of fractional derivatives in the diffusion equation [8, 9]. These generalizations can be derived, *e.g.*, by considering a random walker with either long-tailed waiting times (giving rise to a fractional time derivative) or long-tailed jump-length distributions leading

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to fractional space derivates and known as a Levy flight [8, 9]. A second generalization of the classical diffusion equation sometimes used to model anomalous diffusion is the so-called porous-media equation

$$\frac{\partial}{\partial t}P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)=-\frac{\partial}{\partial\overrightarrow{r}}\cdot\overrightarrow{u}\left(\overrightarrow{r},t\right)P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)+\frac{\partial}{\partial\overrightarrow{r}}\cdot\overleftrightarrow{D}\cdot\frac{\partial}{\partial\overrightarrow{r}}P^{\mu}\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right). \quad (2)$$

As its name indicates, this equation was established for particular physical systems [10], but it has also been proposed as a phenomenological "non-extensive" extension of classical diffusion [11, 12]. In one dimension and in the absence of drift, $\overrightarrow{u}(\overrightarrow{r},t)=0$, this equation admits of power law solutions of the form

$$P\left(r,t;0,0\right)=A\,t^{-\frac{1}{\mu+1}}\left(1+A^{1-\mu}\frac{1-\mu}{\mu\left(\mu+1\right)}\frac{r^2t^{-\frac{2}{\mu+1}}}{2D}\right)^{\frac{1}{\mu-1}}, \quad (3)$$

where the constant A is fixed by normalization. This function can be written more suggestively as

$$P\left(r,t;0,0\right)=A\,t^{-\frac{1}{\mu+1}}\,e_{2-\mu}\left(-A^{1-\mu}\frac{1}{\mu\left(\mu+1\right)}\frac{r^2t^{-\frac{2}{\mu+1}}}{2D}\right), \quad (4)$$

where the so-called q-exponential is defined by

$$e_q\left(x\right)=\left(1+\left(1-q\right)x\right)^{\frac{1}{1-q}}, \quad (5)$$

which has the property that $\lim_{q\to1}e_q(x)=e^x$. Note that for $q<1$, one restricts the domain to $1+(1-q)x>0$ and assumes that $e_q(x)=0$ otherwise. For this reason, the exponents are generally unconstrained although one expects that $\mu>0$ so as to avoid singularities.

Notice that eq. (2) can be viewed as a classical diffusion equation with the effective diffusion coefficient $\mu\overleftrightarrow{D}P^{\mu-1}(\overrightarrow{r},t;\overrightarrow{r}_0,0)$. Since concentration-dependent and density-dependent diffusion coefficients are commonly used in the scientific literature, this does not differ radically from classical diffusion: what is unusual is that the effective diffusion coefficient vanishes when the probability (or concentration) vanishes.

We consider here a collection of atoms moving under Newtonian dynamics and concentrate on describing the probability of finding a tagged particle, say the 0th particle, at position $\overrightarrow{r}$ at time t given it begins at position $\overrightarrow{r}_0$ at time $t=0$,

$$P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)=\left\langle\delta\left(\overrightarrow{q}\left(t\right)-\overrightarrow{r}\right)\delta\left(\overrightarrow{q}\left(0\right)-\overrightarrow{r}_0\right)\right\rangle_0, \quad (6)$$

where the position of the tagged particle is $\overrightarrow{q}(t)$ and the notation $\langle\ldots\rangle_0$ indicates an ensemble average over some distribution of initial conditions for the other, non-tagged, particles. Differentiation of eq. (6) with respect to time leads to the exact equation

$$\frac{\partial}{\partial t}P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)=-\frac{\partial}{\partial\overrightarrow{r}}\cdot\overrightarrow{u}\left(\overrightarrow{r},t\right)P\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)+\frac{\partial}{\partial\overrightarrow{r}}\cdot\overrightarrow{J}, \quad (7)$$

with the current

$$\overrightarrow{J}\left(\overrightarrow{r},t;\overrightarrow{r}_0,0\right)=-\left\langle\overrightarrow{v}'\left(t\right)\delta\left(\overrightarrow{q}\left(t\right)-\overrightarrow{r}\right)\delta\left(\overrightarrow{q}\left(0\right)-\overrightarrow{r}_0\right)\right\rangle_0, \quad (8)$$

where $\overrightarrow{u}(\overrightarrow{r},t)$ is the average macroscopic velocity, $\overrightarrow{v}(t)$ is the instantaneous velocity of the tagged particle and its peculiar velocity is $\overrightarrow{v}'(t)=\overrightarrow{v}(t)-\overrightarrow{u}(\overrightarrow{r},t)$. The idea of linear-response theory is that, aside from convection and in the absence of driving forces or boundary conditions, the distribution should relax toward a uniform distribution. Hence, one expects the current to be proportional, in some sense, to gradients of the distribution and indeed the simplest assumption that $\vec{J} \propto \vec{\nabla} P$ gives the usual phenomenological Fick's law. Higher-order terms are expected to involve higher-order gradients. Such an expansion is most easily developed in Fourier space by noting that the Fourier transform of the current and the distribution are

$$\begin{aligned} \widetilde{\vec{J}}\left(\vec{k}, t; \vec{r}_0, 0\right) &= -\left\langle \vec{v}'(t) \exp\left[i\vec{k}\cdot\vec{q}(t)\right] \delta\left(\vec{q}(0) - \vec{r}_0\right)\right\rangle_0, \quad (9)\\ \widetilde{P}\left(\vec{k}, t; \vec{r}_0, 0\right) &= \left\langle \exp\left[i\vec{k}\cdot\vec{q}(t)\right] \delta\left(\vec{q}(0) - \vec{r}_0\right)\right\rangle_0, \quad (10) \end{aligned}$$

and expanding their ratio to get a series of the form

$$\widetilde{\vec{J}}/\widetilde{P} = -i\vec{k}\cdot\overleftrightarrow{D}(t) + \ldots\ , \quad (11)$$

thus giving the desired gradient expansion [13]. In general, the diffusion coefficient, which is given by an Einstein relation, is time dependent on microscopic time scales characterized by the time between atomic collisions but in the long-time limit appropriate to hydrodynamics it tends toward a constant value.

Comparison of eqs. (2) and (7) suggests that the key assumption in the use of the generalized diffusion equation is that the current is no longer most simply described by gradients in the distribution function, but rather by gradients in the distribution raised to some power. In order to generalize the linear-response argument, we proceed by defining the Fourier transform of the μ-th power of the distribution to be

$$\widetilde{P}_\mu\left(\vec{k}, t; \vec{r}_0, 0\right) = \int \mathrm{d}\vec{r}\ \exp\left[i\vec{k}\cdot\vec{r}\right] P^\mu\left(\vec{r}, t; \vec{r}_0, 0\right), \quad (12)$$

and expand in the wave vector to obtain

$$\widetilde{\vec{J}}/\widetilde{P}_\mu = -i\vec{k}\cdot\overleftrightarrow{D}_\mu + \ldots\ , \quad (13)$$

which gives

$$\begin{aligned} \overleftrightarrow{D}_\mu(t) &= \left\langle \vec{q}(t)\,\vec{v}'(t)\,\delta\left(\vec{q}(0) - \vec{r}_0\right)\right\rangle_0 \Big/ \int \mathrm{d}\vec{r}\ P^\mu\left(\vec{r}, t; \vec{r}_0, 0\right)\\ &= \overleftrightarrow{D}_1(t) \Big/ \int \mathrm{d}\vec{r}\ P^\mu\left(\vec{r}, t; \vec{r}_0, 0\right), \quad (14) \end{aligned}$$

where $\overleftrightarrow{D}_1(t)$ is the classical diffusion coefficient which is the same as that occurring in eq. (11). Note that by expressing $\vec{q}(t)$ in terms of the time-integral of the velocity, the diffusion coefficient becomes a function of the velocity auto-correlation function as expected,

$$\overleftrightarrow{D}_\mu(t) = \int_0^t \left\langle \vec{v}(t')\,\vec{v}'(t)\,\delta\left(\vec{q}(0) - \vec{r}_0\right)\right\rangle_0 \mathrm{d}t' \Big/ \int \mathrm{d}\vec{r}\ P^\mu\left(\vec{r}, t; \vec{r}_0, 0\right). \quad (15)$$

Then, keeping only the lowest order in (13), we obtain the generalized advection-diffusion equation

$$\frac{\partial}{\partial t} P\left(\vec{r}, t; \vec{r}_0, 0\right) = -\frac{\partial}{\partial \vec{r}}\cdot\vec{u}\left(\vec{r}, t\right) P\left(\vec{r}, t; \vec{r}_0, 0\right) + \frac{\partial}{\partial \vec{r}}\cdot\overleftrightarrow{D}_\mu(t)\cdot\frac{\partial}{\partial \vec{r}} P^\mu\left(\vec{r}, t; \vec{r}_0, 0\right), \quad (16)$$

with a generalized Einstein relation, eq. (15), relating the diffusion coefficient to the underlying microscopic dynamics and corresponding distribution function. Note that even on hydrodynamic time scales, for which $\overleftrightarrow{D}_1(t)$ can be replaced by $\overleftrightarrow{D}_1 = \lim_{t\to\infty} \overleftrightarrow{D}_1(t)$, $\overleftrightarrow{D}_\mu(t)$ remains time dependent due to its dependence on $P^\mu(\overrightarrow{r}, t; \overrightarrow{r}_0, 0)$. We have no proof that distributions evolving under this equation remain positive definite, but it will be shown below that in the absence of drift, solutions to eq. (16) are closely related to those of the original porous-media equation so that if the latter are positive-definite, then so are the former.

Scaling solutions of eq. (16) in the absence of drift ($\overrightarrow{u} = 0$) are easily examined. For simplicity, consider the approximation, expected to be valid on hydrodynamic time scales, $\overleftrightarrow{D}_1(t) \sim \lim_{t\to\infty} \overleftrightarrow{D}_1(t) \equiv \overleftrightarrow{D}_1$, and suppose that in d-dimensions the distribution assumes the form $P(\overrightarrow{r}, t; \overrightarrow{r}_0, 0) = t^{-da} F(r/t^a)$ for some exponent a (note that the prefactor is dictated by normalization). Then, one has

$$\begin{aligned}\int \mathrm{d}\overrightarrow{r}\; P^\mu\left(\overrightarrow{r}, t; \overrightarrow{r}_0, 0\right) &= \int \mathrm{d}\overrightarrow{r}\; t^{-d\mu a} F^\mu(r/t^a) \\ &= S_d t^{-d(\mu-1)a} \int_0^\infty F^\mu(x) x^{d-1}\,\mathrm{d}x\,,\end{aligned} \tag{17}$$

with $x \equiv t^{-a}|\overrightarrow{r}|$ and where S_d is the area of the d-dimensional hypersphere. The generalized diffusion coefficient is then

$$\overleftrightarrow{D}_\mu(t) = t^{d(\mu-1)a} \overleftrightarrow{D}'_\mu\,, \tag{18}$$

where

$$\overleftrightarrow{D}'_\mu \equiv \left(S_d \int_0^\infty F^\mu(x) x^{d-1}\,\mathrm{d}x\right)^{-1} \overleftrightarrow{D}_1 \tag{19}$$

is a time-independent coefficient. Substitution into eq. (16) gives, after simplification,

$$-a t^{-da-1}\left[dF(x) + xF'(x)\right] = t^{-a(d+2)} \frac{\partial}{\partial \overrightarrow{x}} \cdot \overleftrightarrow{D}'_\mu \cdot \frac{\partial}{\partial \overrightarrow{x}} F^\mu(x)\,, \tag{20}$$

which is only valid for $a = \frac{1}{2}$. The generalized diffusion equation given here therefore describes ordinary diffusion when there is no drift. However, the distributions are not Gaussian. For example, in one dimension the scaling equation becomes

$$-\frac{1}{2}F(x) - \frac{1}{2}x\frac{\mathrm{d}}{\mathrm{d}x}F(x) = D'_\mu \frac{\mathrm{d}^2}{\mathrm{d}x^2} F^\mu(x)\,, \tag{21}$$

which is again solved by the canonical q-exponential form as

$$F(x) = Ae_{2-\mu}\left(-\frac{A^{1-\mu}}{2\mu(\mu+1)D'_\mu}x^2\right), \tag{22}$$

or, with $\mu = 2-q$,

$$P(r,t;0,0) = A\,t^{-1/2}\left(1 - (1-q)\frac{A^{q-1}}{(2-q)(3-q)}\frac{r^2}{2D'_\mu t}\right)^{\frac{1}{1-q}}. \tag{23}$$

The mean-squared displacement is then obtained straightforwardly from (23); with $r^* = r/\sqrt{D'_\mu t}$, one has

$$\begin{aligned}\langle r^2(t)\rangle &= \int_0^\infty \mathrm{d}r\, r^2\, P(r,t;0,0) \\ &= D'_\mu t \int_0^\infty \mathrm{d}r^*\, r^{*2} A\left(1 - (1-q)\frac{A^{q-1}}{(2-q)(3-q)}\frac{r^{*2}}{2}\right)^{\frac{1}{1-q}}.\end{aligned} \tag{24}$$

Thus, in the absence of drift, eq. (16) describes normal diffusion in the sense that the mean-squared displacement grows linearly with time, but it generalizes classical diffusion as the distribution (23) takes on the form typical of non-extensive systems.

Although eq. (16) is formally the same as eq. (2), there is an additional self-consistency implied by the Einstein relation (15) which raises the question as to whether or not these descriptions can be regarded in any sense as being the same. In some cases they are, because eq. (16) is of first order in time so that any time dependence generated by the self-consistency can be hidden by a non-linear change in the time variable. For example, in the absence of drift, let $Q(\overrightarrow{r}, s; \overrightarrow{r}_0, 0)$ be a solution to eq. (2), written with the variable s instead of t, and having initial condition $P(\overrightarrow{r}, 0; \overrightarrow{r}_0, 0)$. Then it is easy to see that the solution of eq. (16) is $P(\overrightarrow{r}, t; \overrightarrow{r}_0, 0) = Q(\overrightarrow{r}, s(t); \overrightarrow{r}_0, 0)$ where the time variables are related by the implicit equation

$$t\left(s\right) = \int_0^s \left(\int \mathrm{d}\overrightarrow{r}\; Q^{\mu}\left(\overrightarrow{r}, \sigma; \overrightarrow{r}_0, 0\right)\right) \mathrm{d}\sigma. \tag{25}$$

To illustrate this, consider again the case of one-dimensional diffusion with no drift term. The solution of the porous media equation (2) is given by (3) which, with the replacement $t \to s$, is what is called here Q. Substitution into eq. (25) gives

$$t\left(s\right) = \int_0^s \left(\int \mathrm{d}\overrightarrow{r}\; Q^{\mu}\left(\overrightarrow{r}, \sigma; \overrightarrow{r}_0, 0\right)\right) \mathrm{d}\sigma = C s^{\frac{2}{\mu+1}}\,, \tag{26}$$

for some constant C, thus recovering eq. (22).

It is interesting that eq. (16) is very similar to the equation recently derived by Abe and Thurner [6], where the derivation begins with the classical picture based on a random walker which jumps from position $r + \Delta$ at time t to position r at time $t + \tau$ with a jump probability $\phi(\Delta) = \phi(-\Delta)$, so that the probability that the walker be at r at time $t + \tau$ is given by

$$P\left(r, t + \tau\right) = \int P\left(r + \Delta, t\right) \phi\left(\Delta\right)\, \mathrm{d}\Delta. \tag{27}$$

They consider the more general case in which the probability $P(r, t)$ occurring in the integral is replaced by the so-called escort probability [14]

$$F\left(r, t\right) = \frac{P^{\nu}\left(r, t\right)}{\int P^{\nu}\left(r, t\right) \mathrm{d}r}\,, \tag{28}$$

with the result that the diffusion equation becomes

$$\frac{\partial}{\partial t} P\left(r, t\right) = D_{\nu}\left(t\right) \frac{\partial^2}{\partial r^2} P^{\nu}\left(\overrightarrow{r}, t\right) + \frac{1}{\tau}\left(F\left(r, t\right) - P\left(\overrightarrow{r}, t\right)\right) \tag{29}$$

with $D_{\nu}(t)$ defined as in eq. (15). This result (29) is somewhat difficult to interpret as its derivation involves taking the limit $\tau \to 0$ in which case the second term on the right is problematic. Nevertheless, the result is strikingly similar to our nonlinear-response result including the definition of the time-dependent diffusion coefficient.

In this paper, we have developed a method whereby a standard derivation yields typically non-extensive expressions by generalizing a key ansatz, *i.e.* a generalization of standard linear-response arguments which gives rise to a q-diffusion equation including a generalization of the Einstein relation for the diffusion coefficient. The equation is similar in structure to the porous-media equation but with the important difference that the diffusion coefficient depends on the solution of the equation which leads to the fact that, in the absence of drift, the diffusion process is classical with mean-squared displacement increasing linearly with time. Nevertheless, the new q-diffusion equation admits of the now well-known q -exponential distribution which is often postulated as a description of nonequilibrium systems. Comparison of our results with the similar results of Abe and Thurner indicates how "nonextensive" expressions can arise without the explicit introduction of escort probabilities.

REFERENCES

[1] Swinney H. L. and Tsallis C. (Editors), *Anomalous Distributions, Nonlinear Dynamics, Nonextensivity*, *Physica D*, **193** (2004) 1-356.
[2] Gell-mann M. and Tsallis C. (Editors), *Nonextensive Entropy - Interdisciplinary Applications* (Oxford University Press, New York) 2004.
[3] Tsallis C., *Physica D*, **193** (2004) 3.
[4] Beck C. and Cohen E. D. G., *Physica A*, **321** (2003) 267.
[5] Hanel R. and Thurner S., *Physica A*, **351** (2005) 260.
[6] Abe S. and Thurner S., *Anomalous diffusion in view of Einstein's 1905 theory of Brownian motion*, to be published in *Physica A* (2005).
[7] Boon J. and Yip S., *Molecular Hydrodynamics* (Dover, New York) 1991.
[8] Metzler R. and Klafter J., *Phys. Rep.*, **339** (2000) 1.
[9] Metzler R. and Klafter J., *J. Phys. A*, **37** (2004) R167.
[10] Muskat M., *The Flow of Homogeneous Fluids through Porous Media* (McGraw-Hill, New York) 1937.
[11] Plastino A. R. and Plastino A., *Physica A*, **222** (1995) 347.
[12] Tsallis C. and Bukman D. J., *Phys. Rev. E*, **54** (1996) R2197.
[13] Dufty J. W., *Phys. Rev. A*, **30** (1984) 1465.
[14] Beck C. and Schlogl F., *Thermodynamics of Chaotic Systems* (Cambridge University Press, Cambridge) 1993, Chapt. 9.