Physical Properties in the Absence of Thermal Noise: Effective Temperature in Nonextensive Statistical Mechanics

F.D. Nobre, E.M.F. Curado
CBPF - Brazil

A.M.C. Souza
UFS - Brazil

- Nonlinear Fokker-Planck Equation:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial\{A(x)\Psi[P(x,t)]\}}{\partial x} + \frac{\partial}{\partial x}\left\{\Omega[P(x,t)]\frac{\partial P(x,t)}{\partial x}\right\}$$

$\Psi[P(x,t)]$ and $\Omega[P(x,t)]$: positive, finite, integrable, differentiable (at least once)

$$A(x) = -d\phi(x)/dx$$

$$P(x,t)|_{x\to\pm\infty} = 0\ ;\ \left.\frac{\partial P(x,t)}{\partial x}\right|_{x\to\pm\infty} = 0\ ;\ A(x)\Psi[P(x,t)]|_{x\to\pm\infty} = 0\ (\forall t)$$

- H-Theorem and Nonlinear FP Equation:

$$S[P] = \int_{-\infty}^{\infty} dx \; g[P(x,t)] \; ; \; g(0) = g(1) = 0 \; ; \; \frac{d^2 g}{dP^2} \leq 0$$

$$F = U - \gamma S \; ; \quad U = \int_{-\infty}^{\infty} dx \; \phi(x) P(x,t)$$

- Condition for the H-Theorem:

$$-\gamma \; \frac{d^2 g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]}$$

- Examples of FPEs and Associated Entropies

a) FPE Associated with BG Entropy

$$\Psi[P(x,t)] = P(x,t) \ ; \quad \Omega[P(x,t)] = D \ (\text{constant})$$

$$\frac{dg}{dP} = -\frac{D}{T}\ln P + C \quad \Rightarrow \quad g[P] = -k_{\mathrm{B}}\, P \ln P$$

b) FPE Associated with Tsallis Entropy

A.R. Plastino and A. Plastino (1995)

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial[A(x)P(x,t)]}{\partial x} + D\mu\frac{\partial}{\partial x}\left\{[P(x,t)]^{\mu-1}\frac{\partial P(x,t)}{\partial x}\right\}$$

$$\Psi[P(x,t)] = P(x,t) \; ; \quad \Omega[P(x,t)] = D\mu[P(x,t)]^{\mu-1}$$

$$g[P] = -\frac{D}{\gamma}\,\frac{P^\mu}{\mu-1} + CP \quad \Rightarrow \quad g[P] = k\,\frac{P-P^\mu}{\mu-1}$$

$$(k = D/\gamma)$$

$$P(x,t) = B(t)[1+\beta(t)(1-\mu)x^2]_+^{1/(\mu-1)}$$

PRL 105, 260601 (2010) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2010

Thermostatistics of Overdamped Motion of Interacting Particles

J. S. Andrade, Jr.,[1,3] G. F. T. da Silva,[1] A. A. Moreira,[1] F. D. Nobre,[2,3] and E. M. F. Curado[2,3]

[1]*Departamento de Física, Universidade Federal do Ceará, 60451-970 Fortaleza, Ceará, Brazil*

[2]*Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, 22290-180, Rio de Janeiro-RJ, Brazil*

[3]*National Institute of Science and Technology for Complex Systems, Rua Xavier Sigaud 150, 22290-180, Rio de Janeiro-RJ, Brazil*

(Received 8 August 2010; published 22 December 2010)

We show through a nonlinear Fokker-Planck formalism, and confirm by molecular dynamics simulations, that the overdamped motion of interacting particles at $T = 0$, where T is the temperature of a thermal bath connected to the system, can be directly associated with Tsallis thermostatistics. For sufficiently high values of T, the distribution of particles becomes Gaussian, so that the classical Boltzmann-Gibbs behavior is recovered. For intermediate temperatures of the thermal bath, the system displays a mixed behavior that follows a novel type of thermostatistics, where the entropy is given by a linear combination of Tsallis and Boltzmann-Gibbs entropies.

DOI: 10.1103/PhysRevLett.105.260601 PACS numbers: 05.10.Gg, 05.20.−y, 05.40.Fb, 05.45.−a

- Physical system: interacting particles under overdamped motion

- Disordered type-II superconductors

➡ interacting overdamped vortices

$$\eta \mathbf{v}_i = \mathbf{F}_i^{\mathrm{pp}} + \mathbf{F}_i^{\mathrm{ext}} \qquad (i = 1, 2, \cdots, N)$$

$$\mathbf{F}_i^{\mathrm{pp}} = \frac{1}{2} \sum_{j \neq i} B^{\mathrm{pp}}(r_{ij})\ \hat{\mathbf{r}}_{ij}\ ; \quad B^{\mathrm{pp}}(r_{ij}) = f_0 K_1(r_{ij}/\lambda)$$

- Introducing uncorrelated thermal noise:

$$\eta \mathbf{v}_i = \mathbf{F}_i^{\mathrm{pp}} + \mathbf{F}_i^{\mathrm{ext}} + \mathbf{F}_i^{\mathrm{th}} \qquad (i = 1, 2, \cdots, N)$$

$$\langle \mathbf{F}_i^{\mathrm{th}}(t) \rangle = 0 \; ; \qquad \langle \mathbf{F}_i^{\mathrm{th}}(t) \cdot \mathbf{F}_i^{\mathrm{th}}(t') \rangle = 2 k_B T \eta \; \delta(t - t')$$

$$\frac{\partial P(x,t)}{\partial t} = \ldots \; + k_{\mathrm{B}} T \; \frac{\partial^2 P(x,t)}{\partial x^2}$$

- The following analysis $\longrightarrow$ T=0

- Coarse graining $\Rightarrow$ density $\rho(\mathbf{r}, t)$

$$\rho(\mathbf{r}, t) \approx \rho(0, t) + \mathbf{r} \cdot \nabla \rho(\mathbf{r}, t)$$

$$\mathbf{F}^{\mathrm{pp}} = \frac{1}{2} \int d^2 r \, \rho(\mathbf{r}, t) B^{\mathrm{pp}}(r) \hat{\mathbf{r}} \approx a \nabla \rho(\mathbf{r}, t)$$

$$a = \pi \int_0^\infty dr \; r^2 B^{\mathrm{pp}}(r) = 2\pi f_0 \lambda^3$$

- For simplicity: $\rho(\mathbf{r}, t) \equiv \rho(x, y, t) \quad (d = 2)$

- Using continuity equation with:

$$\mathbf{J} = \rho \mathbf{v} \quad \text{and} \quad \mathbf{F}^{\text{ext}} = -A(x)\hat{\mathbf{x}}$$

$$\eta \frac{\partial \rho(\mathbf{r},t)}{\partial t} = \nabla \cdot \left\{ \rho(\mathbf{r},t) \left[a \nabla \rho(\mathbf{r},t) + \mathbf{F}^{\text{ext}} \right] \right\}$$

$$= \frac{\partial}{\partial x} \left\{ \rho(\mathbf{r},t) \left[a \, \frac{\partial \rho(\mathbf{r},t)}{\partial x} - A(x) \right] \right\}$$

- For fixed y $\rightarrow$ introduce P(x,t) ($\eta = 1$):

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial [A(x)P(x,t)]}{\partial x} + 2D\frac{\partial}{\partial x}\left\{P(x,t)\frac{\partial P(x,t)}{\partial x}\right\}$$

$$D = k\gamma = \lim_{N,L_y\to\infty}\frac{N\pi f_0\lambda^2}{L_y} = n\pi f_0\lambda^2$$

γ $\rightarrow$ Effective Temperature

- From now on: $A(x) = -\alpha x \qquad (\alpha > 0)$

- Entropy: $S[P] = k\{1 - \int_{-\infty}^{\infty} dx\ [P(x,t)]^2\ \}$

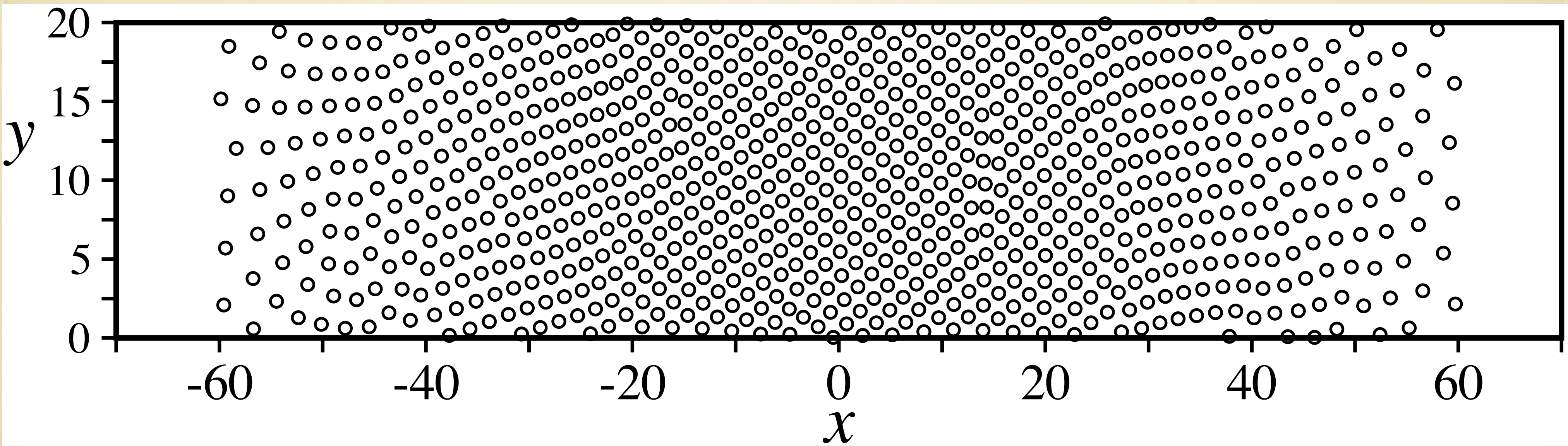
$$P(x,t) = B(t)[1 - \beta(t)x^2]_+$$

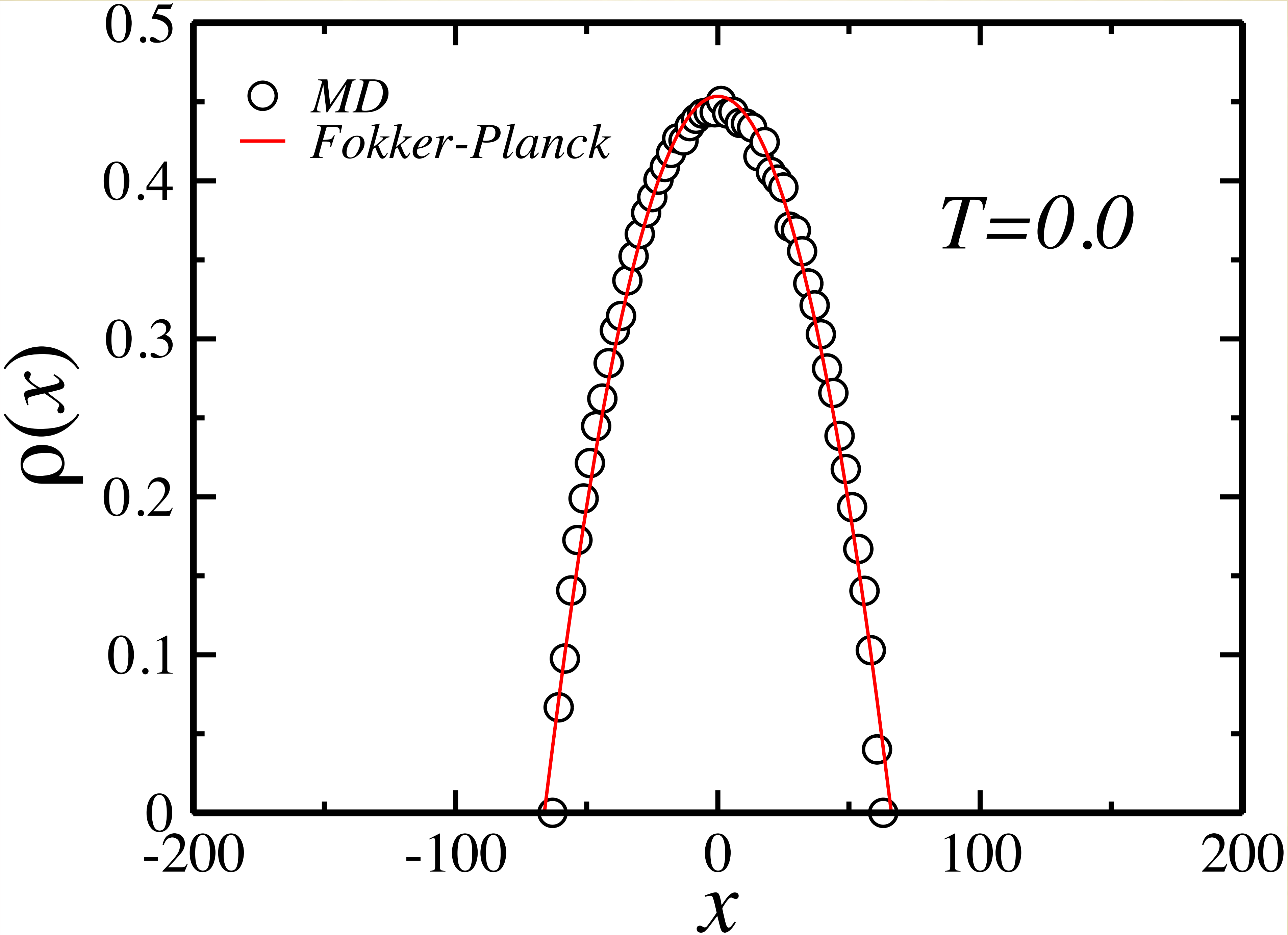
- Molecular Dynamics Simulations (2d):

$$L_x = 100\lambda \ ; \quad L_y = 20\lambda \ \text{(pbc)}$$

$$N = 800 \ ; \quad \alpha = 10^{-3} f_0/\lambda$$

Stationary state:




MD
Fokker-Planck
T=0.0
ρ(x)
x
0.5
0.4
0.3
0.2
0.1
0
-200
-100
0
100
200

PHYSICAL REVIEW E **85**, 021146 (2012)

Time evolution of interacting vortices under overdamped motion

Mauricio S. Ribeiro,[1,*] Fernando D. Nobre,[1,†] and Evaldo M. F. Curado[1,2,‡]

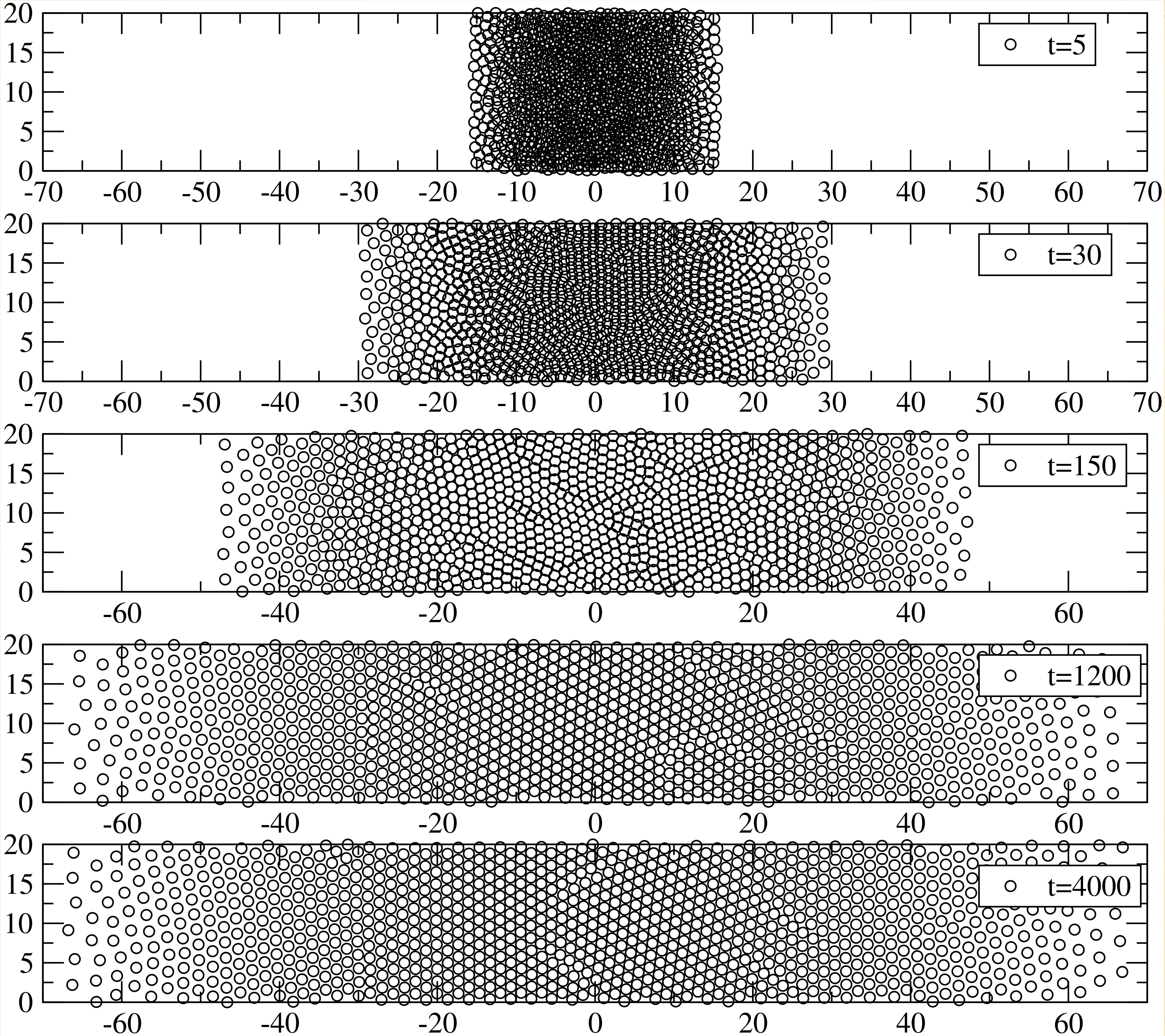
[1]*Centro Brasileiro de Pesquisas Físicas and National Institute of Science and Technology for Complex Systems, Rua Xavier Sigaud 150, Rio de Janeiro, RJ 22290-180, Brazil*

[2]*Laboratoire APC, Université Paris Diderot, 10 rue A. Domon et L. Duquet, 75205 Paris, France*

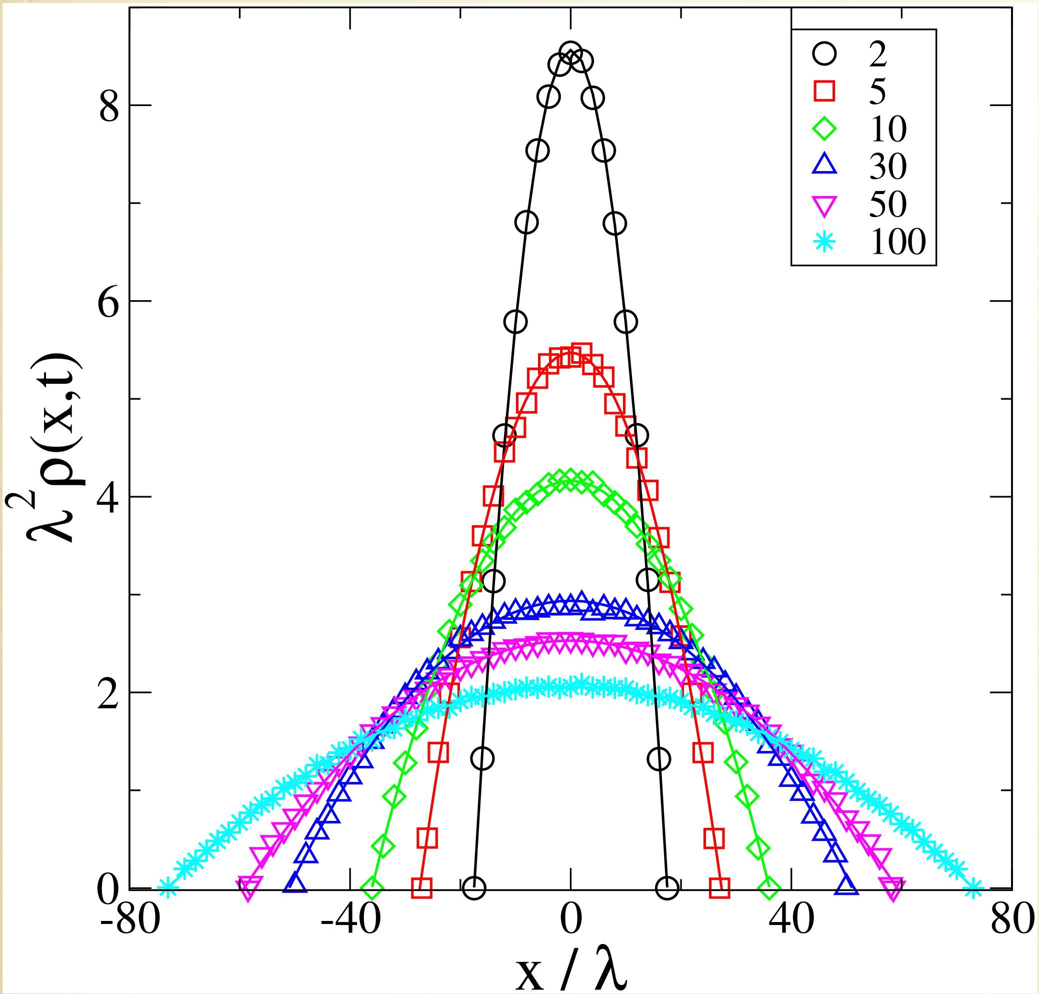
(Received 15 December 2011; published 27 February 2012)

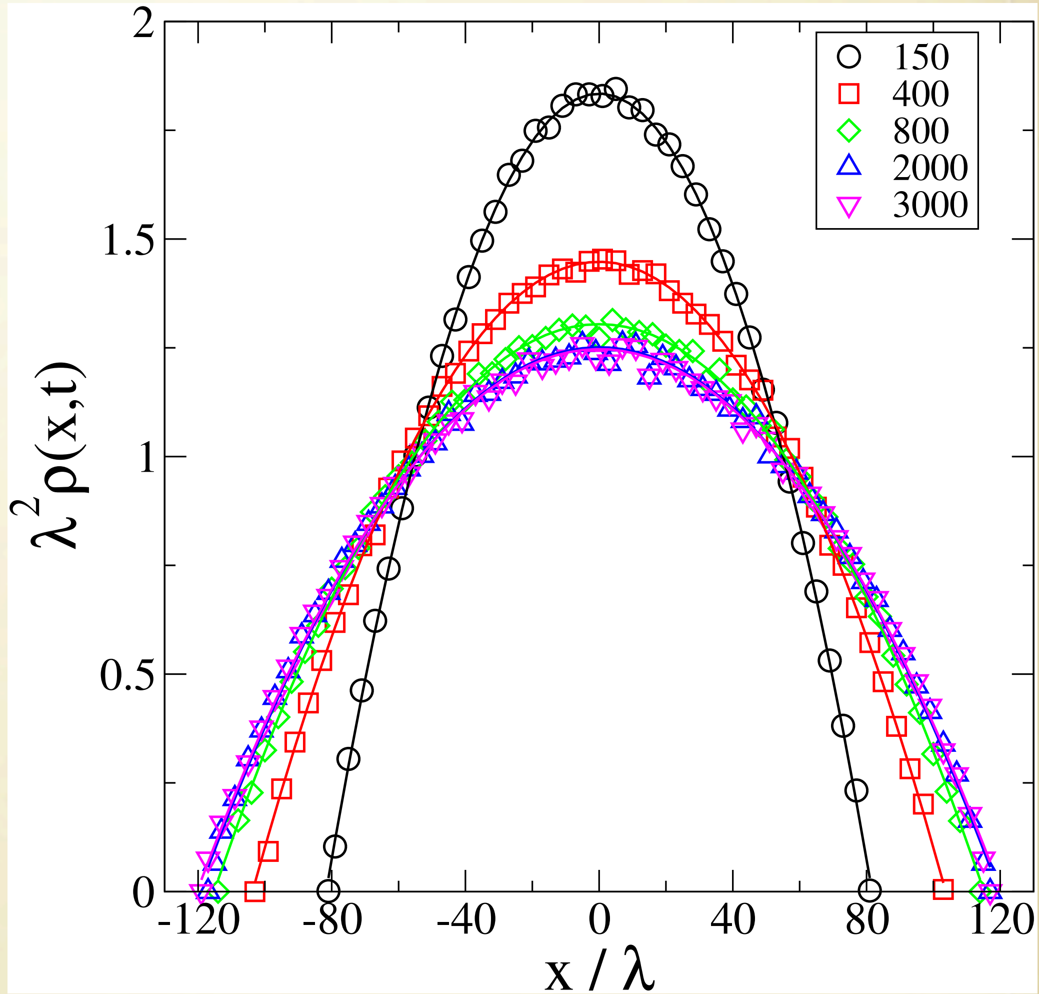
A system of interacting vortices under overdamped motion, which has been commonly used in the literature to model flux-front penetration in disordered type-II superconductors, was recently related to a nonlinear Fokker-Planck equation, characteristic of nonextensive statistical mechanics, through an analysis of its stationary state. Herein, this connection is extended by means of a thorough analysis of the time evolution of this system. Numerical data from molecular-dynamics simulations are presented for both position and velocity probability distributions $P(x,t)$ and $P(v_x,t)$, respectively; both distributions are well fitted by similar q-Gaussian distributions, with the same index $q = 0$, for all times considered. Particularly, the evolution of the system occurs in such a way that $P(x,t)$ presents a time behavior for its width, normalization, and second moment, in full agreement with the analytic solution of the nonlinear Fokker-Planck equation. The present results provide further evidence that this system is deeply associated with nonextensive statistical mechanics.

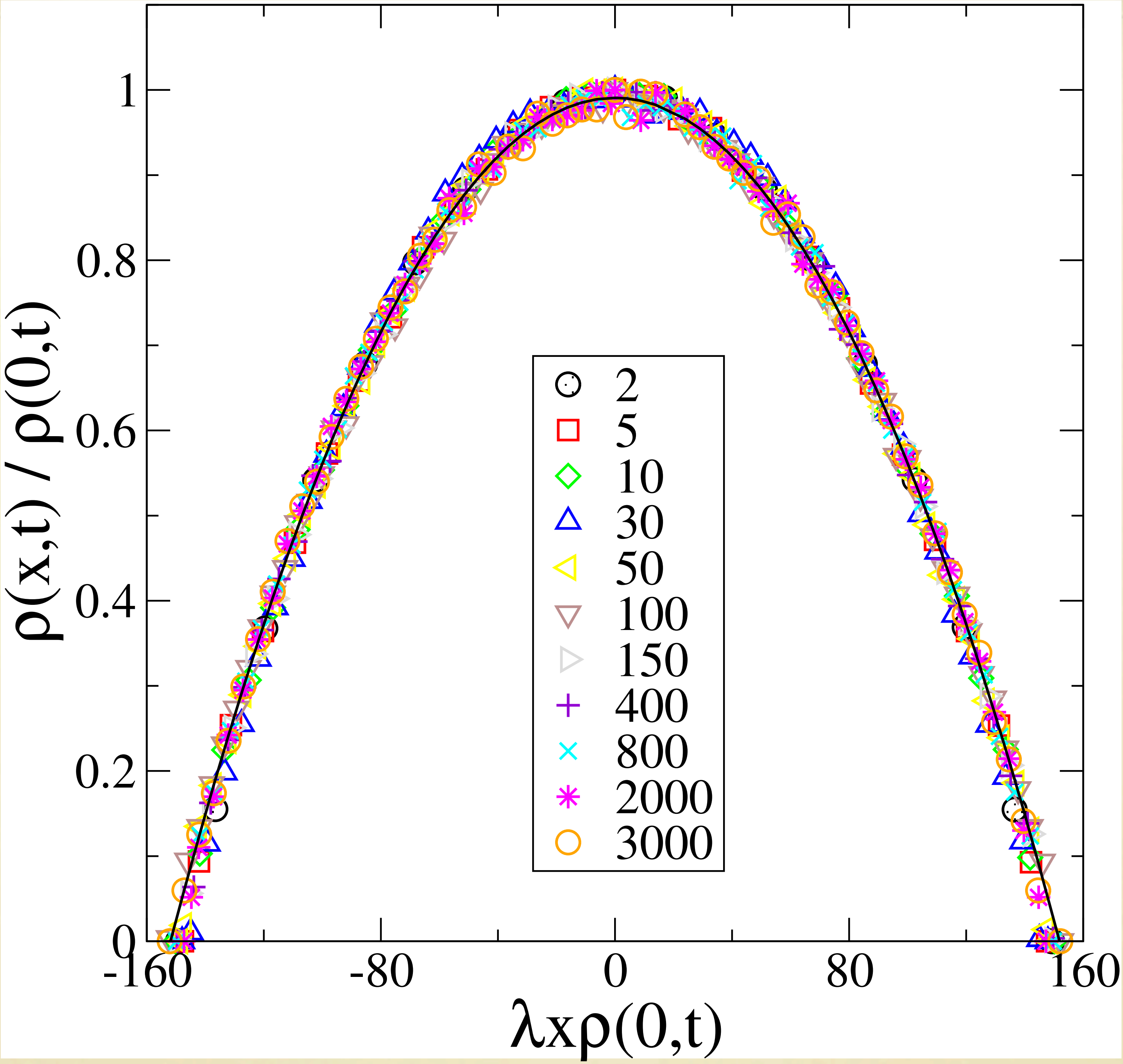
DOI: 10.1103/PhysRevE.85.021146 PACS number(s): 05.40.Fb, 05.10.Gg, 05.20.−y


t=5
t=30
t=150
t=1200
t=4000

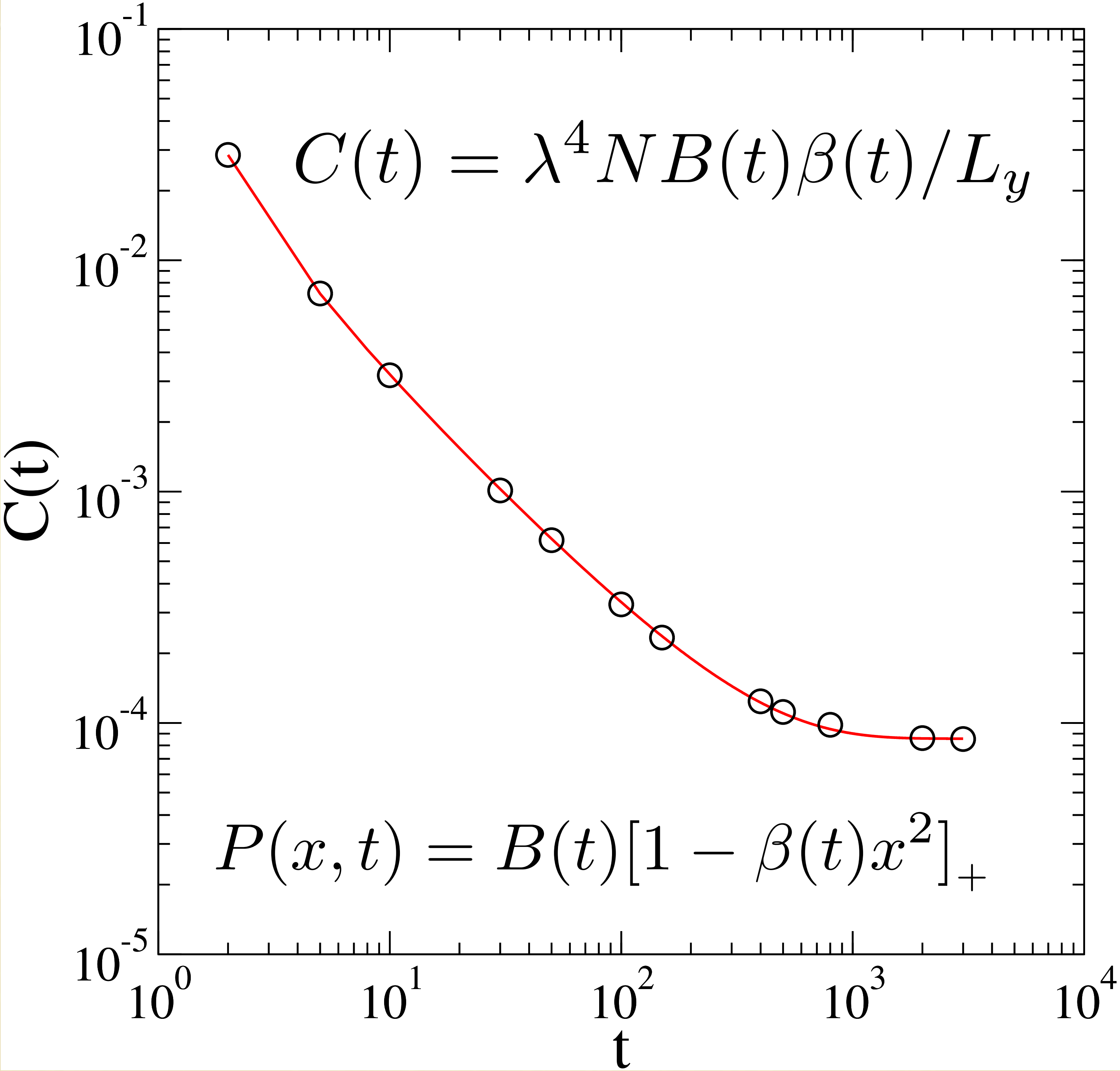
$$a = (5.87 \pm 0.02) f_0 \lambda^3 \quad \Longleftrightarrow \quad a = 2\pi f_0 \lambda^3$$







1
0.8
0.6
0.4
0.2
0
-160
-80
0
80
160
λxρ(0,t)
ρ(x,t) / ρ(0,t)
2
5
10
30
50
100
150
400
800
2000
3000


$C(t) = \lambda^4 N B(t) \beta(t) / L_y$
$P(x,t) = B(t)[1 - \beta(t) x^2]_+$
C(t)
t
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}

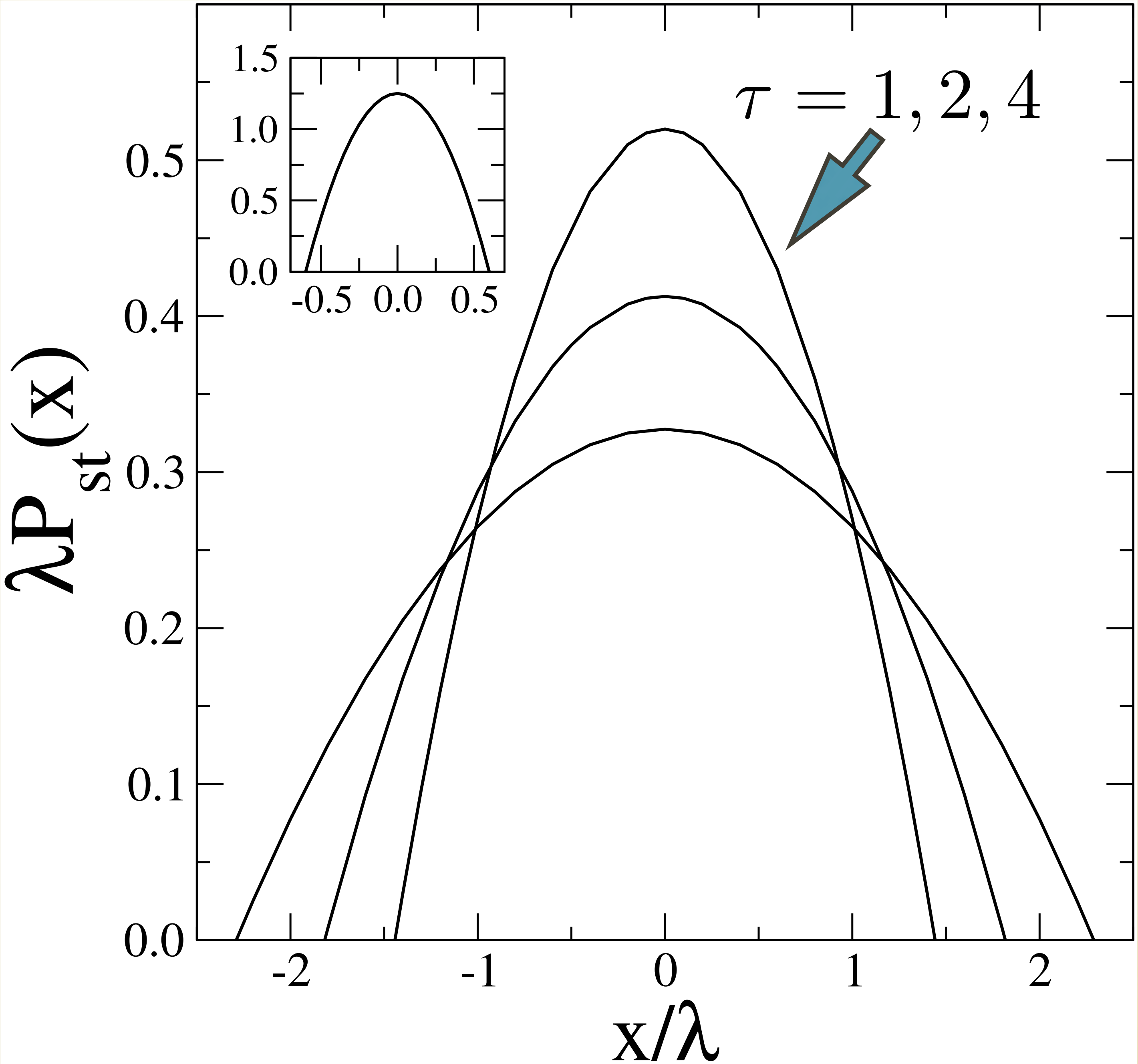
- Analysis of Stationary State:

$$D = k\gamma = \lim_{N, L_y \to \infty} \frac{N\pi f_0 \lambda^2}{L_y} = n\pi f_0 \lambda^2$$

Dimensionless variable: $\tau = \frac{k\gamma}{\alpha\lambda^2} = \frac{n\pi f_0}{\alpha}$

$$P_{\mathrm{st}}(x) = \frac{\alpha}{4D\lambda}(x_e^2 - x^2) = \frac{1}{4\tau\lambda}\left[\left(\frac{x_e}{\lambda}\right)^2 - \left(\frac{x}{\lambda}\right)^2\right]$$

$$(|x| < x_e) \qquad x_e = (3D\lambda/\alpha)^{1/3} = (3\tau)^{1/3}\lambda$$



$$\langle x^2 \rangle = \frac{1}{5}(3\tau)^{2/3}\lambda^2$$

$$\langle x^2 \rangle \sim \gamma^{2/3}$$

Dynamics:

$$\langle x^2 \rangle \sim t^{2/3}$$

? ?

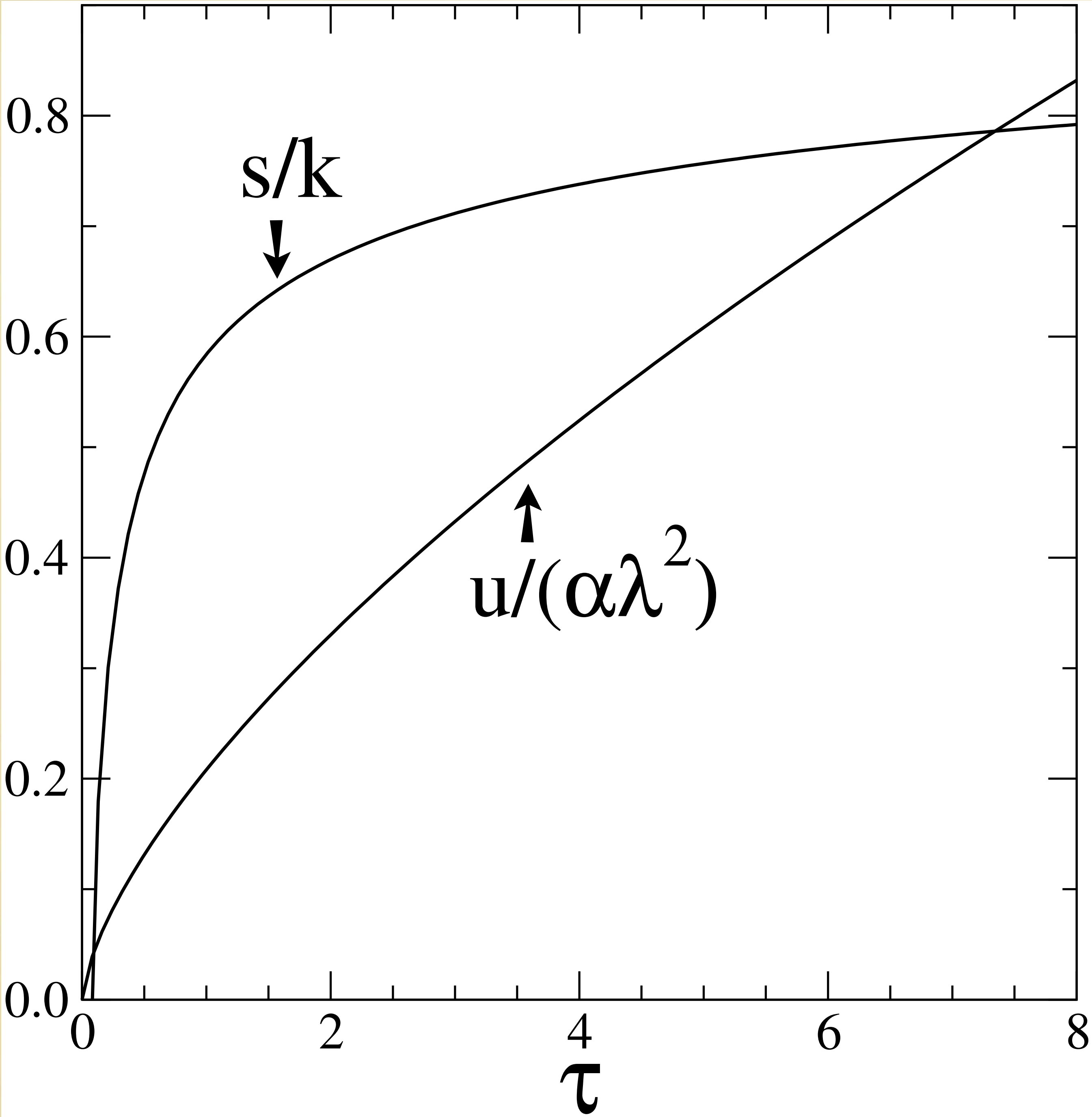
$$\langle x^2 \rangle \sim (\gamma t)^{2/3}$$

$$u = \int_{-x_e}^{x_e} dx \; \frac{\alpha x^2}{2} \; P_{\mathrm{st}}(x) = \frac{3^{2/3}}{10} \; \alpha\lambda^2 \; \tau^{2/3}$$

$$s = k \left[1 - \frac{1}{5} \left(\frac{9}{\tau} \right)^{1/3} \right]$$

$$s(u) = k \left[1 - \frac{3}{5} \left(\frac{\alpha\lambda^2}{10u} \right)^{1/2} \right]$$

$$\frac{\partial s(u)}{\partial u} = \frac{1}{\gamma}$$



$$s < 0$$

$$\text{for} \quad \tau < 0.072$$

$$f = \alpha\lambda^2 \left[\frac{3^{5/3}}{10}\,\tau^{2/3} - \tau\right] \Rightarrow \frac{\partial f}{\partial \gamma} = -s$$

$$c = \frac{\partial u}{\partial \gamma} = \gamma \frac{\partial s}{\partial \gamma} = -\gamma \frac{\partial^2 f}{\partial^2 \gamma} = \frac{3^{2/3}}{15}\,k\tau^{-1/3}$$

Energy Fluctuations: $\langle E^2 \rangle - \langle E \rangle^2 = \frac{18}{7}\,\gamma^2 c^2$

Suggests $\Rightarrow$ $\langle E^2 \rangle - \langle E \rangle^2 \propto (k\gamma)^2 \left(\frac{c}{k}\right)^{2-q}$

Conclusions

- Physical system for Tsallis statistics
- Associated Entropy:

$$S[P] = k[1 - \int_{-\infty}^{\infty} dx \; P^2(x,t)] \qquad (T=0)$$

- Effective Temperature: $k\gamma = n\pi f_0 \lambda^2$

➡ Similar behavior for physical properties

- Collaborators:

J.S. Andrade Jr. (UFC - CE)

E.M.F. Curado (CBPF - RJ)

G.F.T. da Silva (UFC - CE)

A.A. Moreira (UFC - CE)

M.S. Ribeiro (CBPF - RJ)

A.M.C. Souza (UFS - SE)

Thursday, May 3, 2012

Thursday, May 3, 2012

- Collaborators:

J.S. Andrade Jr. (UFC - CE)

E.M.F. Curado (CBPF - RJ)

G.F.T. da Silva (UFC - CE)

A.A. Moreira (UFC - CE)

M.S. Ribeiro (CBPF - RJ)

V. Schwämmle (CBPF - RJ)

Linear Fokker-Planck Equation:

$$\frac{\partial P(x,t)}{\partial t} = -\mu \, \frac{\partial \{A(x)P(x,t)\}}{\partial x} + D \, \frac{\partial^2 P(x,t)}{\partial x^2}$$

$$A(x) = -d\phi(x)/dx$$

$$P(x,t)|_{x\to\pm\infty} = 0 \ ; \ \left.\frac{\partial P(x,t)}{\partial x}\right|_{x\to\pm\infty} = 0 \ ; \ A(x)P(x,t)|_{x\to\pm\infty} = 0 \ (\forall t)$$

$$\int_{-\infty}^{\infty} dx \ P(x,t) = \int_{-\infty}^{\infty} dx \ P(x,t_0) = 1 \quad (\forall t)$$

H-Theorem and FP Equation:

$$F = U - TS \; ; \; U = \int_{-\infty}^{\infty} dx \; \phi(x) P(x,t) \; ; \; S = -k_B \int_{-\infty}^{\infty} dx \; P(x,t) \ln P(x,t)$$

$$\begin{aligned} \frac{dF}{dt} &= \frac{\partial}{\partial t} \left(\int_{-\infty}^{\infty} dx \; \phi(x) P(x,t) + k_B T \int_{-\infty}^{\infty} dx P(x,t) \ln P(x,t) \right) \\ &= \int_{-\infty}^{\infty} dx \; \{\phi(x) + k_B T [\ln P(x,t) + 1]\} \frac{\partial P(x,t)}{\partial t} \end{aligned}$$

FPE and Integration by Parts :

$$\begin{aligned} \frac{dF}{dt} &= -\int_{-\infty}^{\infty} dx \left(\mu \frac{d\phi(x)}{dx} P(x,t) + D \frac{\partial P}{\partial x} \right) \left(\frac{d\phi(x)}{dx} \right. \\ &+ \left. \frac{k_B T}{P} \frac{\partial P}{\partial x} \right) = -\mu \int_{-\infty}^{\infty} dx P(x,t) \left(\frac{d\phi(x)}{dx} + \frac{k_B T}{P} \frac{\partial P}{\partial x} \right)^2 \leq 0 \end{aligned}$$

- Remark: "duality" $q \rightarrow (2-q)$
- Extremization of entropy:

$$U = \int_{-\infty}^{\infty} dx\ \phi(x) P(x,t) \quad \text{or} \quad U = \int_{-\infty}^{\infty} dx\ \phi(x) P^q(x,t)$$

In the first case: $\mu = 2 - q$

- Present application: $\mu = 2 \quad \Rightarrow \quad q = 0$
- Entropy: $S[P] = k\{1 - \int_{-\infty}^{\infty} dx\ [P(x,t)]^2\ \}$

- Remark: “duality” $q \to (2-q)$
- Extremization of entropy:

$$U = \int_{-\infty}^{\infty} dx \; \phi(x) P(x,t) \quad \text{or} \quad U = \int_{-\infty}^{\infty} dx \; \phi(x) \Gamma[P(x,t)]$$

In the first case: $\mu = 2 - q$

- Next application: $\mu = 2 \quad \Rightarrow \quad q = 0$
- Entropy: $S[P] = k\{1 - \int_{-\infty}^{\infty} dx \; [P(x,t)]^2 \}$