Thermostatistics of Interacting Particles Under Overdamped Motion

Thermostatistics of Overdamped Motion of Interacting Particles

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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.

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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 :

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

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:

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

$$F = U - \frac{1}{\beta}\, S\ ; \quad U = \int_{-\infty}^{\infty} dx\ \phi(x) P(x,t)$$

- Condition for the H-Theorem:

$$-\frac{1}{\beta} \frac{d^2 g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]}$$

- Examples of FPEs and Associated Entropies

a) FPE Associated with BG Entropy

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

$$\frac{dg}{dP} = -\beta D \ln P + C \quad \Rightarrow \quad g[P] = -k_B P \ln P$$

b) FPE Associated with Tsallis Entropy

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

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

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

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

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

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

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

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

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

- Physical system: interacting particles under overdamped motion
- Disordered type-II superconductors

➡ interacting overdamped vortices

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

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

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

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

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

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

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

- Using continuity equation with:

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

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

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

- For fixed y $\Rightarrow$ introduce P(x,t):

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

$$D = \frac{\pi n f_0 \lambda^3}{\eta} \quad \Rightarrow \quad D = \mu k_B \theta$$

"Einstein-like" relation

$\theta = f_0 \lambda / k_B$ $\Rightarrow$ "temperature"

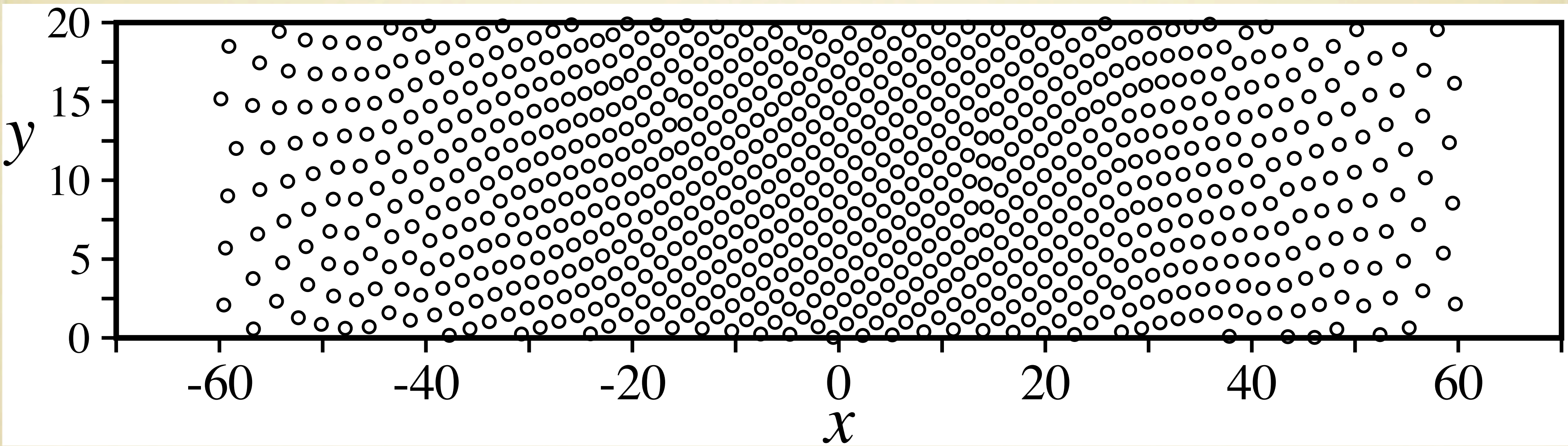
$\mu = \pi n \lambda^2 / \eta$ $\Rightarrow$ effective mobility

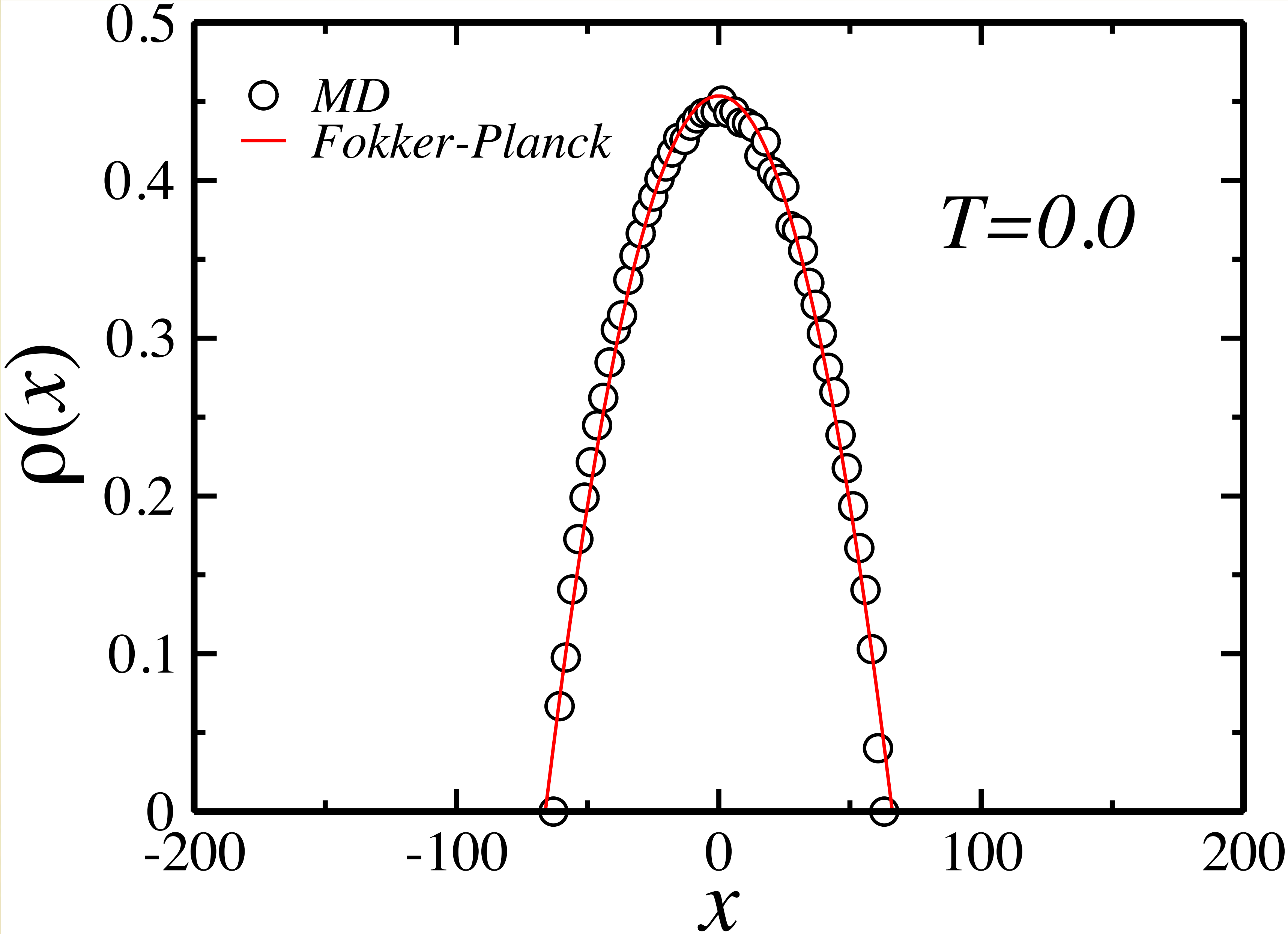
Molecular Dynamics Simulations (2d):

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

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

Stationary state:





$$D \approx 2.41\ n f_0 \lambda^3/\eta \quad \text{(MD)}$$

- Introducing uncorrelated thermal noise:

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

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

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

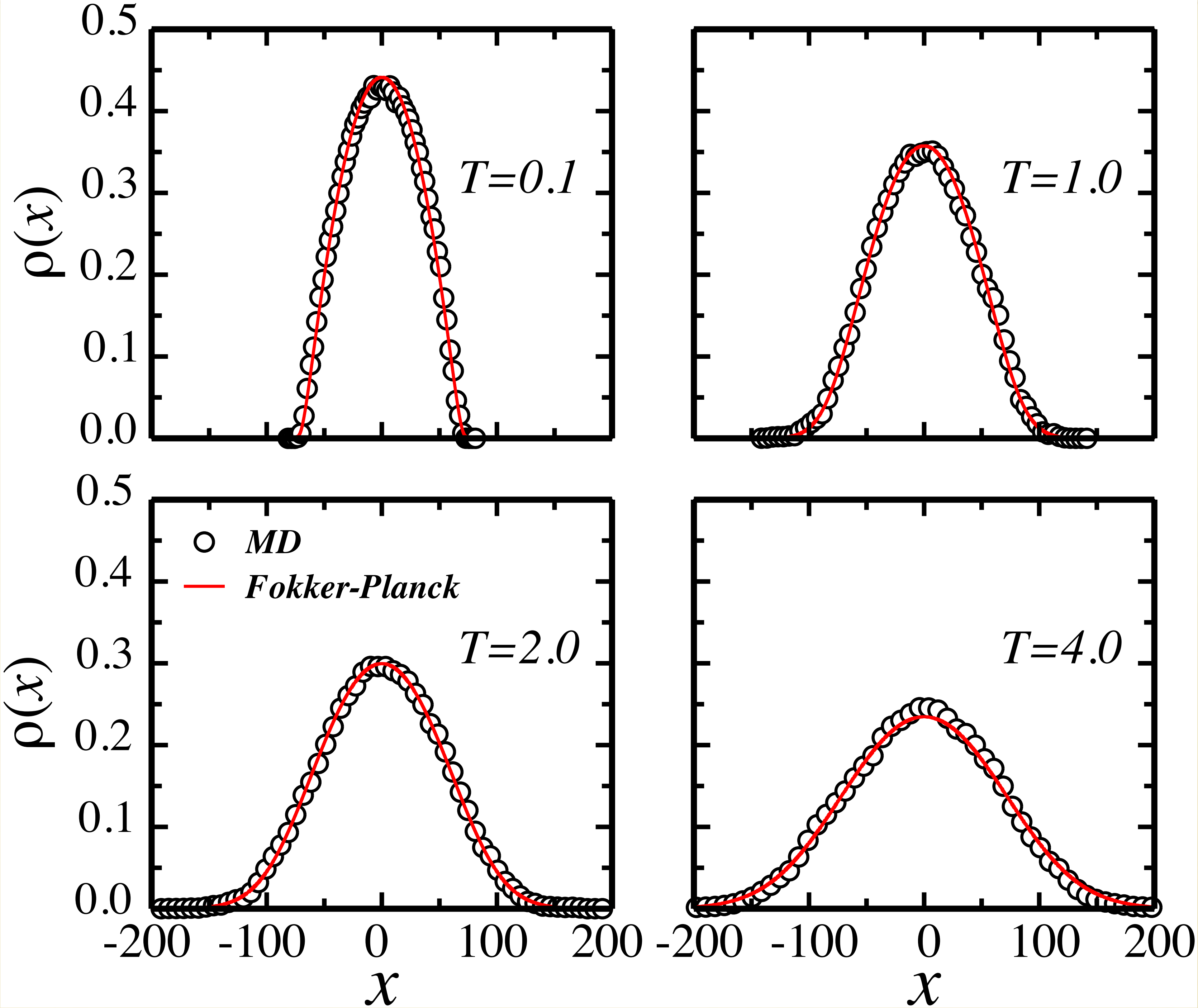
$$+ k_B T \frac{\partial^2 \rho(\mathbf{r}, t)}{\partial x^2}$$

- Stationary-state solution:

$$\rho(x) = \frac{k_B T}{a} \; W \left\{ \frac{a\rho(0)}{k_B T} \; \exp\left[\frac{a\rho(0)}{k_B T} - \frac{\alpha x^2}{2 k_B T} \right] \right\}$$

- W-Lambert function:

$$W(z) \exp\left[W(z)\right] = z$$


T=0.1
T=1.0
T=2.0
T=4.0
MD
Fokker-Planck
ρ(x)
x
0.0
0.1
0.2
0.3
0.4
0.5
-200
-100
0
100
200

- Entropy:

$$S[P] = \frac{D}{\bar{\gamma}}[1 - \int_{-\infty}^{\infty} dx \;P^2(x,t)]$$

$$-\frac{k_B T}{\bar{\gamma}} \int_{-\infty}^{\infty} dx \;P(x,t) \ln P(x,t)$$

Conclusions

- Physical system for Tsallis Statistics
- Associated Entropy:

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

$$S[P] = \frac{D}{\bar{\gamma}}[1 - \int_{-\infty}^{\infty} dx\ P^2(x,t)]$$

$$-\frac{k_B T}{\bar{\gamma}} \int_{-\infty}^{\infty} dx\ P(x,t) \ln P(x,t) \qquad (T \neq 0)$$

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PHYSICA A

Non-extensive statistical mechanics and generalized Fokker–Planck equation

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Abstract

A non-linear, generalized Fokker–Planck (GFP) equation is studied whose exact stationary solutions are the maximum entropy distributions introduced by Tsallis in his generalization of Statistical Mechanics. In the case of a constant or linearly varying drift, the time dependent solutions of the GFP equation are seen to obey a suitable form of the celebrated H-theorem. The temporal changes of Tsallis' entropies are seen to be given in terms of the Fisher's information measure. Particular time-dependent solutions of the GFP equation of the maximum (Tsallis') entropy form are obtained.