EUROPHYSICS LETTERS 15 September 2004

Europhys. Lett., **67** (6), pp. 1052–1053 (2004)

DOI: 10.1209/epl/i2004-10156-y

Reply

Reply to the Comment by J. D. Bao on "The Fluctuation-Dissipation Theorem fails for fast superdiffusion"

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(received 12 February 2004; accepted in final form 23 July 2004)

PACS. 05.10.Gg – Stochastic analysis methods (Fokker-Planck, Langevin, etc.).
PACS. 05.40.Ca – Noise.
PACS. 05.40.Jc – Brownian motion.

In his comment [1] (hereafter referred to as Bao), the author claims that the violation of the Fluctuation-Dissipation Theorem (FDT) is due to the choice of the initial condition for the distribution function: First, the comment shows a generalization and confirmation of our results. Second, it opens up a discussion on an interesting and unresolved topic which deserves the attention of our community. However, there are few points that must be clarified.

In our article [2] we discussed the behavior of the mean-square value of a dynamical variable $A(t)$, and the mean-square displacement of the quantity $y(t) = \int_0^t A(t')\mathrm{d}t'$. The variable $A(t)$ is governed by a generalized Langevin equation (GLE), and we set the intial conditions as $\langle A(0)\rangle = 0$. The asymptotic behavior of $\langle y^2(t)\rangle \sim t^\alpha$ as $t \to \infty$ can be divided into two regimes. For $0 < \alpha < 2$, the FDT works [3–8]. For the fast superdiffusion (FSD), *i.e.* $\alpha \geq 2$, the FDT does not work [2].

Bao modifies our work by introducing an arbitrary distribution of values $A(0)$ at the origin. After a long time, his distribution acquires an effective temperature T_{eff} of the form

$$\frac{T_{\mathrm{eff}}}{T} = 1 + R^2(t \to \infty)\left(\frac{T_0}{T} - 1\right), \tag{1}$$

where $R(t)$ is the correlation function $R(t) = \langle A(t)A(0)\rangle / \langle A(0)A(0)\rangle$. Here, T and T_0 are the temperatures of the heat bath and of the system at the initial state. The above equation generalizes our resut, obtained for $T_0 = 0$. Now, it was explicitly demonstrated [2] that for fast superdiffusion $R(t \to \infty) \neq 0$; consequently, $T_{\mathrm{eff}} \neq T$. Bao correctly states that *if the system is at equilibrium, $T_0 = T$, it will remain at equilibrium, $T_{\mathrm{eff}} = T$, even for fast superdiffusion.* This is an expected although important result, which we did not obtain. Again, our aim was to prove that for fast superdiffusion the system never reaches an equilibrium and the FDT fails. This is quite clear from the above expression, where $T_{\mathrm{eff}} \neq T$, except for $T_0 = T$. The system acquires an effective temperature found out in many complex relaxation processes where the FDT fails as well [9–12]. Consequently, Bao confirms our conclusion. Moreover, we connect the failure of the FDT with the failure of ergodicity [8]. The failure of those concepts has implications in many areas, ranging from anomalous reaction rate [13] to chaos synchronization [14].

In the first paragraph of our article, and at the conclusion, we state that Kubo's FDT does not work for a system far from equilibrium. However, Bao confuses the initial conditions we set with the dynamics of the motion. The variables are evaluated at equilibrium, $\langle\ \rangle_{\text{eq}}$, but the FDT itself is a detailed balanced mechanism that slows down particles with average temperature higher than the heat reservoir and accelerates those with lower temperature. Consequently, a detailed balanced argument is the way the system reaches equilibrium. In the context of non-equilibrium statistical physics, the FDT applies in the linear-response regime [3–8]. This is similar to quantum mechanics, where one uses the unperturbed states as a basis to obtain results for the perturbed system.

Diffusion is itself a way through which a system searches for homogeneity in particles and energy densities, so even when local equilibrium is assumed, the whole process is out of equilibrium evolving to reach global equilibrium. The far-from-equilibrium conditions [2] are not a consequence of the initial conditions, rather they are a consequence of the process. In the range $0 < \alpha < 2$, and $R(t \to \infty) = 0$, diffusion takes place and the system reaches an equilibrium independent of the initial conditions, while for $\alpha \geq 2$, and $R(t \to \infty) \neq 0$, the FSD is probably some kind of activated process, and equilibrium is not achieved unless the system is already at equilibrium, for that the FDT does not work. This basic phenomenon has impact in many areas of physics, and so does the general assumption connected with it. Consequently, it is fundamental to understand precisely if one can reckon with the FDT and ergodicity.

Now a structural question is if there is an equilibrium state for a ballistic motion. If one follows the precise analysis of Lee [8], those sytems are not ergodic and the answer is that there is no equilibrium state for this case. However, for such a rich system it would be safe to say that the question still remains open.

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This work was supported by CAPES, FINEP, CNPq and FINATEC.

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