Brownian Colloids under Non Homogeneous Temperature

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Langevin and Fokker–Planck equations have been the most used paradigm in the studies of Brownian particles motion. These equations give the correct Boltzmann equilibrium statistics and incorporate interesting nonequilibrium aspects such as the dynamical evolution to equilibrium and allows the incorporation of non equilibration elements such flows of matter and temperature gradients.

In this last situation the standard form of the Langevin equation needed some revisions due to the presence of multiplicative white noise. This problem was already studied and appropriate Fokker-Planck [1] and Langevin equations were derived [1, 2].

This study starts with the following Langevin equation for noninteracting classical Brownian particles,

$$\ddot{z} = -\hat{\gamma}_0 \dot{z} - V'(z) + g(z)\xi(\tau), \tag{1}$$

where $V(z)$ is an external potential and $\xi(\tau)$ is the thermal Gaussian white noise with zero mean and correlation $< \xi(\tau)\,\xi(\tau') >= 2\delta(\tau - \tau')$. All variables and parameters have been rescaled to be dimensionless. Temperature $\hat{T}(z)$ is spatially dependent but the following local fluctuation dissipation relation is fulfilled,

$$g(z)^2 = \hat{\gamma}_0 \hat{T}(z). \tag{2}$$

Brownian motion of colloidal particles under the following spatially dependent temperature $\hat{T}(z) = 1 + 0.1z$, is studied in the spatial domain $z \in [0, 10]$.

The nonequilibrium steady densities $P_{st}(z, v)$ and $P_{st}(z)$ are evaluated and the underdamped and overdamped regimes are discussed. The existence of local equilibrium is characterized as a function of the friction parameter. Correct Langevin equations and their numerical simulations are derived.

Is is important to determine if the local kinetic energy equipartition theorem

$$< v^2(z) >_{st} = \hat{T}(z), \tag{3}$$

is fulfilled or it is friction dependent. Numerical simulations show that the underdamped and overdamped regimens are separated by de condition $\hat{\gamma}_0 = 1$, As $\hat{\gamma}_0$ is a dimensionless parameter it has to be expressed in terms of the physical parameters such as,

$$\hat{\gamma}_0 = \gamma_0 \sqrt{\frac{x_0^2}{m k_B T_0}}, \tag{4}$$

where γ_0 is the Stokes friction, m the Brownian particle mass, x_0 and T_0 are characteristic length and temperature of the specific system. When the friction is also temperature dependent the criteria have to be applied locally.

Let us take here, such as representative example, a parabolic potential fixed at the center of the system ,

$$\ddot{z} = -\hat{\gamma}_0 \dot{z} - \hat{k}(z - 5) + \sqrt{\hat{\gamma}_0 \hat{T}(z)}\,\eta(\tau). \tag{5}$$

Results of numerical simulations for two friction values $\hat{\gamma}_0 = 6$ and $\hat{\gamma}_0 = 0.05$ are presented in Fig. 1, where numerical results for the kinetic energy equipartition theorem are plotted. Here we see also important deviations for low friction.

Nonequilibrium state distributions for the overdamped regime were checked satisfactorily by numerical simulations. Actually it was shown that in the overdamped regime local equilibrium is also fulfilled ($\hat{\gamma}_0 = 6$ in Fig. 1). With respect the underdamped regime, numerical results show important deviations with the overdamped regime. When the space covered by a particle with a thermal velocity $v \sim \sqrt{\hat{T}}$ is of order of the system size, then particles do not feel the local temperature and the equipartition theorem is violated locally ($\hat{\gamma}_0 = 0.05$ in Fig. 1). In this regime the local kinetic energy equipartition theorem is lost, and particles feel the averaged temperature $\bar{T} = 1.5$ in any place of the system.

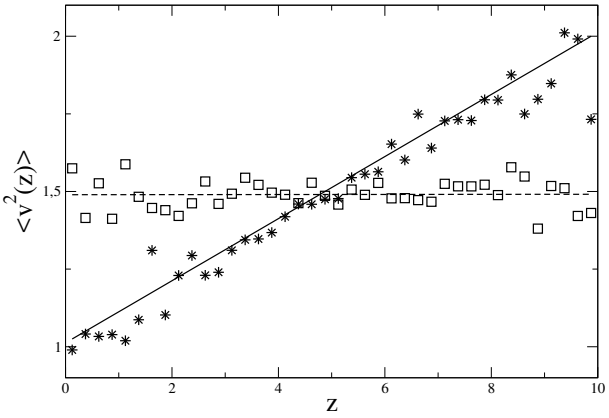

Figure 1: Local second moment for the harmonic potential: $< v^2(z) > \sim$ kinetic energy. Continuous line corresponds to the energy equipartition theorem (3), and the dashed line is a guide of the mean temperature$\bar{T} = 1.5$. Numerical results for $\hat{\gamma}_0 = 6$ (stars) and $\hat{\gamma}_0 = 0.05$ (squares).

[1] J. M. Sancho, M. San Miguel, and D. Dürr, J. Stat. Phys. **28**, 291 (1982).

[2] J. M. Sancho, Phys, Rev. E **84**, 062102 (2011)

[3] J. M. Sancho, Phys. Rev. E **92**, 062110(2015).