Fluctuation Theorem for the DLD Model

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Abstract

The applicability of Zwanzig-Caldeira-Leggett (ZCL) [1] model is rather simple to explain the physical phenomena associated with a generalized brownian motion. In the usual formulation, one should specify the stochastic force ξ, which arises from interaction with some fluctuating homogeneous field $\xi(t)$. However, more generally, this force may arise from the interaction with a disordered potential $\xi(x,t) = -\nabla U(x,t)$. In the latter case the spatial auto-correlations of the force plays a role. In this poster, we want to elucidate some points of the 'diffusion, localization and dissipation' model (DLD) [2,3], possible thermodynamic effects, and also non-equilibrium fluctuations caused by the local interaction.

Model

As in the ZCL model, the classical DLD model considers a motion of a particle under the influence of bath which is composed of infinitely many oscillators. However, in this case, the particle interacts locally with the n oscillator through $u(x-x_n)$, where x_n is the location of the corresponding oscillator. The DLD Hamiltonian is

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_I + \mathcal{H}_B, \tag{1}$$

$$\mathcal{H}_S = \frac{p^2}{2m} + V(x), \tag{2}$$

$$\mathcal{H}_I = -\sum_n c_n\, q_n,\, u(x-x_n), \tag{3}$$

$$\mathcal{H}_B = \sum_n \frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 q_n^2, \tag{4}$$

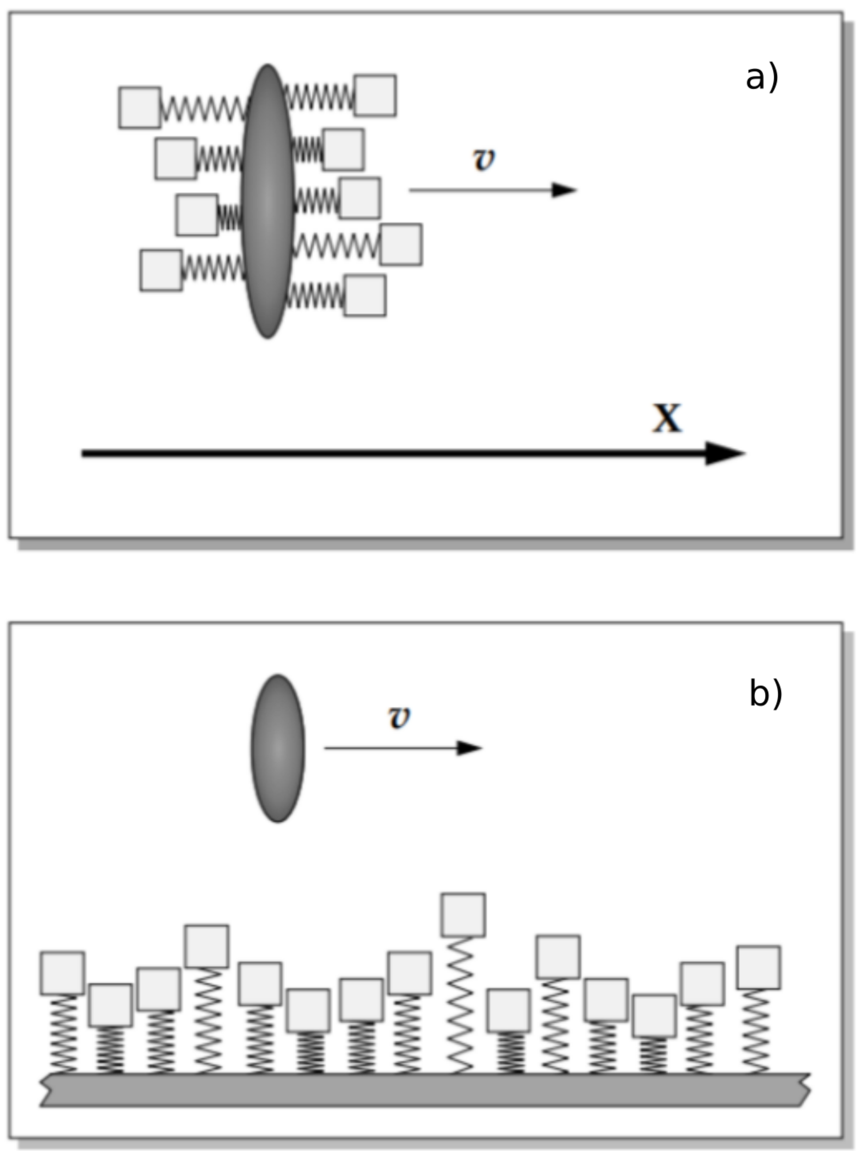

Figure 1: ZCL model (fig. a) and DLD model (fig. b) in perspective.

Future perspectives

We expect to proceed with studying

- the possible implications to the steady state given the range σ
- the DLD fluctuation theorem
- the thermodynamics of the DLD model (linear response, entropy production)

DLD Kramers Equation

- A master equation is derived for the DLD model [2]

$$\frac{\partial}{\partial t}\varrho = -\frac{p}{m}\frac{\partial}{\partial x}[\varrho] + V'(x)\frac{\partial}{\partial p}[\varrho] + \gamma\frac{\partial}{\partial p}[G_F * p\varrho] + \nu\,(G_N * \varrho)\,, \tag{5}$$

where

$$G_F(p,\sigma) \equiv \mathcal{FT}\left\{\frac{w'(r)}{r}\right\},$$

$$G_N(p,\sigma) \equiv \frac{1}{\hbar^2}\mathcal{FT}\left\{w(r) - w(0)\right\}.$$

- As $\sigma = l/\hbar \to 0$, the standard Kramers equation is restored

$$\frac{\partial}{\partial t}\varrho = \gamma\frac{\partial}{\partial p}[p\varrho] + \nu\frac{\partial^2}{\partial p^2}[\varrho].$$

That means, the Zwanzig–Caldeira–Leggett (ZCL) model [1] constitutes a special formal limit of the DLD model [2,3].

For DLD model, the correlations of the stochastic force satisfy

$$\langle \zeta(x,t)\zeta(x',t')\rangle = w(x-x')\phi(t-t'),$$

where, due to the local interaction with bath modes, the space correlation function w reads

$$w(x) = \int_{-\infty}^{\infty} u(x-x')u(x')dx'. \tag{6}$$

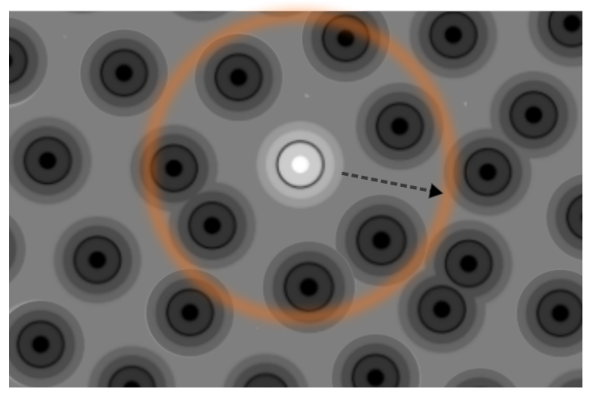

Figure 2: Representation of the range of interaction, described by σ, between the system (white particle) and the bath oscillators (black ones).

DLD Langevin Equation

- Starting from first principles in classical mechanics, a Langevin equation can be derived for the DLD model:

$$m\frac{\partial^2}{\partial t^2}x = -V'(x) + \int_0^t ds\,\left[\gamma(t-s)w''(x(t)-x(s))\right]\frac{\partial}{\partial t}x(s) + \zeta(t). \tag{7}$$

- Non-Markovian effects are present in the previous Langevin equation. However, when considering an Ohmic bath, i.e., $\gamma(t) = \gamma\delta(t)$, the resulting equation is the standard Langevin equation, since

$$\int_0^t dt\,\left[\gamma(t-s)w''(x(t)-x(s))\right]\frac{\partial}{\partial t}x(s) = \gamma w''(0)\frac{\partial}{\partial t}x(t) = -\gamma\frac{\partial}{\partial t}x(t).$$

DLD Smoluchowski Equation

- In fact, it is simpler to treat the master equation (5) in an overdamped regime. An overdamped master equation is given as follows

$$\frac{\partial}{\partial t}\rho = \frac{\partial}{\partial x}\left[\frac{V'(x)}{\gamma}\rho\right] + \frac{\nu}{\gamma^2}\mathcal{G}_N(x,\varsigma) * \rho, \qquad \mathcal{G}_N(x,\varsigma) = \frac{1}{\varsigma}\left[\frac{1}{\sqrt{\varsigma}}\exp\left(-\frac{x^2}{2\varsigma}\right) - \delta(x)\right], \tag{8}$$

- where $\varsigma \sim \sigma/\gamma$. A solution can be found for a harmonic potential and hence a steady state

$$\phi(k,t) = \mathcal{FT}_{x\to k}\{\rho(x,t)\} = \exp\left[-\frac{1}{\lambda}\left(\int^{ke^{-\lambda t}} dk'\frac{\mathcal{G}_N(k')}{k'} - \int^{k} dk'\frac{\mathcal{G}_N(k')}{k'}\right) - ikxe^{-\lambda t}\right],$$

$$\rho(x) = \lim_{t\to\infty}\rho(x,t) = \sqrt{\frac{\lambda}{2\pi D_0}}\exp\left[-\frac{\lambda x^2}{D_0} + \sum_{n=0}^{\infty} D_n\frac{\lambda^{2n+2}}{D_0^{2n+2}(2n+2)}x^{2n+2}\right], \tag{9}$$

where $D_n \sim \varsigma^n$. As $\varsigma \to 0$, i.e., $D_n \to 0$, the standard Ornstein Uhlenbeck solution is restored

$$\rho(x) = \sqrt{\frac{\lambda}{2\pi D_0}}\exp\left[-\frac{\lambda x^2}{D_0(t)}\right].$$

References

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