Easy as π: The Fluctuation-Dissipation Relation

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Newtonian mechanics defines the equation of motion as

$$m\ddot{x} = F \tag{1}$$

where m is the mass of a body, $\ddot{x}$ is the second derivative of the coordinates x of the body with respect to time t, and F is the total force applied to the body.

When a body is submerged into a fluctuating environment, the force F can be split into three parts: external F_e, drag F_d, and random R

$$F = F_e + F_d + R$$

Drag force F_d is proportional to velocity $\dot{x}$ with some drag coefficient γ: $F_d = -\gamma\dot{x}$. The random part R represents random forces the body experiences from the environment. Let us assume that R is sampled from some distribution with the variance $\langle R^2\rangle$. This variance depends on the time frame δ during which the force R is applied. Additionally we assume that R does not depend on the body state, does not have an average force $\langle R\rangle = 0$, and does not correlate with itself at times greater than δ, i.e.:

$$\langle R_t R_\tau\rangle = \begin{cases} 0, & \text{if} \quad 0 < \tau < t - \delta \\ \langle R^2\rangle, & \text{if} \quad t - \delta < \tau < t \end{cases} \tag{2}$$

where τ and t are two points in time ($0 < \tau < t$). Here and further the index t is implied if not specified.

Now we would like to establish a relationship between the drag coefficient γ and the random force R. Let us place the body into the environment without an external force:

$$m\ddot{x} = -\gamma\dot{x} + R \tag{3}$$

The body will experience some random movements due to fluctuations in the environment. In an equilibrium state the kinetic energy of the body, $e = m\dot{x}^2/2$, on average does not change, remaining equal to some value $E = \langle e\rangle$. Multiplying eq. 3 by $m\dot{x}$ one finds

$$m^2\ddot{x}\dot{x} = -m\gamma\dot{x}^2 + mR\dot{x}$$

which is

$$m\dot{e} = -2\gamma e + mR\dot{x}$$

because

$$\dot{e} = \frac{d}{dt}\frac{m\dot{x}^2}{2} = \frac{m}{2}\frac{d}{dt}\dot{x}^2 = m\ddot{x}\dot{x}$$

On average e does not change $\langle\dot{e}\rangle = 0$:

$$m\langle\dot{e}\rangle = 0 = -2\gamma\langle e\rangle + m\langle R\dot{x}\rangle$$

which gives us the first relation

$$m\langle R\dot{x}\rangle = 2\gamma E \tag{4}$$

Now let us go back to eq. 3 and integrate it

$$m\int_0^t \ddot{x}_\tau d\tau = -\gamma\int_0^t \dot{x}_\tau d\tau + \int_0^t R_\tau d\tau$$

$$m\dot{x} - m\dot{x}_0 = -\gamma x + \gamma x_0 + \int_0^t R_\tau d\tau$$

Multiplying this equation by R (remember that index t is implicit $R \equiv R_t$) and taking the average we find:

$$m\langle R\dot{x}\rangle - m\langle R\dot{x}_0\rangle = -\gamma\langle Rx\rangle + \gamma\langle Rx_0\rangle + \langle R_t\int_0^t R_\tau d\tau\rangle$$

Since R does not depend on x, $\dot{x}_0$ or x_0, the following terms are zeros: $\langle R\dot{x}_0\rangle = \langle R\rangle\langle\dot{x}_0\rangle = 0$, $\langle Rx\rangle = \langle R\rangle\langle x\rangle = 0$, and $\langle Rx_0\rangle = \langle R\rangle\langle x_0\rangle = 0$:

$$m\langle R\dot{x}\rangle = \langle R_t\int_0^t R_\tau d\tau\rangle = \int_0^t\langle R_t R_\tau\rangle d\tau = \langle R^2\rangle\delta$$

The last integral is taken using eq. 2 because the integration up to $t - \delta$ is zero and between $t - \delta$ and t is a constant.

This gives us the second relation:

$$m\langle R\dot{x}\rangle = \langle R^2\rangle\delta \tag{5}$$

Combining eq. 4 and eq. 5 we get:

$$\boxed{\langle R^2\rangle\delta = 2\gamma E} \tag{6}$$

This formula sets the relationship between the strength of the random force, the drag coefficient and the average kinetic energy of the body in the equilibrium state.

The relationship within eq. 6 suggests how to simulate eq. 1 with fluctuations. First place the body into the environment without an external force and initial velocity, and observe the average kinetic energy E. Given that the drag force F_d is known, the coefficient γ can be calculated at each moment in time $\gamma = F_d/\dot{x}$. When integrating with a time step δ, R obeys a distribution with a variance

$$\sigma_R^2 = \langle R^2\rangle = \frac{2\gamma E}{\delta}$$

By introducing a random value $\widetilde{r}$, sampled from a distribution with a variance

$$\sigma_r^2 = \langle r^2\rangle = 2\gamma E$$

the random force $\widetilde{R}$ has to be expressed as

$$\widetilde{R} = \frac{\widetilde{r}}{\sqrt{\delta}}$$

which can be used in a time step integration of eq. 1:

$$\dot{x}(t+\delta) = \dot{x}(t) + \frac{\delta}{m}(F_e + F_d + \widetilde{R})$$

The integration for the random force works differently – its contribution is proportional to the square root of the time step δ:

$$\dot{x}(t+\delta) = \dot{x}(t) + \frac{1}{m}(F_e\delta + F_d\delta + \widetilde{r}\sqrt{\delta})$$

Note that $\widetilde{r}$ depends on γ and E but not on δ.