

THE FLUCTUATION - DISSIPATION THEOREM

For a linear system at thermal equilibrium we have that the Power Spectral Density $S_{xx}(\omega)$ of the observable x is :

$$S_{xx}(\omega) = 4\hbar\alpha'' \cdot \left\{ \frac{1}{2} + \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1} \right\} \quad (1)$$

where α'' is the imaginary part of the response :

$$(2) \quad X(\omega) = \alpha(\omega) \cdot F(\omega) \text{ and } \alpha(\omega) = \alpha'(\omega) + i\alpha''(\omega)$$

The relation (1) is known as F-D Theorem.

(1) is valid in the classical and quantum regimes.

Let's see the classical limit of (1).

In the classical limit $\frac{\hbar\omega}{kT} \ll 1$

Considering that $kT \approx 25 \text{ meV}$ at $300K$ and that $\hbar\omega \approx 1.24 \text{ eV}$ for a radiation of $1\mu\text{m}$, then :

$$\frac{\hbar\omega}{kT} = 1.24 \left(\frac{1\mu\text{m}}{\lambda} \right) \cdot \frac{300K}{0.025 \cdot T} = 14880 \left(\frac{1\mu\text{m}}{\lambda} \right) \cdot \left(\frac{1K}{T} \right)$$

Since $\lambda = \frac{c}{f}$ where $c = 3 \cdot 10^{14} \mu\text{m/s} = 3 \cdot 10^{14} \mu\text{m} \cdot \text{Hz}$ we have also that

$$\frac{\hbar\omega}{kT} \approx 0.05 \left(\frac{f}{1\text{GHz}} \right) \cdot \left(\frac{1K}{T} \right) \quad (3)$$

(2)

The expression (3) helps us to identify the limit of the classical limit.

so, considering $\frac{\hbar\omega}{kT} \ll 1$, from (1) we have :

$$S_{xx}(\omega) \approx 4\hbar\alpha'' \left\{ \frac{1}{2} + \frac{kT}{\omega\hbar} \right\} \approx 4\hbar\alpha'' \left\{ \frac{kT}{\hbar\omega} \right\} = \\ = \frac{4kT}{\omega} \cdot \alpha'' \quad (4)$$

The random behaviour of x could be explained as the result of a random force F acting on a noiseless x .

Since $\tilde{x} = x \tilde{F}$ Then

$$S_{xx} = |\alpha|^2 S_{ff} \quad (5)$$

and hence :

$$S_{ff} = 4\hbar \frac{\alpha''}{\alpha\alpha^*} \left\{ \dots \right\} \xrightarrow[\text{classical limit}]{\text{classical}} \frac{4kT}{\omega} \frac{\alpha''}{\alpha\alpha^*} \quad (6)$$

A final remark : once the observable x has been identified the associated force F is the one that the product $-x \cdot F$ correspond to a perturbation to the Hamiltonian of x .

So, the product $x \cdot F$ must correspond to an energy.

Now, let's apply the F-D Theorem to a Brownian particle. (3)

Be a particle of mass m placed in a fluid that causes a viscous force of constant γ to the particle.

If the particle is driven by a force F then the dynamical equation is:

$$m\ddot{x} = -\gamma\dot{x} + F \quad (7)$$

The F-D Theorem says that even if $F=0$ $x(t) \neq 0$
Therefore we are forced to write eq. (7) with the following:

$$m\ddot{x} = -\gamma\dot{x} + F + f \quad (8)$$

f is a random force that respect eq. (6). Later we will give the expression of S_{ff} . For the moment let's calculate the response α . Writing (7) in the frequency domain we have :

$$\alpha = \frac{\tilde{X}}{\tilde{F}} = \frac{-1}{m\omega^2 + i\omega\gamma} \quad (9)$$

where $\tilde{X}(\omega) = \int_{-\infty}^{\infty} x(t) e^{i2\pi f t} dt$ and $x(t) = \int_{-\infty}^{\infty} \tilde{X}(2\pi f) e^{-i2\pi f t} df$

then

$$\alpha'' = \frac{\alpha - \alpha^*}{2i} = \frac{-1}{2i} \left[\frac{1}{m\omega^2 + i\omega\gamma} - \frac{1}{m\omega^2 - i\omega\gamma} \right] = \frac{\omega\gamma}{m^2\omega^2 \left(\omega^2 + \frac{\gamma^2}{m^2} \right)} \quad (10)$$

(4)

In the classical limit:

$$S_{xx}(\omega) = \frac{4kT}{\omega} \alpha'' = \frac{4kT}{m} \frac{\gamma/m}{\omega^2(\omega^2 + \frac{\gamma^2}{m^2})} \quad (11)$$

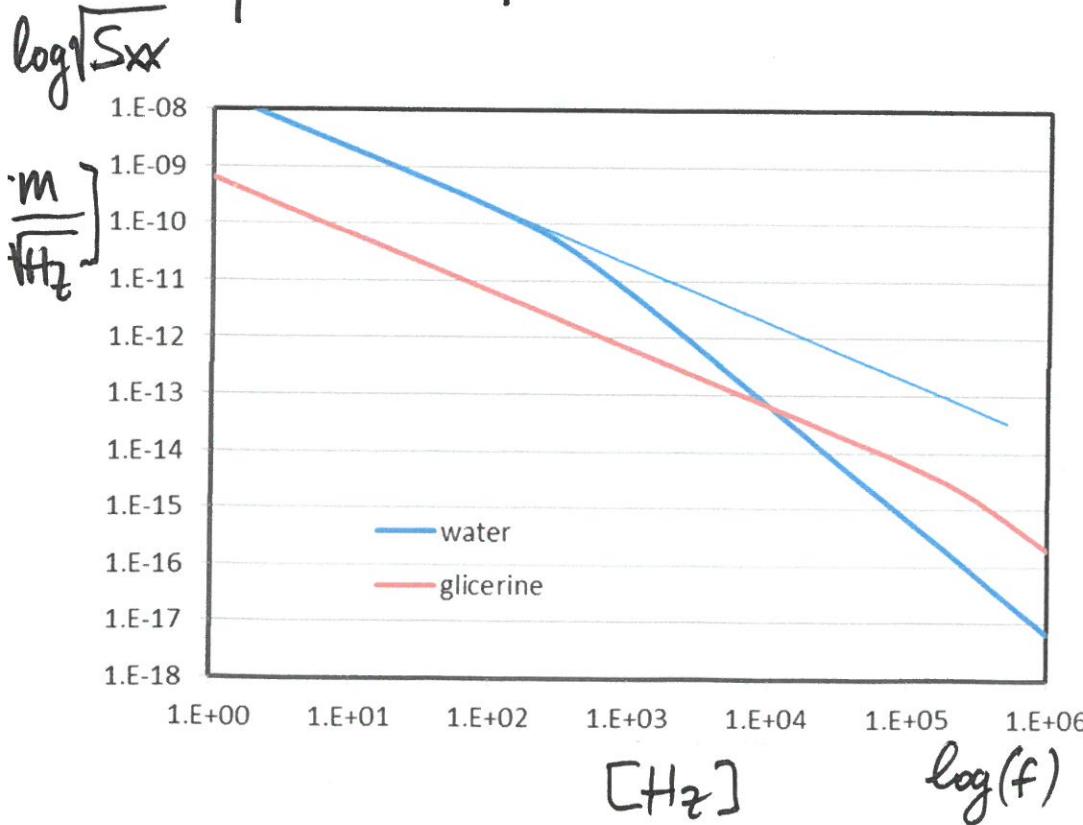
Let's do some numerical estimates.

A grain of pollen has a diameter of $100\text{ }\mu\text{m}$. Assuming it has the density of water:

$$m = \rho \frac{4}{3} \pi r^3 = 10^3 \cdot \frac{4}{3} \pi (5 \cdot 10^{-5})^3 \approx 5 \cdot 10^{-10} \text{ kg}$$

Using the Stokes formula: $\gamma = 6\pi\eta r$

	Water	Glycerine	$\sqrt{\frac{4kT}{m}} = 2\sqrt{\frac{0.025 \cdot 1.6 \cdot 10^{-19}}{5 \cdot 10^{-10}}} =$
η	10^{-3} Pas	1 Pas	
γ	$10^{-6} \frac{\text{Ns}}{\text{m}}$	$10^3 \frac{\text{Ns}}{\text{m}}$	
γ/m	$2 \cdot 10^3 \text{ s}^{-1}$	$2 \cdot 10^6 \text{ s}^{-1}$	$\approx 5.7 \frac{\mu\text{m}}{\text{Hz}}$



We can estimate the rms value of the displacement knowing that

$$\int \frac{dx}{x^2(x+a^2)} = -\frac{1}{a^2 \cdot x} - \frac{\arctan(\frac{x}{a})}{a^3}$$

Then:

$$\begin{aligned} x_{rms}^2 &= \int_0^\infty S_{xx} df = \frac{4kT}{m} \cdot \frac{a}{2\pi} \left[-\frac{\pi}{2} + \frac{1}{a^2 \Omega} + \frac{\arctan(\frac{\Omega}{a})}{a^3} \right] = \\ &= \frac{4kT}{m} \frac{1}{2\pi a^2} \left[\frac{a}{\Omega} + \frac{\Omega}{a} - \frac{\pi}{2} \right] \text{ if } \frac{\Omega}{a} \ll 1 \end{aligned}$$

Replacing $a = \frac{\gamma}{m}$ and integrating from $\Omega = 2\pi \cdot 1$

$$x_{rms}^2 = \frac{4kT}{m} \frac{1}{2\pi \gamma} \left[\frac{1}{2\pi} - \frac{\pi}{2\frac{\gamma}{m}} + \frac{2\pi}{(\frac{\gamma}{m})^2} \right] \approx \frac{kT}{m\pi^2 \frac{\gamma}{m}}$$

$$x_{rms} = \frac{2.85 \cdot 10^{-6}}{\pi \cdot \sqrt{2 \cdot 10^3}} \approx 20 \text{ nm} \text{ in water}$$

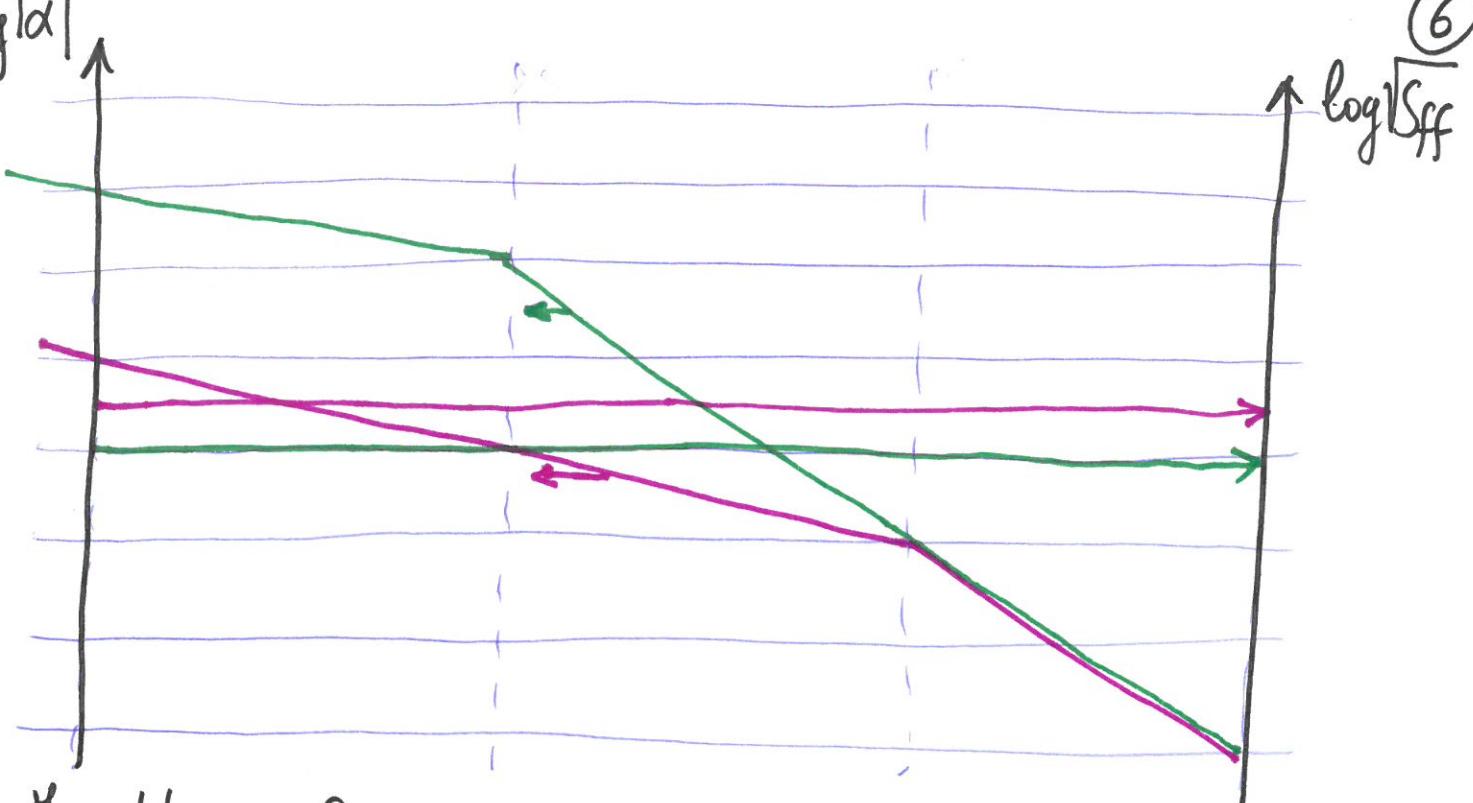
In glycerine the rms is about 30 times lower.

Let's see what is the amplitude spectral density of the fluctuating force f .

$$S_{ff} = \frac{S_{xx}}{|a|^2} \quad \text{from (9)} \quad aa^* = \frac{1}{m^2 \omega^4 + \omega^2 \gamma^2} = \frac{1}{m^2 \omega^2 \left(\omega^2 + \frac{\gamma^2}{m^2} \right)}$$

Therefore, from (11), we have

$$S_{ff} = \frac{4kT \gamma}{m^2} \frac{1}{\omega^2 \left(\omega^2 + \frac{\gamma^2}{m^2} \right)} \cdot m^2 \omega^2 \left(\omega^2 + \frac{\gamma^2}{m^2} \right) = 4kT \gamma \quad (12)$$



In this plot $\gamma = 10 \gamma_\infty$

We have seen that in order to calculate the thermal noise one needs of the "good" dynamical equation. For the Brownian particle that is eq.(7) or (8) but the real important ingredient is to have the good model for the dissipative part of the dynamics.

let's see why α'' is associated with the dissipation.

Under a periodic force $\tilde{F} = f_0 \operatorname{Re}\{e^{i\omega t}\}$ the observable X has a periodic motion with $\tilde{x} = \alpha \cdot \tilde{F}$. Our aim is to calculate the work done by the external force in one period :

$$W = \int_0^T F dx = \int_0^T F \cdot v \cdot dt \quad (13)$$

$$\begin{aligned}
 \text{Now, } V(t) &= \frac{d}{dt} X(t) = \frac{d}{dt} \operatorname{Re}\{\alpha \cdot F\} = \\
 &= \frac{d}{dt} \left\{ \frac{\alpha F + \alpha^* F^*}{2} \right\} = \frac{f_0}{2} \frac{d}{dt} \left\{ \alpha e^{i\omega t} + \alpha^* e^{-i\omega t} \right\} = \\
 &= i\omega \frac{f_0}{2} \left\{ \alpha e^{i\omega t} - \alpha^* e^{-i\omega t} \right\} \quad (14)
 \end{aligned}$$

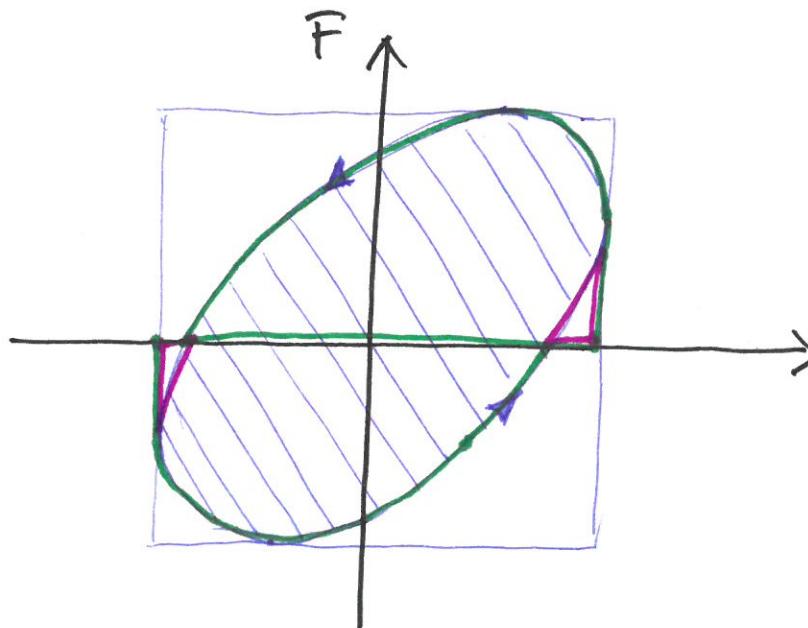
So, the instantaneous power $P = F \cdot V$ is :

$$\begin{aligned}
 P &= \frac{f_0}{2} \left\{ e^{i\omega t} + e^{-i\omega t} \right\} \cdot i\omega \frac{f_0}{2} \left\{ \alpha e^{i\omega t} - \alpha^* e^{-i\omega t} \right\} = \\
 &= \frac{i\omega f_0^2}{4} \left\{ -\alpha^* + \alpha + \alpha e^{2i\omega t} - \alpha^* e^{-2i\omega t} \right\} \quad (15)
 \end{aligned}$$

The terms depending on time give a null contribution after the integration in (13) because the integral is over a period.

Knowing that $\alpha = \alpha' + i\alpha'' \rightarrow \alpha - \alpha^* = 2i\alpha''$ hence

$$W = \frac{i\omega f_0^2}{4} \cdot 2i\alpha'' \cdot T = -\pi f_0^2 \alpha'' \quad (16)$$



the shaded area, being covered anti-clockwise, gives a negative integral.