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Master QLMN - Université Paris-Saclay

TD 3 - Non-equilibrium Statistical Physics
Langevin model - CORRECTION

1 Fluctuation of polarizability for a dielectric particle.

In this short exercise, we will derive an expression of the dipole moments fluctuations using a Langevin model, instead of the fluctuation dissipation theorem.

The differential equation describing the exponential decay can be written :

$$\frac{d\vec{p}}{dt} + \gamma\vec{p} = \vec{0}$$

We now add a noise term $\vec{f}$ accounting for the fluctuations of the dipole momentum :

$$\frac{d\vec{p}}{dt} + \gamma\vec{p} = \vec{f}$$

We assume that the fluctuations are delta-correlated, so that

$$\langle f_i(t) f_j(t+\tau)\rangle = |f|^2 \delta_{ij}(\tau)$$

In other words, different components of the noise have no correlation whatsoever whereas a single component is delta-correlated. This assumption is only valid if the typical correlation time of the noise is much shorter than the characteristic time of evolution of the dipole, so if the correlation time scale is much inferior to $\frac{1}{\gamma}$.

Now that we have a more explicit model for this random noise, we will see how it affects the fluctuations of the dipole. We write the dynamic equation in the harmonic regime, working on windowed functions p_T and f_T so that all quantities are square integrable :

$$\begin{aligned}(-i\omega + \gamma)p_{i,T}(\omega) &= f_{i,T}(\omega)\\ p_{i,T}(\omega) &= \frac{1}{\gamma - i\omega} f_{i,T}(\omega)\\ I_p(\omega) &= I_f(\omega)\frac{1}{\gamma^2 + \omega^2}\end{aligned}$$

showing that the power spectral density of the dipole fluctuations are connected to the power spectral density of the fluctuations of the noise. We have a model for the fluctuations of this noise, meaning that we will be able to compute the correlation of the dipole momentum using our model for the random noise. In particular, we know that the fluctuations are delta-correlated. In other words, the noise is a white noise, and its PSD is constant over its whole spectrum and we note $I_f(\omega) = I_f$.

$$\begin{aligned}\langle p(t)p(0)\rangle &= \int_{-\infty}^{+\infty} I_p(\omega)e^{-i\omega t}\frac{d\omega}{2\pi} \\ &= I_f \int_{-\infty}^{+\infty} \frac{1}{\gamma^2+\omega^2}e^{-i\omega t}\frac{d\omega}{2\pi} \\ &= I_f\frac{e^{-\gamma t}}{2\gamma}\text{for t} > 0\end{aligned}$$

We need the exact value of the noise PSD. We can immediately write :

$$I_f = \int \langle f_i(t)f_i(0)\rangle e^{i\omega t}dt = \int |f|^2\delta(t)e^{i\omega t}dt = |f|^2$$

And $\langle p(t)p(0)\rangle = |f|^2\frac{e^{-\gamma t}}{2\gamma}$.

We will derive the exact value of f using what we know of the fluctuations at equilibrium, usign the results of the previous tutorials and by noting the value of the correlation function at $t = 0$ is equal to the total power of the fluctuations at equilbrium :

$$\langle p_i(0)p_i(0)\rangle = C_{pp}(0) = \sigma_{pp}^2 = k_BT\chi_0$$

We finally get $|f|^2 = 2\gamma k_BT\chi_0$, and $\langle p(t)p(0)\rangle = k_BT\chi_0e^{-\gamma t}$.

The power spectral density can be derived by taking the Fourier transform of the previous expression :

$$I_p(\omega) = \int \langle p(t)p(0)\rangle e^{i\omega t}dt = \frac{2\gamma k_BT\chi_0}{\omega^2+\gamma^2}$$

2 Fluctuations of elongation of a spring

Writing the equation of motion in the Langevin model gives :

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

where the deterministic part of the force is given by the viscous term and spring reaction, and the random part given by R. In harmonic regime introducing the eigenfrequency of the system without dissipation $\omega_0^2 = \frac{k}{m}$, we get :

$$\left(-m\omega^2 - im\omega\gamma + m\omega_0^2\right)x(\omega) = R(\omega)$$

Taking the squared modulus of the Fourier transform the square integrable signal and random force $x_T(\omega)$ and $R_T(\omega)$, we can connect both PSDs :

$$I_x(\omega) = \frac{1}{m^2}\frac{I_R(\omega)}{|\omega_0^2 - \omega^2 - i\omega\gamma|^2}$$

In order to move to the correlation function, we need to take the Fourier Transform of the previous expression, following Wiener-Khinchine's theorem.

$$\langle x(t)x(t+\tau)\rangle = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}I_{xx}(\omega)e^{-i\omega\tau} = \frac{I_R}{2\pi m^2}\int_{-\infty}^{+\infty}d\omega\frac{e^{-i\omega\tau}}{|\omega_0^2-\omega^2-i\omega\gamma|^2}$$

We will compute this integral using the residue theorem. We replace this integral over $\mathbb{R}$ by an integral over a subspace of $\mathbb{C}$. We will first rewrite the denominator of the previous fraction to identify the poles of the integrand.

$$|\omega_0^2-\omega^2-i\omega\gamma|^2 = (\omega_0^2-\omega^2-i\omega\gamma)(\omega_0^2-\omega^2-i\omega\gamma)^*$$

We have a product of two polynoms of second order, complex conjugates of each other. We therefore have a total of 4 roots, for instance ω_1 and ω_2 and their complex conjugates.

$$\omega^2+i\omega\gamma-\omega_0^2 \rightarrow \Delta = 4\omega_0^2-\gamma^2$$

In order to simplify the upcoming expressions, we introduce the notation $\omega_0' = \frac{1}{2}\sqrt{4\omega_0^2-\gamma^2}$. Note that ω_0' is a real positive number, as we consider that viscous term is smaller that the eignefrequency of the system, preventing overdamping. The four poles of our integrands are :

$$\omega_1 = \frac{-i\gamma}{2}+\omega_0' = \frac{-i\gamma}{2}+\frac{\sqrt{4\omega_0^2-\gamma^2}}{2}$$

$$\omega_2 = \frac{-i\gamma}{2}-\omega_0'$$

$$\omega_1^* = \frac{i\gamma}{2}+\omega_0'$$

$$\omega_2^* = \frac{i\gamma}{2}-\omega_0'$$

$$\langle x(t)x(t+\tau)\rangle = \frac{I_R}{2\pi m^2}\int_{-\infty}^{+\infty}d\omega\frac{e^{-i\omega\tau}}{(\omega-\omega_1)(\omega-\omega_2)(\omega-\omega_1^*)(\omega-\omega_2^*)}$$

We can now explicitly use the residue theorem. We perform the integration in the complex plane instead of doing it on the real axis only. In other words, ω is now considered a complex number.

We choose a contour in the complex plane comprising the real axis and a half circle, so that the integral over the arc of the circle goes to zero (Jordan's lemma). This requires that the numerator, $e^{-i\omega\tau}$ goes to zero when ω goes to infinity in modulus. Taking τ as a real positive number, we can write :

$$\lim_{\omega\to+\infty}e^{-i\omega\tau} = 0 \Leftrightarrow \Im(\omega) < 0$$

In other words, we will use a contour in the lower half-plane, where ω will explore negative values of its imaginary part.

The lower half-space comprises two poles out of the four : ω_1 and ω_2, which both have a negative imaginary part.

We use the notation $f : \omega \to \frac{e^{-i\omega\tau}}{(\omega-\omega_1)(\omega-\omega_2)(\omega-\omega_1^*)(\omega-\omega_2^*)}$. The residue theorem gives :

$$\begin{aligned}
\langle x(t)x(t+\tau)\rangle &= \frac{I_R}{2\pi m^2}(-2i\pi)\left[\mathrm{Res}(f,\omega_1)+\mathrm{Res}(f,\omega_2)\right] \\
&= \frac{-iI_R}{m^2}\left[\frac{e^{-i\omega_0'\tau}e^{-\gamma\tau/2}}{(-i\gamma)(2\omega_0')(-i\gamma+2\omega_0')}+\frac{e^{+i\omega_0'\tau}e^{-\gamma\tau/2}}{(-\omega_0')(-i\gamma-2\omega_0')(-i\gamma)}\right] \\
&= \frac{+I_R}{m^2}\frac{e^{-\gamma\tau/2}}{2\gamma\omega_0'}\left[\frac{e^{-i\omega_0'\tau}}{(-i\gamma+2\omega_0')}-\frac{e^{+i\omega_0'\tau}}{(-i\gamma-2\omega_0')}\right]
\end{aligned}$$

In order to simplify the expression, let's focus on the denominators.

$$z = 2\omega_0' - i\gamma = |z|e^{i\mathrm{Arg}(z)}$$

with $|z| = \sqrt{4\omega_0'^2+\gamma^2} = \sqrt{4\omega_0^2-\gamma^2+\gamma^2} = 2\omega_0$, and $\mathrm{Arg}(z) = -\phi = \arctan(-\frac{\gamma}{2\omega_0'})$. Therefore, we can write :

$$2\omega_0' - i\gamma = 2\omega_0 e^{-i\phi}$$

and

$$-2\omega_0' - i\gamma = -2\omega_0 e^{i\phi}$$

Reinjecting the last two results in the correlation function :

$$\begin{aligned}
C_{xx}(\tau) = \langle x(t)x(t+\tau)\rangle &= \frac{+I_R}{m^2}\frac{e^{-\gamma\tau/2}}{2\gamma\omega_0'}\left[\frac{e^{-i\omega_0'\tau}}{(-i\gamma+2\omega_0')}-\frac{e^{+i\omega_0'\tau}}{(-i\gamma-2\omega_0')}\right] \\
&= \frac{+I_R}{m^2}\frac{e^{-\gamma\tau/2}}{2\gamma\omega_0'}\left[\frac{e^{-i\omega_0'\tau}}{2\omega_0 e^{-i\phi}}+\frac{e^{+i\omega_0'\tau}}{2\omega_0 e^{i\phi}}\right] \\
&= \frac{+I_R}{m^2}\frac{e^{-\gamma\tau/2}}{2\gamma\omega_0'}\left[\frac{e^{-i(\omega_0'\tau-\phi)}+e^{i(\omega_0'\tau-\phi)}}{2\omega_0}\right] \\
&= \frac{I_R}{2m^2\gamma\omega_0\omega_0'}\exp(-\gamma\tau/2)\cos(\omega_0'\tau-\phi)
\end{aligned}$$

Our expression of the correlation function still depends on I_R, yet unknown. In order to calculate this value, we use the expression of the fluctuations of the system : indeed, we have $\langle x^2\rangle = \sigma_x^2 = C_{xx}(\tau = 0)$ and from the equipartition theorem, at equilibrium : $\frac{1}{2}k\langle x^2\rangle = \frac{k_BT}{2}$.

$$\begin{aligned}
\langle x^2\rangle &= \frac{I_R}{2m^2\gamma\omega_0\omega_0'}\cos(-\phi) = \frac{k_BT}{m\omega_0^2} \\
I_R &= \frac{2\gamma m k_BT\sqrt{1-\frac{\gamma^2}{4\omega_0^2}}}{\cos(\phi)}
\end{aligned}$$

and finally :

$$\langle x(t)x(t+\tau)\rangle = \frac{k_BT}{m\omega_0^2}\frac{\cos(\omega_0\tau - \phi)\exp(-\gamma\tau/2)}{\cos(\phi)}$$