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TD 2 Physique Statistique Hors équilibre
Fluctuation-Dissipation Theorem

1 Polarizability of a Dielectric Particle

Derive the complex susceptibility $\chi(\omega)$.
We recall here the results of the previous tutorial.

We consider a dielectric particle much smaller than the excitation wavelength. In presence of a static electric field E_0, the particle has a dipole moment $\vec{p_0}$ given by its static susceptibility χ_0. When the electric field is switched off, the amplitude of the dipole moment decays exponentially with a time constant $\tau = 1/\gamma$.

Derive the relaxation function Ψ **and the linear response** $\chi(t)$**(t)** .

Let's define the origin of time when the electric field is switched off. For $t < 0$, we have the relation $\vec{p_0} = \chi_0 \vec{E_0}$. For $t > 0$, the dipole decays exponentially and we can write $\vec{p}(t) = \chi_0 \vec{E_0} \exp(-\frac{t}{\tau})$.The relaxation function is therefore : $\Psi(t) = \chi_0 e^{-\frac{t}{\tau}}$.

Following the textbook results, the response is given by :

$$\chi(t) = -\frac{d\psi(t)}{dt} H(t)$$

where $H(t)$ is the Heaviside function. We obtain immediately $\chi(t) = \frac{\chi_0}{\tau} e^{-\frac{t}{\tau}} H(t)$.
The complex susceptibility is given by the Fourier transform of the linear response :

$$\begin{aligned}\chi(\omega) &= \int_{-\infty}^{+\infty} \chi(t') e^{i\omega t'} dt' \\ &= \int_{0}^{+\infty} \frac{\chi_0}{\tau} e^{-\frac{t'}{\tau} + i\omega t'} dt' \\ &= \frac{\chi_0}{\tau} \frac{-1}{i\omega - \frac{1}{\tau}} = \frac{\chi_0}{1 - i\omega\tau}\end{aligned}$$

Fluctuations of the dipole moment .

The power spectral density of the fluctuations can be derived following two different options : either using the relaxation function to derive the correlation function, then using the Wiener-Khinchine theorem ; or using the susceptibility and the fluctuation-dissipation theorem.

Using the relaxation function, we can write for positive t :

$$\Psi(t) = \beta C_{pp}(t) = \beta \langle p(t)p(0) \rangle == \frac{1}{k_B T} \chi_0 e^{-t/\tau}$$

The relaxation function is defined for positive time, and describes the evolution of the system when the generalized force driving the system out of equilibrium is switched off.

The correlation function $C_{pp}(t)$ describes fluctuations at equilibrium of a stationary, random process. Stationarity implies :

$$C_{pp}(t) = \langle p(t)p(0)\rangle = \langle p(t+t_0)p(t_0)\rangle$$

In the correlation function, t is not to be understood as being a specific date, but more as being a time difference, time interval between which we want to measure the correlations in the fluctuations of the system. The correlation function is therefore defined for both positive and negative t : We have then $C_{pp}(t) = C_{pp}(-t)$. In other words,

$$C_{pp}(t) = \frac{1}{\beta}\chi_0 e^{-|t|/\tau}$$

We now use the W-K theorem :

$$\begin{aligned}
I_{pp}(\omega) &= k_B T\chi_0 \int_{-\infty}^{+\infty} C_{pp}(t)e^{i\omega t} \\
&= k_B T\chi_0 \left[\int_0^{+\infty} e^{(-1/\tau+i\omega)t} + \int_{-\infty}^{0} e^{(1/\tau+i\omega)t}\right] \\
&= k_B T\chi_0 \left[\frac{-1}{-1/\tau+i\omega} + \frac{1}{1/\tau+i\omega}\right] \\
&= \frac{2k_B T\chi_0/\tau}{\omega^2+1/\tau^2}
\end{aligned}$$

Using the susceptibility and the fluctuation dissipation theorem :

$$\begin{aligned}
\chi(\omega) = \frac{\chi_0}{1-i\omega\tau} \rightarrow I_{pp}(\omega) &= \frac{2k_B T}{\omega}\Im(\chi(\omega) \\
&= \frac{2k_B T}{\omega}\Im\left(\frac{\chi_0}{1-i\omega\tau}\right) \\
&= \frac{2k_B T}{\omega}\frac{\omega\tau\chi_0}{1+\omega^2\tau^2} = \frac{2k_B T\chi_0/\tau}{\omega^2+1/\tau^2}
\end{aligned}$$

2 Fluctuations of a torsion oscillator

In this problem, we will follow two paths to make a connection between the fluctuations of the system at equilibrium on one hand, and to the correlation function of the system on the other hand.

First, we will model the system by writing the equation of motion of the mirror when driven by an external harmonic torque, then we will derive the susceptibility of the system to derive the power spectral density and the correlations of the system using the fluctuation-dissipation theorem and the Wiener-Khinchine theorem.

2.1 Equilibrium Fluctuations

In statistical physics, a state of the system is defined by the two conjugated variables of angular position θ and angular momentum $p = J\dot{\theta}$. The classical approximation is valid if the energy difference between two consecutives state energy of the system is much less than $k_B T$. The rotation hamiltonian can be expressed as $H_r = \frac{p^2}{2J}$. Two quantum number j and m_j are associated to this hamiltonian, and the rotation energies are given by $\epsilon_r = Bj(j+1)$ with $B = \frac{\hbar^2}{2J}$.

Consecutive energy levels around Bj^2 are separated by an amount on the order of $2jB$. They move away from each other when j increrases. The classical approximation eventually fails at some temperature, but we will consider it valid in our situation, as B is a tiny number and j a large quantum number so that Bj^2 is around $k_B T$ at room temperature and $\Delta E \approx Bj << Bj^2$.

The energy of a state is the sum of its kinetic and potential energy :

$$E_r = \frac{1}{2}J\dot{\theta}^2 + \frac{1}{2}C\theta^2 = \frac{p^2}{2J} + \frac{C\theta^2}{2}$$

The partition function can be written in the most general way as : $Z = \sum_r e^{-\beta E_r}$. We consider now the classical approximation so that the discrete sum over all states r is replaced by an integral over the phase space of conjugated coordinates θ and p, related to the only degree of freedom in our problem (rotation along the axis of the torsion wire) :

$$\sum_r \rightarrow \int \frac{dpd\theta}{h}$$

where h accounts for the elementary volume of a state in the phase space in the classical approximation. We now compute the partition function :

$$\begin{aligned} Z &= \int \frac{d\theta dp}{h} e^{-\beta E(\theta,p)} \\ &= \int \frac{d\theta dp}{h} e^{-\beta(\frac{p^2}{2J}+\frac{C\theta^2}{2})} \\ &= \frac{1}{h}\left[\int_{-\infty}^{+\infty} e^{-\beta\frac{p^2}{2J}}dp\right]\left[\int_{-\infty}^{+\infty} e^{-\beta\frac{C\theta^2}{2}}d\theta\right] \end{aligned}$$

where we identify the integral of two gaussian functions. Knowing that $\int e^{-au^2}du = \sqrt{\frac{\pi}{a}}$, we finally get :

$$Z = \frac{1}{h}\sqrt{\frac{2J\pi}{\beta}}\sqrt{\frac{2\pi}{\beta C}} = \frac{k_B T}{\hbar\omega_0}$$

with $\omega_0 = \sqrt{\frac{C}{J}}$. We can easily derive the mean energy from now, using different techniques.

First, we can use the equipartition theorem : we have a one-degree-of-freedom harmonic oscillator problem, with one quadratic contribution to the energy coming from θ and potential energy, and another one coming from $\dot{\theta}$ and kinetic energy. We can directly write :

$$\langle E\rangle = \frac{k_B T}{2} + \frac{k_B T}{2} = k_B T$$

Alternatively, we can directly the relations between ensemble averages and the logarithm of the partition function :

$$\langle E\rangle = -\frac{\partial \ln Z}{\partial\beta} = -\frac{\partial}{\partial\beta}\left[-\ln\beta - \ln\hbar\omega_0\right] = \frac{1}{\beta} = k_B T$$

Finally, we can write that the mean energy is given by :

$$\langle E\rangle = \frac{C}{2}\langle\theta^2\rangle + \frac{J}{2}\langle\dot{\theta}^2\rangle$$

In order to compute the mean energy, we need to calculate the average values $\langle\theta^2\rangle$ and $< \dot{\theta}^2 >$. We use the definition of such averages, using the probability distribution :

$$\begin{aligned} \langle\theta^2\rangle &= \sum_r P_r\theta_r^2 \\ &= \frac{1}{Z}\int \frac{dpd\theta}{h} e^{-\beta(\frac{p^2}{2J}+\frac{C\theta^2}{2})}\theta^2 \\ &= \frac{1}{Z}\frac{\partial}{\partial C}\left[\int \frac{dpd\theta}{h} e^{-\beta(\frac{p^2}{2J}+\frac{C\theta^2}{2})}\right] \times \left(\frac{-2}{\beta}\right) \\ &= \frac{1}{Z}\frac{\partial Z}{\partial C} \times \left(\frac{-2}{\beta}\right) = -2k_B T\frac{\partial \ln Z}{\partial C} \end{aligned}$$

Using our previous result $Z = \frac{k_B T}{\hbar}\sqrt{\frac{J}{C}}$, we get :

$$\langle \theta^2 \rangle = -2k_B T \frac{\partial}{\partial C}[-\frac{1}{2}\ln C] = \frac{k_B T}{C},$$

and we can use a completely similar approach, with derivatives along J, to get $\langle \dot{\theta}^2 \rangle = \frac{k_B T}{J}$. This approach could let us derive $\langle \theta^2 \rangle$ along the way. We have access to the fluctuations of the system at equilibrium :

$$\begin{aligned}\sigma_\theta^2 = \langle \theta^2 \rangle - \underbrace{\langle \theta \rangle^2}_{=0} \\ &= \frac{k_B T}{C} \\ &= \int d\omega I_{\theta\theta}(\omega) \\ &= C_{\theta\theta}(0) \\ &= \frac{2k_B T}{\pi}\int_0^{+\infty} \frac{\chi"(\omega)}{\omega}\end{aligned}$$

2.2 Temporal Correlation of Fuctuations from the Fluctuation-Dissipation Theorem

An external driving torque $C_0 e^{-i\omega t}$ is applied to the system. The equation of motion reads :

$$J\ddot{\theta} = \Gamma(t) - C\theta - \gamma J\dot{\theta}$$

where $\Gamma(t) = C_0 e^{-i\omega t}$ is the applied torque, C is the torsion coefficient, and γ is the fluid friction coefficient. In the harmonic regime, we now can write :

$$(-J\omega^2 - \gamma J i\omega + C)\theta(\omega) = \Gamma(\omega).$$

Using the notation $\omega_0^2 = \frac{C}{J}$, we now have :

$$\theta(\omega) = \underbrace{\frac{1}{C - \gamma J\omega i - J\omega^2}}_{\text{Susceptibility:}\chi(\omega)}\Gamma(\omega) = \frac{C}{J}\frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma}\Gamma(\omega)$$

We now use the fluctuation-Dissipation theorem to derive the power spectral density of the fluctuations in position of the system from the susceptibility :

$$\begin{aligned}I_{\theta\theta}(\omega) &= \frac{2k_B T}{\omega}\Im(\chi(\omega)) \\ &= \frac{2k_B T}{\omega}\Im\left[\frac{C}{J}\frac{(\omega_0^2 - \omega^2 + i\gamma\omega)}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2}\right] \\ &= \frac{2k_B T C\gamma}{J}\frac{1}{\underbrace{[(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2]}_{\text{Lorentzian shape close to }\omega_0}}\end{aligned}$$

The previous expression shows that the power spectral density of the fluctuations follow a somewhat resonant behavior around ω_0, the eigenfrequency of the system.

We now apply the Wiener-Khinchine theorem to derive the correlation function $C_{\theta\theta}(t)$ of the angular fluctuations. The theorem states that the correlation function is the Fourier transform of the power spectral density :

$$C_{\theta\theta}(t) = \frac{2k_B T C\gamma}{J}\int \frac{e^{-i\omega t}}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2}\frac{d\omega}{2\pi}$$

Recalling the results of the previous tutorial :

At the end of the previous session, we derived the relation between the fluctuations of a dipole moment at equilibrium and the response, which was in this case a *static* response :

$$\sigma_{pi}^2 = \frac{\chi_0}{\beta} = k_B T \chi_0$$

Using this result and noting that $\chi_0 = \chi(\omega = 0)$, we can write :

$$\chi_0 = \frac{2}{\pi} \int_0^{+\infty} d\omega \frac{\chi^{"}(\omega)}{\omega}$$

This results connects the static response to an integral over the dissipative part, a special result coming from the Kramers-Kronig relations.