Master 2 Physique | ENS-Lyon
Deuxième Année | Université Lyon I

PHYSIQUE STATISTIQUE HORS EQUILIBRE

Transport coefficients and Kubo formulas: Shear viscosity

The aim of this exercise is to establish the expression of the shear viscosity η as a function of a self-correlation function. This expression is similar to the Kubo formula for the diffusion coefficient D.

1) The evolution of the local velocity $\overline{\vec{u}}(\vec{r},t)$ is described by the Navier-Stokes equation:

$$m\rho\frac{\partial\overline{\vec{u}}}{\partial t}(\vec{r},t) = -\vec{\nabla}P + \eta\Delta\overline{\vec{u}}$$

where m is the mass of one molecule, ρ is the numeric density and P the pressure. $\overline{\vec{u}}(\vec{r},t)$ represents the average of the dynamical quantity $\vec{u}(\vec{r},t)$ on a small, but macroscopic, volume:

$$\overline{\vec{u}}(\vec{r},t) = \frac{1}{v}\int_v \vec{u}(\vec{r}-\vec{r}\,',t)d\vec{r}\,'$$

and

$$\vec{u}(\vec{r},t) = \frac{1}{\rho}\sum_{i=1}^{N}\vec{v}_i(t)\delta(\vec{r}-\vec{r}_i(t))$$

where $i = 1,..,N$ is the index of the (identical) particles in the system. We define $\overline{\vec{j}}(\vec{k},t) = \int d\vec{r}\mathrm{e}^{-i\vec{k}.\vec{r}}\ \overline{\vec{u}}(\vec{r},t)$. Show that the transverse components (perpendicular to $\vec{k}$) of $\overline{\vec{j}}$, denoted as $\overline{j}_{\perp\alpha}$ ($\alpha = 1,2$), verify the equation of evolution:

$$m\rho\frac{\partial\overline{j}_{\perp\alpha}}{\partial t}(\vec{k},t) = -k^2\eta\overline{j}_{\perp\alpha}(\vec{k},t)$$

2) We denote $\vec{z}$ the axis bearing $\vec{k}$, and $\vec{x}$ is an axis perpendicular to $\vec{z}$. Consider the correlation function:

$$C(\vec{k},t) = <\sum_{i=1}^{N}\sum_{j=1}^{N}\dot{x}_i(t)\dot{x}_j(0)\mathrm{e}^{-ik[z_i(t)-z_j(0)]}>$$

Show that, for small k, we can write:

$$C(\vec{k},t) = C(\vec{k},0)\left(1 - \frac{k^2\eta t}{\rho m} + ...\right)$$

Show that:

$$C(\vec{k},0) = \frac{Nk_BT}{m}$$

3) Deduce from that result the following expression of the shear viscosity η:

$$\eta = \frac{1}{2Vk_BT\ t} < \sum_{i=1}^{N}\sum_{j=1}^{N} p_{x_i}(t)p_{x_j}(0)[z_i(t) - z_j(0)]^2 >$$

where V is the volume and $p_{x_i} = m\dot{x}_i$. To find this result, identify the coefficients of k^2 in both parts of the first equation of question 2).
4) Show that we can also write:

$$\eta = \frac{1}{2Vk_BT\ t} < \left[\sum_{i=1}^{N}\{z_i(t)p_{x_i}(t) - z_i(0)p_{x_i}(0)\}\right]^2 >$$

Here, we shall use the fact that the system is isolated, and is in equilibrium.
5) We can also note that:

$$\frac{d}{dt}\{z_i(t)p_{x_i}(t)\} = \frac{p_{z_i}(t)p_{x_i}(t)}{m} + z_i(t)F_{x_i}(t)$$

where $F_{x_i}(t)$ is the component along x of the force exerting on the molecule i.
Show finally that:

$$\eta = \frac{1}{Vk_BT}\int_0^{+\infty} dt < J(0)J(t) >$$

where

$$J = \sum_{i=1}^{N}\left(\frac{p_{z_i}p_{x_i}}{m} + z_iF_{x_i}\right)$$