Transport coefficients and Kubo formulas: Shear viscosity

The aim of this exercise is to establish the expression of the shear viscosity \( \eta \) 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 \( \vec{u}(\vec{r},t) \) is described by the Navier-Stokes equation:

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

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

\[
\vec{u}(\vec{r},t) = \frac{1}{V} \int_V \vec{u}(\vec{r} - \vec{r}',t)d\vec{r}'
\]

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 \( \vec{j}(\vec{k},t) = \int d\vec{r} e^{-i\vec{k}\cdot\vec{r}} \vec{u}(\vec{r},t) \). Show that the transverse components (perpendicular to \( \vec{k} \)) of \( \vec{j}_\alpha \), denoted as \( j_{\perp\alpha} \) \( (\alpha = 1, 2) \), verify the equation of evolution:

\[
m \rho \frac{\partial j_{\perp\alpha}}{\partial t}(\vec{k},t) = -k^2 \eta j_{\perp\alpha}(\vec{k},t)
\]

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

\[
C(\vec{k},t) = \langle \sum_{i=1}^{N} \sum_{j=1}^{N} \dot{x}_i(t)\dot{x}_j(0) e^{-ik|z_i(t) - z_j(0)|} \rangle
\]
Show that, for small \( k \), we can write:

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

Show that:

\[
C(\vec{k}, 0) = \frac{N k_B T}{m}
\]

3) Deduce from that result the following expression of the shear viscosity \( \eta \):

\[
\eta = \frac{1}{2V k_B T} \left< \sum_{i=1}^{N} \sum_{j=1}^{N} p_{x_i}(t)p_{x_j}(0)[z_i(t) - z_j(0)]^2 \right>
\]

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:

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

Here, we shall use the fact that the system is isolated, and is in equilibrium.

5) We can also note that:

\[
\frac{d}{dt} \left\{ z_i(t)p_{x_i}(t) \right\} = \frac{p_{z_i}(t)p_{x_i}(t)}{m} + z_i(t)F_{x_i}(t)
\]

where \( F_{x_i}(t) \) is the component along \( x \) of the force exerting on the molecule \( i \).

Show finally that:

\[
\eta = \frac{1}{V k_B T} \int_{0}^{+\infty} dt < J(0)J(t) >
\]

where

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