Master de Sciences de la Matière, deuxième année
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NONEQUILIBRIUM STATISTICAL PHYSICS
Première Session, Janvier 2006, durée 3h

Rheology of brownian elastic dumbbells

An elastic dumbbell is made of two identical Brownian particles connected by a Hookean spring. We consider a dilute solution of such dumbbells in a solvent, as a crude model for a polymer solution.
The equation of motion for the particle 1 of a dumbbell is of the Langevin type

$$M\frac{d\mathbf{V}_1}{dt} = -\zeta\mathbf{V}_1 - K(\mathbf{X}_1 - \mathbf{X}_2) + \mathbf{R}_1(t)$$

and similarly for particle 2

$$M\frac{d\mathbf{V}_2}{dt} = -\zeta\mathbf{V}_2 - K(\mathbf{X}_2 - \mathbf{X}_1) + \mathbf{R}_2(t)$$

Here $\mathbf{X_i}$ is the position of particle i, $\mathbf{V_i}$ its velocity (bold letters correspond to vectors). K is the spring constant of the Hookean spring, and $\mathbf{R_i}$ is the random force.

1. Describe the properties of the random forces $\mathbf{R}_i(t)$, within the Langevin model. How is the random force connected to the friction ζ in an equilibrium system ?

2. Show that the equations of motion can be transformed into an equation of motion for the center of mass coordinate, $\mathbf{C} = (\mathbf{X}_1 + \mathbf{X}_2)/2$, and the relative coordinate $\mathbf{U} = \mathbf{X}_2 - \mathbf{X}_1$

3. Write these equations in the Langevin form, by defining appropriate frictions, masses and random forces. SHow that by using the proper mass and friction, the fluctuation dissipation relation is obeyed by these frictions and random forces.

4. Write the Fokker-Planck equation for the distribution functions of $d\mathbf{C}/dt = \mathbf{W}$ and $\mathbf{C}$, $\psi(\mathbf{W}, \mathbf{C}, t)$

5. Write the Fokker-Planck equation for the distribution functions of $d\mathbf{U}/dt = \mathbf{V}$ and $\mathbf{U}$, $\phi(\mathbf{U}, \mathbf{V}, t)$

6. What is the equilibrium solution for $\phi(\mathbf{U}, \mathbf{V})$?

7. From now on consider the **strong friction** limit, so that the acceleration terms can be ignored in the Langevin equations. Write the equations of motion for $\mathbf{U}$ and $\mathbf{C}$ in the standard Langevin form, $dX/dt = -F(X) + R(t)$. Give the values of the functions $F(X)$ and $R(t)$ in each case.

8. Show that the distribution function of the internal dumbbell coordinate $\mathbf{U}$, $\psi(\mathbf{U}, t)$, obeys the following partial differential equation (where $\zeta' = \zeta/2$)

$$\zeta'\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial U_\alpha}(KU_\alpha\psi) + k_BT\frac{\partial^2\psi}{\partial U_\alpha\partial U_\alpha}$$

Greek indexes correspond to the components of the vector $\mathbf{U}$. Summation over repeated indexes is implicitly assumed.

9. The dumbbell is now in a position dependent velocity field $\mathbf{W}(\mathbf{X})$. This velocity field is assumed to be homogeneous, i.e. of the form $\mathbf{W} = [\kappa]\mathbf{X}$ where $[\kappa]$ is a fixed tensor.

$$W_\alpha(X) = \kappa_{\alpha\beta} X_\beta$$

The friction force on a particle is now $-\zeta(d\mathbf{X}/dt - \mathbf{W}(\mathbf{X}))$. Show that the evolution equation for $\psi(\mathbf{U}, t)$ is now

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial U_\alpha}\left(\left(\frac{K}{\zeta'} U_\alpha - \kappa_{\alpha\beta} U_\beta\right)\psi\right) + \frac{k_B T}{\zeta'}\frac{\partial^2 \psi}{\partial U_\alpha \partial U_\alpha}$$

10. It can be shown that the contribution to the stress tensor arising from the Hookean dumbbells in solution is

$$\sigma_{\alpha\beta} = nK < U_\alpha U_\beta >$$

where n is the number density of dumbbells, and the average is taken with the statistical weight $\psi(U, t)$. Check that $\sigma_{\alpha\beta}$ has the correct dimensions for a stress tensor. Show that the evolution equation for ψ can be transformed into an equation for the components of the stress tensor, of the form

$$\frac{d\sigma_{\alpha\beta}}{dt} - -\sigma_{\alpha\gamma}\kappa_{\beta\gamma} - \kappa_{\alpha\gamma}\sigma_{\gamma\beta} = \frac{2k_B T}{\zeta'}\delta_{\alpha\beta} - \frac{2K}{\zeta'}\sigma_{\alpha\beta}$$

(note: the order of indexes in the above equation is important. Recall that $[\kappa]$ is not, in general, a symmetric tensor).

11. Consider the case of a simple steady (time independent) shear flow, $\kappa_{xz} = \dot{\gamma}$ and all other components of κ are equal to zero. Compute the value of σ_{xz} and the viscosity of the system.

12. Compute the difference $\sigma_{xx} - \sigma_{zz}$ (first normal stress difference) as a function of $\dot{\gamma}$. What i sth ephysical implication of this normal stress difference, in terms of the forces exerted by a moving fluid ?