Statistical Physics and Computer Simulations
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Exercise Sheet 5

1. **Green–Kubo Formula for the Shear Viscosity**

   We start from the low Reynolds number equations of motion for an incompressible fluid with flow velocity $\vec{u}(\vec{r}, t)$, mass density ρ, shear viscosity η, kinematic viscosity $\nu = \eta/\rho$, pressure p,

$$
\begin{aligned}
\nabla \cdot \vec{u} &= 0, &(1)\\
\rho \frac{\partial}{\partial t} \vec{u} &= \eta \nabla^2 \vec{u} - \nabla p, &(2)
\end{aligned}
$$

   and assume that the flow is confined to a 3–dimensional box of size $V = L^3$ with periodic boundary conditions. The Hamiltonian of this system can be written as

$$
H = \frac{\rho}{2} \int_V d^3\vec{r}\, \vec{u}^2. \tag{3}
$$

   Expand the flow field in a Fourier series with respect to the spatial coordinates, and write the Hamiltonian as well as the equations of motion in terms of these Fourier modes. Show that the incopressibility constraint forces us to restrict our attention to *transversal* modes, where the amplitude is perpendicular to the wave vector. For example, you may assume that the wave vector is oriented in x direction, while the amplitude is parallel to the z axis. Show that the pressure term is irrelevant for these modes.

   Now assume that the system is in thermal equilibrium. From the Stokes equation, construct a phenomenological model for the time–displaced autocorrelation function of a mode. In terms of the amplitude, consider the scalar product (not the tensor product).

   Hint: Take a look at lecture 17 and the phenomenological model that we constructed for the momentum relaxation of a Brownian particle. Take into account the equipartition theorem. *Have care:* Make sure you count the number of degrees of freedom in the mode correctly, taking into account incompressibility.

Finish the phenomenological treatment by calculating the Fourier transform of this correlation function with respect to time. You should find a fairly familiar form.

Now, we consider the same system from a microscopic (atomistic) point of view, assuming that the microscopic Hamiltonian is

$$H = \sum_i \frac{\vec{p}_i^2}{2m} + \sum_{i<j} U\left(|\vec{r}_i - \vec{r}_j|\right). \tag{4}$$

Show that a suitable microscopic expression for the flow field is given by

$$\vec{u}(\vec{r}, t) = \rho^{-1} \sum_i \vec{p}_i \delta(\vec{r} - \vec{r}_i(t)), \tag{5}$$

and calculate its spatial Fourier transform. Now consider again one particular transversal mode. Assume that this mode can be considered as a slow variable in the sense of the Mori–Zwanzig formalism. Calculate the various terms in the memory equation. For the memory function, you may assume that the projection operator Q can be ignored, since we are discussing a long–wavelength hydrodynamic variable. After focussing attention on the leading–order behavior for small k, taking into account Newton's third law, and employing a Markov approximation to the memory function, your results should coincide with those of the phenomenological approach. Use this to finally derive the Green–Kubo formula for the shear viscosity, in terms of a time integral of the stress–stress autocorrelation function. Useful literature on this topic is the book by Hansen and McDonald, Theory of Simple Liquids.

The xz component of the stress is, in analogy to the expression derived in Sheet 4 (virial theorem)

$$P_{xz} = \frac{1}{Vm} \sum_i p_{ix} p_{iz} + \frac{1}{V} \sum_i F_{iz} x_i. \tag{6}$$

2. **The Box–Muller Algorithm**
Let u_1, u_2 be two independent random numbers, uniformly distributed between zero and one. Furthermore, let

$$x_1 = \sqrt{-2 \ln u_1} \sin(2\pi u_2), \tag{7}$$

$$x_2 = \sqrt{-2 \ln u_1} \cos(2\pi u_2). \tag{8}$$

Calculate the probability density for the pair (x_1, x_2) by means of the Jacobi determinant.