"Many particle systems out of equilibrium" Problems, Series 1, 2006-07.

Problem 1. Microscopic pressure tensor

a) Show that the microscopic momentum density $\boldsymbol{G}^{micr}(\boldsymbol{r}, t)$ satisfies the local conservation law

$$\frac{D\boldsymbol{G}^{micr}(\boldsymbol{r},t)}{Dt} = \frac{\rho^{micr}(\boldsymbol{r},t)}{m}\boldsymbol{F}^{ext}(\boldsymbol{r})$$
$$-\nabla\cdot\Big[\mathsf{P}^{micr}(\boldsymbol{r},t) + (\boldsymbol{G}^{micr} - \rho^{micr}\boldsymbol{u}(\boldsymbol{r},t))\boldsymbol{u}\Big] - \boldsymbol{G}^{micr}\nabla\cdot\boldsymbol{u} \qquad (1)$$

For brevity the arguments $(\boldsymbol{r}, t)$ were omitted after the first appearance. For an N-particle system with Hamiltonian

$$H = \sum_i \left[\frac{p_i^2}{2m} + V^{ext}(\boldsymbol{r}_i)\right] + \sum_{i<j}\phi(r_{ij}) \qquad (2)$$

the microscopic pressure tensor is defined as

$$\begin{aligned}\mathsf{P}^{\mathsf{micr}}(\boldsymbol{r},t) &= \sum_i m(\boldsymbol{v}_i - \boldsymbol{u}(\boldsymbol{r},t))(\boldsymbol{v}_i - \boldsymbol{u}(\boldsymbol{r},t))\delta(\boldsymbol{r}-\boldsymbol{r}_i) + \\ &\quad \sum_{i<j}\int_0^1 d\lambda\, \boldsymbol{r}_{ij}\boldsymbol{F}_{ij}\delta(\boldsymbol{r}-\lambda\boldsymbol{r}_i-(1-\lambda)\boldsymbol{r}_j). \qquad (3)\end{aligned}$$

Here $\boldsymbol{F}_{ij} \equiv -\nabla_{\boldsymbol{r}_{ij}}\phi(r_{ij})$.

b) Show that, on averaging, Eq. (1) reduces to Eq. (16) of the lecture notes. You may use the identities

$$\langle\boldsymbol{G}^{micr}(\boldsymbol{r},t)\rangle = \rho(\boldsymbol{r},t)\boldsymbol{u}(\boldsymbol{r},t); \qquad \langle\mathsf{P}^{micr}(\boldsymbol{r},t)\rangle = \mathsf{P}(\boldsymbol{r},t)$$

Problem 2. Virial theorem

Derive the virial theorem: this states that the pressure in a d-dimensional simple fluid may be obtained as

$$p = nk_BT + \frac{n^2}{2d}\int d\boldsymbol{r}\, g(r)rF(r). \qquad (4)$$

Here n is the average number density, $n = N/V$, of the system and $g(r)$ is the *pair correlation function*. For a homogeneous system this is defined as the ratio of the probability of finding a particle at a distance r from a given particle and that of finding it at an arbitrary position. This may be formulated in an equation as

$$\langle \sum_{i \neq j} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\delta(\boldsymbol{r}' - \boldsymbol{r}_j) \rangle = n^2 g(|\boldsymbol{r} - \boldsymbol{r}'|).$$

Problem 3. The energy equation

In some books (e.g. McQuarrie "*Statistical Mechanics*" and D.J. Evans and G.P. Morriss, "*Statistical Mechanics of Nonequilibrium Liquids*") the equation for heat conduction is given in the form

$$\frac{DT}{Dt} = \frac{1}{\rho c_v} \nabla^2 T.$$

In other books (e.g. Landau-Lifshitz "*Fluid Mechanics*") the same equality appears with c_p instead of c_v. Check which equation is correct, or, if the answer is not unique, under which conditions which equation is correct. Hint: start by rewriting

$$\frac{D\hat{\epsilon}}{Dt} = \left(\frac{\partial \hat{\epsilon}}{\partial T}\right)_\rho \frac{DT}{Dt} + \left(\frac{\partial \hat{\epsilon}}{\partial \rho}\right)_T \frac{D\rho}{Dt},$$

with $\hat{\epsilon}$ the energy density, and combine the resulting equation with the continuity equation to obtain an equation for T alone.