"Many particle systems out of equilibrium" Problems, Series 8, 2006-07.

Problem 17. Kubo's linear response formalism

a) Show that, in the Grand canonical ensemble, the Kubo product between operators A and B that both commute with the number operator N, assumes the form

$$\langle A|B\rangle_G = \frac{1}{\beta}\int_0^\beta d\,\lambda\,\langle A^\dagger \exp -\lambda(H_0-\mu N) B \exp \lambda(H_0-\mu N)\rangle_G, \quad (1)$$

with $\langle\rangle_G$ the Grand canonical average.

b) Show that the Kubo products between Fourier components of conserved densities, such as $n(\boldsymbol{k})$ and $\boldsymbol{G}(\boldsymbol{k})$, in the limit $\boldsymbol{k} \to 0$ approach the static correlation functions between the same quantities.

Problem 18. Debye's theory of dielectric response

a) In fluids consisting of electric dipoles with permanent dipole moment $\boldsymbol{\mu}$, it is often a good approximation assuming that each of the dipole moments performs a rotational diffusive motion. In such a process the magnitude of the dipole moment does not change, but the unit vector $\hat{\boldsymbol{\mu}}$ describes a random motion over the unit sphere, that may be described by the equation

$$\frac{\partial P(\theta,\phi,t)}{\partial t} = D_R L^2 P(\theta,\phi,t). \quad (2)$$

Here L^2 is the Laplacian in spherical coordinates at $r = 1$, without the radial contribution. What are the eigenfunctions for this equation and what are their decay rates?

b) Calculate the frequency dependent dielectric constant (both real and imaginary part) for a system with n of these dipoles per unit volume.

c) A classical, rigid diatomic molecule in a dilute gas may be described as performing a uniform rotation in a fixed plane, until it collides with another molecule, after which it will start rotating with a different angular velocity in a different plane. Assume these collisions occur at completely random times with average frequency ν. For small ν only those molecules will contribute to the dielectric response at frequency ω that rotate at almost the same frequency (all other frequencies are damped out by interference). Therefore the dielectric constant may be calculated by evaluating the integrals of the correlation functions of individual molecules up to the time they first collide. Perform this calculation, assuming an equilibrium distribution of angular velocities and orientations of the plane of rotation, average over the distribution of final times and give the frequency dependent dielectric constant. You may simplify the thermal average by assuming $\nu \ll \sqrt{k_B T/I}$, with I the moment of inertia of the molecule with respect to the rotation axis, plus using that the main contributions come from rotation frequencies that are almost resonant with the field frequency.

Problem 19. Combined rotation and vibration

In reality a diatomic molecule will perform oscillations on top of the rotation in the direction connecting the centers of the atoms. Assume these are harmonic oscillations with a fixed frequency ω_0 and a typical amplitude much smaller than the distance between the atoms. Calculate the additional contributions from these to the frequency dependent dielectric constant, under the same assumptions as made in problem 18b.