

22.903 Home Work Set No. 3 (Professor Sow-Hsin Chen) Spring Term 2005. Due May 2, 2005

1. There is a practically important case in light and x-ray scattering from isotropic fluids where the coherent dynamic structure factor can be obtained rigorously. It is called the Rayleigh-Brillouin scattering from fluids obeying linearized hydrodynamic equations. This is the case when radiation is probing long wave length thermal density fluctuations in the fluids. Read J.P. Boon and S. Yip, "Molecular Hydrodynamics", McGraw Hill (1980), p.238-251, and derive the following results.

(A) The coherent intermediate scattering function for fluid of number density n is given by

$$\frac{F(k,t)}{S(k)} = \left(1 - \frac{1}{\gamma}\right) \exp\left[-k^2 \left(\frac{\kappa}{nC_p}\right) t\right] + \frac{1}{\gamma} \exp(-k^2 \Gamma t) [\cos(v_s k t) + b k \sin(v_s k t)] \quad (1)$$

where κ is the thermal conductivity, v_s the adiabatic sound speed, η and η_v the shear and bulk viscosities, and $\gamma = C_p / C_v$, the ratio of specific heats at constant pressure and at constant volume,

$$\Gamma = \frac{1}{2} \left[(\gamma - 1) \left(\frac{\kappa}{nC_p} \right) + \left(\frac{\eta_L}{nm} \right) \right]; \quad \eta_L = \frac{4}{3} \eta + \eta_v,$$

$$b = \frac{1}{\gamma v_s} \left[3\Gamma - \left(\frac{\eta_L}{nm} \right) \right]; \quad v_s = \left(\frac{\gamma}{nm \chi_T} \right)^{1/2}; \quad \chi_T = \text{isothermal compressibility.}$$

(B) The dynamic structure factor is

$$\frac{S(k,\omega)}{S(k)} = \frac{1}{\pi} \left\{ \left(1 - \frac{1}{\gamma}\right) \frac{(\kappa/nC_p) k^2}{\omega^2 + \left[(\kappa/nC_p) k^2 \right]^2} + \frac{1}{2\gamma} \left[\frac{\Gamma k^2 + bk(\omega - v_s k)}{(\omega - v_s k)^2 + (\Gamma k^2)^2} + \frac{\Gamma k^2 + bk(\omega + v_s k)}{(\omega + v_s k)^2 + (\Gamma k^2)^2} \right] \right\}$$

Show from kinematic consideration that in order to measure Brillouin peaks of a fluid with adiabatic sound speed v_s , the incoming speed of neutrons must be larger than v_s .

2. Prove the following Sear's expansion for the rotational intermediate scattering function of a water molecule:

$$\left\langle e^{-i\vec{Q}\cdot\vec{b}(0)} e^{i\vec{Q}\cdot\vec{b}(t)} \right\rangle = \sum_{\ell=0}^{\infty} (2\ell+1) j_{\ell}^2(Qb) \left\langle P_{\ell}(\hat{b}(0) \cdot \hat{b}(t)) \right\rangle. \quad (2)$$

Where \vec{b} is the vector from the center of mass of the molecule to the location of the hydrogen atom which is scattering neutrons. Hint: start by expanding each exponential factor on the left-hand side of the above equation by spherical harmonics and then use the addition theorem of the spherical harmonics to obtain the last factor in this equation. This factor is called the rotational correlation function of the ℓ - th order.

3. In general, the self-intermediate scattering function or the intermediate scattering function of a tagged particle in an inhomogeneous liquid (or confined liquid), is defined as:

$$F_s(\mathbf{Q}, t) = \int \int e^{i\vec{Q}\cdot(\vec{r}-\vec{r}_0)} G_s(\vec{r}, t | \vec{r}_0) p(\vec{r}_0) d^3r d^3r_0 \quad (3)$$

where $G_s(\vec{r}, t | \vec{r}_0)$ is the van-Hove space-time self-correlation function of the tagged particle and $p(\vec{r}_0)$ the equilibrium distribution of the particle under the confining potential $V(r)$. Use this definition to show the following four important properties.

(A) Conservation of probability:

$$F_s(\mathbf{Q} = 0, t) = \int \int G_s(\vec{r}, t | \vec{r}_0) p(\vec{r}_0) d^3r d^3r_0 = 1. \quad (4)$$

(B) Initial condition:

$$G_s(\vec{r}, t = 0 | \vec{r}_0) = \delta(\vec{r} - \vec{r}_0) \quad \text{leads to} \quad F_s(\mathbf{Q}, t = 0) = 1. \quad (5)$$

(C) Equilibrium distribution:

$$G_s(\vec{r}, t = \infty | \vec{r}_0) = p(\vec{r}) = \frac{1}{Z} e^{-V(r)/k_B T} \quad (6)$$

where Z is the normalization factor.

(D) Elastic Incoherent Structure Factor:

$$F_s(Q, t = \infty) = \text{EISF} = \left| \int p(\vec{r}) e^{i\vec{Q} \cdot \vec{r}} d^3r \right|^2 \quad (7)$$

In particular, use the last relation to calculate EISF for the following two cases.

Case One: When the tagged particle is confined inside a sphere of radius a ,

$$\text{EISF} = \left[\frac{3j_1(Qa)}{Qa} \right]^2. \quad (8)$$

Case Two: When the tagged particle is confined in a harmonic potential well,

$$\text{EISF} = \exp \left[-\frac{1}{3} Q^2 \langle r^2 \rangle \right], \quad (9)$$

where $\langle r^2 \rangle$ is the mean square vibrational amplitude of the particle in the well. Calculate this quantity in terms of the parameters of the potential well.