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Advanced Statistical Physics II – Problem Sheet 3

Problem 1 – Kramers-Kroning relation

a) (2P) Consider a single-sided function $\chi(t)$ (i.e. $\chi(t < 0) = 0$). Derive expressions for the real and imaginary part of its Fourier transform in terms of the even part $\chi_e(t) = (\chi(t) + \chi(-t))/2$ only.

b) (2P) Calculate the Fourier transform of sign function $\tilde{\text{sign}}(\omega)$.

Hint: use the regularisation technique presented in the lecture

c) (2P) Using the results of the previous problems, derive the Kramers-Kronig relation for the imaginary part of a single-sided function:

$$\tilde{\chi}''(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\omega' \frac{\tilde{\chi}'(\omega')}{\omega - \omega'} \tag{1}$$

d) (3P) Verify eq. 1 for the function

$$\chi(t) = \theta(t)cos(\overline{\omega}t) \tag{2}$$

Hint: $\theta(t) = \frac{1}{2}(\text{sign(t)} + 1)$

Problem 2 – Convolution integrals

a) (3P) Consider the following function:

$$x(t) = \theta(t)e^{-t/\tau} + \int_{-\infty}^{t} e^{-(t-t')/\tau}x(t')dt' \tag{3}$$

Write down the Fourier transform of $x(t)$ in closed form.
Hint: Remember problem set 0.

Problem 3 – Dipole in 3D

Consider a dipole in an electric field in z-direction with the following Hamiltonian:

$$\mathcal{H} = \mathcal{H}_{kin} - \vec{p}\vec{E} \tag{4}$$

a) (2P) Calculate the partition function $Z(E)$.

b) (2P) Now consider the case in which the the electric field is composed of a constant part E_0 and a perturbation h , i.e. $\vec{E} = (E_0 + h)\vec{\mathbf{e}}_z$.
Calculate $\langle p_z \rangle$ and expand it to linear order in h.

c) (2P) Calculate $\langle p_z^2 \rangle_{h=0} - \langle p_z \rangle_{h=0}^2$ and relate it to the linear response function.

Problem 4 – Onsager's relation

We consider a binary system consisting of a mixture of two solutions with non-uniform temperature and composition. The volume fractions are $\phi_1(\vec{r})$ and $\phi_2(\vec{r}) = 1 - \phi_1(\vec{r})$ and the current of the two components satisfy $\mathbf{J}_1 + \mathbf{J}_2 = 0$, the first one is defined as:

$$\mathbf{J}_1 = -D\nabla\phi_1 - \phi_1\phi_2 D_T \nabla T \tag{5}$$

where D is the gradient diffusion coefficient, D_T thermal diffusion coefficient. We define the heat flow, that is driven by temperature and concentration gradients as:

$$\mathbf{J}_Q = -\lambda\nabla T - D_F \nabla\phi_1 \tag{6}$$

where λ is the thermal conductivity, D_F the Dufour coefficient. The hat indicates volume specific quantities, such as the molecular chemical potential divided by the molecular volume, $\hat{\mu}_k = \mu_k/v_k$.

We now consider a binary system with an initial perturbation away from equilibrium. For sufficiently weak deviations, Onsager established linear relations between the fluxes and forces. The particle currents cancel each other, $\mathbf{J}_2 = -\mathbf{J}_1$, so the system can be reduced to 2 independent flows.

$$\mathbf{J}_1 = L_{1Q}\nabla\frac{1}{T} - L_{11}\frac{\nabla(\hat{\mu}_1 - \hat{\mu}_2)}{T} \tag{7}$$

$$\mathbf{J}_Q = L_{QQ}\nabla\frac{1}{T} - L_{Q1}\frac{\nabla(\hat{\mu}_1 - \hat{\mu}_2)}{T} \tag{8}$$

a) (2P) Compare the two systems and using Onsager's reciprocal relation, find the relation between D_T and D_F.

   Hint: $\hat{\mu}_1 = ln(\phi_1)$