HW (2) Phy211 B

§1 Fluctuation, dissipation, and Linear response

In the lecture, we have shown that if a system with Hamiltonian H subjected to an external perturbation $H_e(t) = B e^{-i\omega t + \eta t}$, then the physical quantity of operator A at time t, satisfies

$$\langle A(t) \rangle = \langle A \rangle - \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt' \, \theta(t-t') \langle | [A(t), B(t')] | \rangle e^{-i\omega t' + \eta t'}$$

where $\langle A \rangle$ is the value of A in thermal equilibrium, $A(t)$ and $B(t')$ are operators of A and B in the Heisenberg picture of H, i.e. $A(t) = e^{\frac{i}{\hbar}Ht} A e^{-\frac{i}{\hbar}Ht}$, $B(t') = e^{\frac{i}{\hbar}Ht'} B e^{-\frac{i}{\hbar}Ht'}$.

Define the retarded Green function as

$$G_r(t-t') = -\frac{i}{\hbar} \theta(t-t') \langle | [A(t), B(t')] | \rangle,$$

where the "$\langle | \cdots | \rangle$" means the expectation value in thermal equilibrium.

1 Lehmann representation:

Prove that: $G_r(t-t') = -\frac{i}{\hbar} \theta(t-t') Z^{-1} \sum_{mn} e^{-\beta E_m} \langle m | B | n \rangle \langle n | A | m \rangle$
$\times e^{-\frac{i}{\hbar}(E_m - E_n)t} \left(e^{\beta(E_m - E_n)} - 1 \right)$, where $Z = \sum_m e^{-\beta E_m}$ and $|m\rangle, |n\rangle$ are eigenstates of the unperturbated Hamiltonian H. The Fourier transform should be

$$G_r(\omega) = Z^{-1} \sum_{mn} e^{-\beta \mathcal{E}_m} \langle m | B | n \rangle \langle n | A | m \rangle \frac{e^{\beta(\mathcal{E}_m - \mathcal{E}_n)} - 1}{\hbar\omega - (\mathcal{E}_m - \mathcal{E}_n) + i\eta}$$

We define the spectra function as

$J(\omega) = -2\,\mathrm{Im}\, G_r(\omega)$, and prove that

$$G_r(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{J(\omega')}{\omega - \omega' + i\eta}\, d\omega' .$$

2° Let us set $A = B$, and define the correlation function

$$S(t-t') = \langle A(t) A(t') \rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} S(\omega) .$$

Show that $S(t-t'=0) = \langle A^2 \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{J(\omega)}{e^{\beta\omega} - 1}\, d\omega .$

$\langle A^2 \rangle$ means the ground state fluctuation, and $J(\omega)$ denotes the dissipation spectra, thus the above expression is called fluctuation-dissipation theorem.

Show that for the case of $A = B$, $J(\omega) > 0$ at $\omega > 0$, and

$J(-\omega) = -J(\omega)$.

3° Consider the example of forced harmonic oscillator

$$H = -\frac{1}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega_0^2 x^2 , \quad H_e = -f(t)\, x(t)$$

define the retarded response function as the displacement-correlation function

$$\chi(t-t') = -\frac{i}{\hbar}\,\theta(t-t')\,\langle|[x(t),\ x(t')]|\rangle\,,$$

Calculate $\chi(\omega)$ and $J(\omega)$, Show $\chi(\omega)$ has the pole at $\pm\omega_0$.

Show that in the classic limit $T \to +\infty$,

$$\langle x^2\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{k_BT}{\omega}\,J(\omega)\,d\omega = \frac{k_BT}{m\omega_0^2}$$ as required by

the equipartition theorem!

§2: Sum-rule (f - longitudinal).

Prove that for inter-acting electron gas, the following relations are exact.

(a) $[[H,\ \rho_q],\ \rho_{-q}] = -\left(\frac{Nq^2}{m}\right)$

(b) $\int_0^{+\infty} d\omega\ \omega\ \mathrm{Im}\,\chi(q,\omega) = +\frac{\pi}{2}$

Where ρ_q is the Fourier component of density operator. N is number of particle, $\chi(q,\omega)$ is the density-density response (vaccum polarization), ω_p: plasmon frequency.

3a) Prove that the 3D plasmon dispersion relation is

$$\omega_q^2 = \omega_p^2 + \frac{3}{5} q^2 v_F^2 \quad \text{where } v_F \text{ is the Fermi velocity}$$

$$\text{and } \omega_p^2 = \frac{4\pi N e^2}{m}$$

(from the evaluation of the zero of $\mathcal{E}(q,\omega)$, at $\frac{\omega}{v_F q} \gg 1$).

b) Derive the plasma frequency through classic equation of motion.

Hint: use the continuity equation and equation of motion

$$\frac{\partial n}{\partial t} + \nabla\cdot(n\vec{v}) = 0, \qquad m\frac{\partial}{\partial t}(n\vec{v}) + m\vec{v}\cdot\nabla(n\vec{v}) = -ne\vec{E}.$$

Expand to the leading order fluctuation $\delta n = n - n_0$. Show

$$\frac{\partial^2}{\partial t^2}\delta n = -\frac{4\pi n_0}{m}\delta n \quad \text{at the leading order.}$$

4) We consider a Jellium model.

a) Show that if the screened interaction is taken as the Thomas-Fermi form, then in the limit of low density region, the Hartree Fock energy of an electron with spin up or down is independent of k, its momentum.

b) Assume a finite spin polarization $P = N\uparrow - N\downarrow$, find the total Hartree-Fock energy in the limit of a). Express the result as a function of density n, Fermi energy $\mathcal{E}_F^0$, polarization P, and Thomas-Fermi vector k_{TF}.

c) Calculate the spin-susceptibility due to Hartree-Fock correction. Compare it with the free system. Is the system possible to be spin-polarized? (ferromag)