Solution to HW 2

1.1 $G_r(t-t') = \frac{-i}{\hbar}\theta(t-t')\langle|[A(t), B(t')]|\rangle$

$$= -\frac{i}{\hbar}\theta(t-t')\, Z^{-1}\sum_m\{\langle m|A(t)B(t')|m\rangle - \langle m|B(t')A(t)|m\rangle\}e^{-\beta E_m}$$

$$= -\frac{i}{\hbar}\theta(t-t')\, Z^{-1}\sum_{m,n}\{\langle m|A(t)|n\rangle\langle n|B(t')|m\rangle - \langle m|B(t')|n\rangle\langle n|A(t)|m\rangle\}e^{-\beta E_m}$$

$$A(t) = e^{iHt/\hbar} A e^{-iHt/\hbar}, \quad B(t') = e^{iHt'/\hbar} B e^{-iHt'/\hbar}$$

$$\Rightarrow G_r(t-t') = -\frac{i}{\hbar}\Theta(t-t')\, Z^{-1}\sum_{m,n}\{e^{i(E_m-E_n)t/\hbar}\cdot e^{+i(E_n-E_m)t'/\hbar}\langle m|A|n\rangle\langle n|B|m\rangle$$

$$- e^{i(E_m-E_n)t'/\hbar} e^{+i(E_n-E_m)t/\hbar}\langle m|B|n\rangle\langle n|A|m\rangle\} e^{-\beta E_m}$$

$$= -\frac{i}{\hbar}\Theta(t-t')\, Z^{-1}\sum_{m,n} e^{i(E_m-E_n)(t-t')/\hbar}\{\langle m|A|n\rangle\langle n|B|m\rangle\}\{e^{-\beta E_m} - e^{-\beta E_n}\}$$

$$= \frac{-i}{\hbar}\Theta(t-t')\, Z^{-1}\sum_{m,n} e^{-\beta E_m} e^{i(E_m-E_n)(t-t')/\hbar}\underbrace{[1 - e^{\beta(E_n-E_m)}]}_{\langle m|A|n\rangle\langle n|B|m\rangle}$$

or exchange. m, n

$$\rightarrow -\frac{i}{\hbar}\Theta(t-t')\, Z^{-1}\sum_{m,n} e^{-\beta E_m}\langle m|B|n\rangle\langle n|A|m\rangle\cdot$$

$$e^{-\frac{i}{\hbar}(E_m-E_n)t}\,[e^{\beta(E_m-E_n)} - 1]$$

$$G_r(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\cdot G_r(t)$$

$$= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} \langle m|B|n\rangle \langle n|A|m\rangle \left(e^{\beta(E_m - E_n)} - 1 \right)$$

$$\cdot \int_{-\infty}^{+\infty} dt \; \left(\frac{-i}{\hbar}\right) \theta(t) \; e^{i\left(\omega - \frac{(E_m - E_n)}{\hbar} + i\eta\right) t}$$

$$= Z^{-1} \sum_{m,n} e^{-\beta E_m} \langle m|B|n\rangle \langle n|A|m\rangle \frac{e^{\beta(E_m - E_n)} - 1}{\omega - (E_m - E_n)/\hbar + i\eta}$$

using the fact $\dfrac{1}{x \pm i\eta} = P\left(\dfrac{1}{x}\right) \mp i\pi\delta(x)$

$$J = -2\,\mathrm{Im}\, G_r(\omega) = Z^{-1} (2\pi\hbar) \sum_{m,n} e^{-\beta E_m} \langle m|B|n\rangle \langle n|A|m\rangle \left(e^{\beta(E_m - E_n)} - 1 \right) \delta\left(\omega - (E_m - E_n)\right)$$

$\Rightarrow$ Since $J(\omega)$ is a sumation over δ-function.

It's easy to show

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

1.2 in the case of $A = B$, similarly to the proof of (1.1)

$$S(t-t') = Z^{-1} \sum_{m,n} \langle m| A(t) |n\rangle \langle n| A(t') |m\rangle \, e^{-\beta E_m}$$

$$= Z^{-1} \sum_{m,n} e^{\frac{i}{\hbar}(E_m - E_n)(t-t')} \, e^{-\beta E_m} \, |\langle m|A|n\rangle|^2$$

at $t = t' \Rightarrow S(t-t'=0) = Z^{-1} \sum_{m,n} e^{-\beta E_m} \, |\langle m|A|n\rangle|^2$

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{J(\omega)}{e^{\beta\omega}-1}\,d\omega = Z^{-1}\sum_{m,n} e^{-\beta E_m}\,\langle m|A|n\rangle\langle n|A|m\rangle \underbrace{\int}_{d\omega}\frac{(e^{\beta(\mathcal{E}_m-\mathcal{E}_n)}-1)\,\delta(\omega-(E_m-E_n))}{e^{\beta\omega}-1}$$

$$= Z^{-1}\sum_{m,n} e^{-\beta E_m}\,|\langle m|A|n\rangle|^2$$

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

From the expression

$$J(\omega) = 2\pi Z^{-1}\sum_{m,n} e^{-\beta E_m}\,|\langle m|A|n\rangle|^2\,(e^{\beta(\mathcal{E}_m-\mathcal{E}_n)}-1)\,\delta(\omega-(\mathcal{E}_m-\mathcal{E}_n))$$

if $\omega > 0 \Rightarrow e^{\beta(\mathcal{E}_m-\mathcal{E}_n)}-1 > 0 \Rightarrow J(\omega) > 0.$

$\omega = \mathcal{E}_m - \mathcal{E}_n$

$$J(-\omega) = 2\pi Z^{-1}\sum_{m,n} e^{-\beta E_m}\,|\langle m|A|n\rangle|^2\,(e^{\beta(\mathcal{E}_m-\mathcal{E}_n)}-1)\,\delta(\omega+(\mathcal{E}_m-\mathcal{E}_n))$$

$$= 2\pi Z^{-1}\sum_{m,n} e^{-\beta E_n}\,|\langle n|A|m\rangle|^2\,(e^{\beta(\mathcal{E}_n-\mathcal{E}_m)}-1)\,\delta(\omega+(\mathcal{E}_n-\mathcal{E}_m))$$

$$= +\,2\pi Z^{-1}\sum_{m,n} e^{-\beta\mathcal{E}_m}\,|\langle m|A|n\rangle|^2\,(1-e^{\beta(\mathcal{E}_m-\mathcal{E}_n)})\,\delta(\omega-(\mathcal{E}_m-\mathcal{E}_n))$$

$$= -J(\omega)$$

1.3 $$\chi(\omega) = Z^{-1} \sum_{m,n} e^{-\beta E_m} |\langle m | x | n \rangle|^2 \frac{e^{\beta(E_m - E_n)} - 1}{\hbar\omega - (E_m - E_n) + i\eta}$$

where $|n\rangle, |m\rangle$ are m, n's eigenstate of harmonic oscillator.

$$x = \sqrt{\frac{\hbar}{m\omega}} \frac{1}{\sqrt{2}} (a + a^\dagger) \Rightarrow |\langle m | a + a^\dagger | n \rangle|^2 = \delta_{m,n+1}\, m + \delta_{m,n-1}\, n$$

$$\Rightarrow \chi(\omega) = Z^{-1} \frac{\hbar}{2m\omega_0^2} \sum_{m,n} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{\hbar\omega - (E_m - E_n) + i\eta} [\delta_{m,n+1}\, m + \delta_{m,n-1}\, n]$$

$$= Z^{-1} \frac{1}{2m\omega_0^2} \left[\sum_m \left\{ \frac{e^{-\beta E_m}(e^{\beta\omega} - 1)m}{\omega - \omega_0 + i\eta} \right\} + \sum_n \left\{ \frac{n e^{-\beta E_n}(1 - e^{\beta\omega})}{\omega + \omega_0 + i\eta} \right\} \right]$$

$$\frac{\sum_m m e^{-\beta E_m}}{Z} = \frac{\sum m e^{-\beta E_m}}{\sum e^{-\beta E_m}} = \frac{\sum m e^{-\beta m \hbar\omega}}{\sum e^{-\beta\hbar\omega}} = \frac{1}{e^{\beta\hbar\omega} - 1}$$

$$\Rightarrow \chi(\omega) = \frac{1}{e^{\beta\hbar\omega} - 1} \frac{1}{2m\omega_0^2} \left[\frac{e^{\beta\omega} - 1}{\omega - \omega_0 + i\eta} + \frac{1 - e^{\beta\omega}}{\omega + \omega_0 + i\eta} \right]$$

$$= \frac{1}{2m\omega_0} \left[\frac{1}{\omega - \omega_0 + i\eta} - \frac{1}{\omega + \omega_0 + i\eta} \right]$$

$$= \frac{1}{2m\omega_0} \frac{2\omega_0}{\omega^2 - \omega_0^2 + i\eta} = \frac{1}{m} \frac{1}{(\omega^2 - \omega_0^2) + i\eta}$$

which agree with classic result.

$$\chi(\omega) = \frac{1}{m}\left[\frac{1}{\omega^2-\omega_0^2+i\eta}\right] \Rightarrow J(\omega) = -2\,\mathrm{Im}\,\chi(\omega) = \frac{2\pi}{m}\,\delta(\omega^2-\omega_0^2)$$

$$= \frac{2\pi}{2m\omega_0}\left[\delta(\omega-\omega_0) - \delta(\omega+\omega_0)\right]$$

The pole of $\chi(\omega)$ is located at $\omega = \pm\omega_0$.

$$\langle x^2\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{J(\omega)}{e^{\beta\omega}-1}\,d\omega = \frac{1}{2m\omega_0}\left[\frac{1}{e^{\beta\omega_0}-1} - \frac{1}{e^{-\beta\omega_0}-1}\right]$$

when $\beta \to 0$

$$e^{\pm\beta\omega_0} - 1 = \pm\beta\omega_0$$

$$\langle x^2\rangle = \frac{1}{2m\omega_0}\,2(\beta\omega_0)^{-1} = \frac{kT}{m\omega_0^2}$$

2. a $\quad H = H_0 + H_{int}$. for inter-acting electron-gas

$$H_{int} = \int \frac{\rho(r)\rho(r')\,dr}{|r-r'|} \quad \text{and} \quad \rho_q = \sum_q e^{iqr}\rho(r), \quad \text{thus}$$

$[\rho_q, H_{int}] = 0$. we only need to calculate $[[H_0, \rho_q]\ \rho_{-q}]$

$$[H_0\ \rho_q] = \sum_{kk'} \varepsilon_k [C_k^+ C_k,\ C_{k'-q}^+ C_{k'}] = \sum_{k} \varepsilon_k [C_k^+ C_{k+q} - C_{k-q}^+ C_k]$$

$$= \sum_k (\varepsilon_k - \varepsilon_{k+q})\ C_k^+ C_{k+q}$$

$$[[H_0, \rho_q]\ \rho_{-q}] = \sum_{kk'} (\varepsilon_k - \varepsilon_{k+q})\ [C_k^+ C_{k+q},\ C_{k'+q}^+ C_{k'}]$$

$$= \sum_k (\varepsilon_k - \varepsilon_{k+q})\ C_k^+ C_k - (\varepsilon_k - \varepsilon_{k+q})\ C_{k+q}^+ C_{k+q}$$

$$= \sum_k (\varepsilon_k - \varepsilon_{k+q} - \varepsilon_{k-q} + \varepsilon_k)\ C_k^+ C_k = -\sum_k [\varepsilon_{k+q} + \varepsilon_{k-q} - 2\varepsilon_k]\ C_k^+ C_k$$

$$\varepsilon_{k+q} + \varepsilon_{k-q} - 2\varepsilon_k = [k^2 + 2kq + q^2 + k^2 - 2kq + q^2 - 2k^2]/2m = \frac{\hbar^2 q^2}{m}$$

$$\Rightarrow [[H_0, \rho_q]\ \rho_{-q}] = -\frac{\hbar^2 q^2}{m} \sum_k C_k^+ C_k = -\frac{\hbar^2 q^2}{m} N$$

2.b. $\quad \chi(q,t) = \mp \frac{i}{\hbar}\,\theta(t)\ \langle |\ \rho[q,t]\ \ \rho(-q,0)| \rangle \cdot \frac{1}{V}$

Follow the reasoning in Prob 1 $\Rightarrow$

$$Im\,\chi(q,\omega) = \frac{\mp Z^{-1}}{V}(\pi) \sum_{m,n} e^{-\beta E_m} |\langle m|\rho_q|n\rangle|^2 (e^{\beta\omega} - 1)\ \delta(\omega - (E_m - E_n))$$

$$\int_0^\infty d\omega\ \omega\ Im\,\chi(q,\omega) = -\frac{Z^{-1}\pi}{2V} \sum_{m,n} (e^{-\beta E_m} - e^{-\beta E_n})(E_m - E_n)\ |\langle m|\rho_q|n\rangle|^2$$

$$= \frac{1}{2}\int_{-\infty}^{+\infty} d\omega\ \omega\ Im\,\chi(q,\omega)$$

$$\langle |[[H, \rho_q] \rho_{-q}]|\rangle = \frac{1}{Z}\sum_m e^{-\beta E_m}\{\langle m|[H,\rho_q]|n\rangle\langle n|\rho_{-q}|m\rangle - \langle m|\rho_{-q}|n\rangle\langle n|[H,\rho_q]|m\rangle\}$$

$$= \frac{1}{Z}\sum_m e^{-\beta E_m}\{(E_m - E_n)\langle m|\rho_q|n\rangle\langle n|\rho_{-q}|m\rangle - \langle m|\rho_{-q}|n\rangle\langle n|\rho_q|m\rangle (E_n - E_m)\}$$

$$= \frac{1}{Z}\sum_m (e^{-\beta E_m} - e^{-\beta E_n})(E_m - E_n)(\langle m|\rho_q|n\rangle\langle n|\rho_{-q}|m\rangle)$$

$$\{[H, \rho_q] \rho_{-q}] = -\frac{Nq^2}{m}$$

$$\Rightarrow \int_0^\infty d\omega\, \omega\, \mathrm{Im}\,\chi(q,\omega) = \frac{Nq^2}{Vm}\cdot\frac{\pi}{2}$$

$\hookrightarrow$ f - sum rule.

More: Similarly.

$$\int_{-\infty}^{+\infty} d\omega \frac{\mathrm{Im}\,\chi(q,\omega)}{\omega} = -\frac{\pi}{ZV}\sum_{n,m} e^{-\beta E_m}\left(\frac{|\langle n|\rho_q^+|m\rangle|^2}{E_n - E_m} - \frac{|\langle n|\rho_q|m\rangle|^2}{E_m - E_n}\right)$$

which is just the real part of $\chi(q, \omega=0)$

$$\Rightarrow \int_0^{+\infty} d\omega \frac{\mathrm{Im}\,\chi(q,\omega)}{\omega} = \frac{1}{2}\int_{-\infty}^{+\infty} d\omega \frac{\mathrm{Im}\,\chi(q,\omega)}{\omega} = \frac{\pi}{2}\,\mathrm{Re}\,\chi(q,\omega=0)$$

$$\lim_{q\to 0} \frac{2}{\pi}\int_0^{+\infty} d\omega \frac{\mathrm{Im}\,\chi(q,\omega)}{\omega} = \mathrm{Re}\,\chi(q\to 0, \omega\to 0) = \frac{\partial n}{\partial \mu}.$$

($\omega \to 0$ first
$q \to 0$ second)