Solution for Homework 1

Problem 1.

a) The current and polarization operators are defined as:

$$j_x = e\sum_{k\sigma}\frac{\partial\epsilon_k}{\partial k_x}c^\dagger_{k\sigma}c_{k\sigma}, \qquad P_x = e\sum_{i\sigma}c^\dagger_{i\sigma}c_{i\sigma}r^x_i$$

Operators in momentum space $c_{k\sigma}$ are related to real space representation $c_{i\sigma}$ as:

$$c_{k\sigma} = \frac{1}{V}\sum_i e^{-ikr_i}c_{i\sigma}, \qquad c^\dagger_{k\sigma} = \frac{1}{V}\sum_i e^{ikr_i}c^\dagger_{i\sigma}$$

so their anticommutators are

$$\{c^\dagger_{k\sigma}, c_{i\sigma}\} = \frac{1}{V}e^{ikr_i}, \qquad \{c_{k\sigma}, c^\dagger_{i\sigma}\} = \frac{1}{V}e^{-ikr_i}$$

We use a relationship

$$[A, BC] = B[A, C] + [A, B]C = -B\{A, C\} + \{A, B\}C$$

to find:

$$\begin{aligned}
[c^\dagger_{k\sigma}c_{k\sigma}, c^\dagger_{i\sigma}c_{i\sigma}] &= c^\dagger_{i\sigma}[c^\dagger_{k\sigma}c_{k\sigma}, c_{i\sigma}] + [c^\dagger_{k\sigma}c_{k\sigma}, c^\dagger_{i\sigma}]c_{i\sigma} = -c^\dagger_{i\sigma}\{c^\dagger_{k\sigma}, c_{i\sigma}\}c_{k\sigma} + c^\dagger_{k\sigma}\{c_{k\sigma}, c^\dagger_{i\sigma}\}c_{i\sigma} \\
&= -\frac{1}{V}e^{ikr_i}c^\dagger_{i\sigma}c_{k\sigma} + \frac{1}{V}e^{-ikr_i}c^\dagger_{k\sigma}c_{i\sigma}
\end{aligned}$$

Now we can evaluate the commutator

$$\begin{aligned}
[j_x, P_x] &= e^2\sum_{ik\sigma}\frac{\partial\epsilon_k}{\partial k_x}r^x_i[c^\dagger_{k\sigma}c_{k\sigma}, c^\dagger_{i\sigma}c_{i\sigma}] \\
&= ie^2\sum_{ik\sigma}\frac{\partial\epsilon_k}{\partial k_x}\frac{1}{V}\left(\frac{\partial}{\partial k_x}(e^{ikr_i}c^\dagger_{i\sigma})c_{k\sigma} + c^\dagger_{k\sigma}\frac{\partial}{\partial k_x}(e^{-ikr_i}c_{i\sigma})\right) \\
&= ie^2\sum_{k\sigma}\frac{\partial\epsilon_k}{\partial k_x}\frac{\partial}{\partial k}c^\dagger_{k\sigma}c_{k\sigma} = -ie^2\sum_{k\sigma}\frac{\partial^2\epsilon_k}{\partial k^2}c^\dagger_{k\sigma}c_{k\sigma} \qquad (1)
\end{aligned}$$

To derive the f-sum rule we use the Kubo formula:

$$\sigma(\omega) = \frac{1}{\omega}\int_0^{+\infty}dte^{i\omega t}\langle[j^\dagger(t), j(0)]\rangle + i\frac{e^2}{\omega}\sum_{k\sigma}\frac{\partial^2\epsilon_k}{\partial k^2}\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle \qquad (2)$$

Noticing that $\partial P/\partial t = j$, integrating by parts Eq.(2) and using the commutator Eq.(1) we get:

$$\sigma(\omega) = i\int_0^{+\infty} dt e^{i\omega t}\langle[j(0), P(t)]\rangle$$

Integrating the conductivity other the frequency we derive the sum rule:

$$\int_{-\infty}^{+\infty} d\omega\sigma(\omega) = i2\pi\int_0^{+\infty} dt\delta(t)\langle[j(0), P(t)]\rangle = i\pi\langle[j, P]\rangle = \pi e^2\sum_{k\sigma}\frac{\partial^2\epsilon_k}{\partial k^2}\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle$$

b) Integrating by parts a Fourier transform of a function we obtain an expansion in $1/\omega$:

$$f(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} f(t) = -\sum_{k=0}^{\infty}(i\omega^{-1})^{k+1}[f^{(k)}(0)]$$

where $[f^{(k)}(0)]$ is a jump of the function $f^{(k)}(t)$ at $t = 0$:

$$[f^{(k)}(0)] \equiv f^{(k)}(0^+) - f^{(k)}(0^-)$$

For example, for a Green's function:

$$G_{ij}(i\omega) = -\frac{1}{i\omega}[G_{ij}(0)] + \frac{1}{(i\omega)^2}[\frac{\partial G_{ij}(0)}{\partial\tau}] - \frac{1}{(i\omega)^3}[\frac{\partial^2 G_{ij}(0)}{\partial\tau^2}] + ... \tag{3}$$

where

$$[G_{ij}(0)] = -\langle c_i c^\dagger_j\rangle - \langle c^\dagger_j c_i\rangle = -\langle\{c_i, c^\dagger_j\}\rangle = -\delta_{ij}$$

$$[\frac{\partial G_{ij}(0)}{\partial\tau}] = -\langle\frac{\partial c_i}{\partial\tau}c^\dagger_j\rangle - \langle c^\dagger_j\frac{\partial c_i}{\partial\tau}\rangle = -\langle[H, c_i]c^\dagger_j\rangle - \langle c^\dagger_j[H, c_i]\rangle = -\langle\{[H, c_i], c^\dagger_j\}\rangle$$

Similarly:

$$[\frac{\partial^2 G_{ij}(0)}{\partial\tau^2}] = -\langle\{[H, c_i], [H, c^\dagger_j]\}\rangle$$

Using $[c^\dagger_{i\sigma}c_{j\sigma}, c_{i\sigma}] = -c_{j\sigma}$ we evaluate:

$$\begin{aligned}
[H, c_{i\sigma}] &= -\sum_{lj} t_{ij}[c^\dagger_{l\sigma}c_{j\sigma}, c_{i\sigma}] + U\sum_l[n_{l\uparrow}n_{l\downarrow}, c_{i\sigma}] + \mu[c^\dagger_{l\sigma}c_{l\sigma}, c_{i\sigma}] \\
&= \sum_j(t_{ij} - \mu\delta_{ij})c_{j\sigma} - Uc_{i\sigma}n_{i\bar{\sigma}} \\
[H, c^\dagger_{i\sigma}] &= -[H, c_{i\sigma}]^\dagger = -\sum_j(t_{ji} - \mu\delta_{ij})c^\dagger_{j\sigma} + Uc^\dagger_{i\sigma}n_{i\bar{\sigma}}
\end{aligned}$$

From where:

$$\{[H, c_{i\sigma}], c^\dagger_{j\sigma}\} = (t_{ij} - \mu\delta_{ij}) - U\delta_{ij}n_{i\bar{\sigma}} \tag{4}$$

$$\{[H, c_{i\sigma}], [H, c^\dagger_{j\sigma}]\} = -\sum_l (t_{il} - \mu\delta_{il})(t_{lj} - \mu\delta_{lj}) + U(t_{ij} - \mu\delta_{ij})(n_{i\bar{\sigma}} + n_{j\bar{\sigma}}) - U^2\delta_{ij} n_{i\bar{\sigma}} n_{j\bar{\sigma}} \quad (5)$$

Assuming no symmetry breaking $\langle n_{i\sigma}\rangle = \langle n\rangle$ for $\forall\ i, \sigma$ we rewrite Eqs.(4,5) in momentum space:

$$[G^{(1)}(0,k)] = \epsilon_k + U\langle n\rangle \quad (6)$$

$$[G^{(2)}(0,k)] = -\epsilon_k^2 - 2U\epsilon_k\langle n\rangle + U^2\langle n^2\rangle \quad (7)$$

With the self-energy $\Sigma(\omega, k) = A_1 + A_2/(i\omega)$ expansion of the Green's function reads:

$$G(\omega, k) = \frac{1}{i\omega - \epsilon_k - \Sigma(\omega, k)} = \frac{1}{i\omega} + \frac{1}{(i\omega)^2}(\epsilon_k + A_1) + \frac{1}{(i\omega)^3}(A_2 + (\epsilon_k + A_1)^2) \quad (8)$$

From Eqs.(3,6,7,8) we obtain:

$$A_1 = U\langle n\rangle$$

$$A_2 = U^2(\langle n^2\rangle - \langle n\rangle^2) = U^2\langle n\rangle(1 - \langle n\rangle)$$