Continue with Green's functions

Electrons in a Solid

$$H = H_0 = \sum_{\bar{k}\sigma} \epsilon_{\bar{k}}\, a^{+}_{\bar{k}\sigma} a_{\bar{k}\sigma}$$

$$N = \sum_{\bar{k}\sigma} a^{+}_{\bar{k}\sigma} a_{\bar{k}\sigma} \qquad \mathcal{H} = H_0 - \mu N$$

Specify A, B

$a_{\bar{k}\sigma} \Leftrightarrow A \qquad \alpha \in \{Ret, Adv, c\}$

$a^{+}_{\bar{k}\sigma} \Leftrightarrow B \qquad \eta = -1$

$$G^{\alpha}_{\bar{k}\sigma}(\epsilon) = \langle\langle a_{\bar{k}\sigma}, a^{+}_{\bar{k}\sigma} \rangle\rangle^{\alpha}_{E}$$ (so-called one-electron Green's function)

EOM
$$E\, G^{\alpha}_{\bar{k}\sigma}(\epsilon) = \hbar \langle [a_{\bar{k}\sigma}, a^{+}_{\bar{k}\sigma}]_{+} \rangle + \langle\langle [a_{\bar{k}\sigma}, \mathcal{H}]_{-}, a^{+}_{\bar{k}\sigma} \rangle\rangle^{\alpha}$$

Examine $[a_{\bar{k}\sigma}, \mathcal{H}]_{-}$

$$[a_{\bar{k}\sigma}, \mathcal{H}]_{-} = \sum_{\bar{k}'\sigma'} (\epsilon_{\bar{k}'\sigma'} - \mu)[a_{\bar{k}\sigma}, a^{+}_{\bar{k}'\sigma'} a_{\bar{k}'\sigma'}]_{-} =$$

$$= \sum_{\bar{k}'\sigma'} (\epsilon_{\bar{k}'\sigma'} - \mu) \left\{ a_{\bar{k}\sigma} a^{+}_{\bar{k}'\sigma'} a_{\bar{k}'\sigma'} - a^{+}_{\bar{k}'\sigma'} a_{\bar{k}'\sigma'} a_{\bar{k}\sigma} \right\} =$$

$$= \sum_{\bar{k}'\sigma'} (\epsilon_{\bar{k}'\sigma'} - \mu)\, a_{\bar{k}\sigma} \left(\cancel{a^{+}_{\bar{k}'\sigma'} a_{\bar{k}'\sigma'}} - \left(\cancel{a^{+}_{\bar{k}'\sigma'} a_{\bar{k}'\sigma'}} - \delta_{\bar{k}\bar{k}'} \delta_{\sigma\sigma'} \right) \right) =$$

$$= (\epsilon_{\bar{k}\sigma} - \mu)\, a_{\bar{k}\sigma}$$

$$E\, G^{\alpha}_{\bar{k}\sigma}(\epsilon) = \hbar + (\epsilon_{\bar{k}\sigma} - \mu)\, G^{\alpha}_{\bar{k}\sigma}(\epsilon) \longrightarrow$$ closed equation for $G^{\alpha}_{\bar{k}\sigma}(\epsilon)$.

$$G^{Ret/Adv}_{\hat{n}\sigma}(\epsilon) = \frac{\hbar}{\epsilon - (\epsilon_{\hat{n}\sigma} - \mu) \pm i0^+}$$ (singularities $\leftrightarrow$ excitation energies)

Spectral density $G^{Ret/Adv}_{AB} = \int_{-\infty}^{\infty} d\epsilon' \frac{S_{AB}(\epsilon')}{\epsilon - \epsilon' \pm i0^+} \rightarrow S_{\hat{n}\sigma}(\epsilon) = \hbar\,\delta(\epsilon - (\epsilon_{\hat{n}\sigma} - \mu))$

Take $G^{Ret}_{\hat{n}\sigma}$, find $G^{Ret}_{\hat{n}\sigma}(t-t')$

$$G^{Ret}_{\hat{n}\sigma}(t-t') = \frac{1}{2\pi\cancel{\hbar}} \int_{-\infty}^{\infty} d\epsilon\, e^{-i\frac{\epsilon}{\hbar}(t-t')} \frac{\cancel{\hbar}}{\epsilon - (\epsilon_{\hat{n}\sigma} - \mu) + i0^+} = \left\{ \tilde{\epsilon} = \epsilon - (\epsilon_{\hat{n}\sigma} - \mu) \right\} =$$

$$= \frac{1}{2\pi} e^{-i(\epsilon_{\hat{n}\sigma} - \mu)(t-t')/\hbar} \underbrace{\int_{-\infty}^{\infty} d\tilde{\epsilon}\, e^{-\frac{i}{\hbar}\tilde{\epsilon}(t-t')} \frac{1}{\tilde{\epsilon} + i0^+}}_{*} =$$

$$\left\{ * = \left\{ \tilde{\epsilon} = \hbar x \right\} = \hbar \int_{-\infty}^{\infty} dx\, e^{-ix(t-t')} \frac{\hbar^{-1}}{x + i0^+} = -2\pi i\, \Theta(t-t') \right\}$$

$$= -i\Theta(t-t')\, e^{-\frac{i}{\hbar}(\epsilon_{\hat{n}\sigma} - \mu)(t-t')}$$

By adding $+i0^+$ we pick the right BC.

Analogously $G^{Adv}_{\hat{n}\sigma}(t-t') = i\,\Theta(t'-t)\, e^{-\frac{i}{\hbar}(\epsilon_{\hat{n}\sigma} - \mu)(t-t')}$

Now calculate $\langle n_{\hat{n}\sigma} \rangle$

$$\langle B(t')A(t) \rangle = \frac{1}{\hbar} \int_{-\infty} d\epsilon \frac{S_{AB}(\epsilon)}{e^{\beta\epsilon} + 1} e^{-\frac{i}{\hbar}\epsilon(t-t')}.$$

$$A(t) \rightarrow a_{\hat{n}\sigma}(t)$$

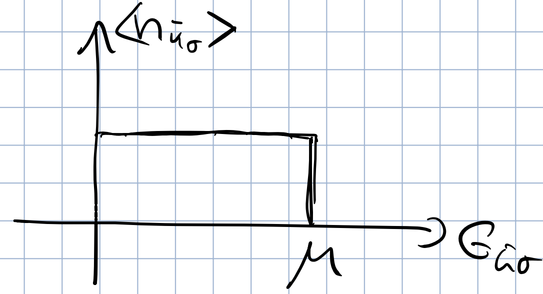
$$B(t) \rightarrow a^{\dagger}_{\hat{n}\sigma}(t)$$

so that

$$\langle a^{\dagger}_{\hat{n}\sigma}(t') a_{\hat{n}\sigma}(t) \rangle \Big|_{t'=t} = \langle a^{\dagger}_{\hat{n}\sigma} a_{\hat{n}\sigma} \rangle = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\epsilon \frac{\hbar\,\delta(\epsilon - (\epsilon_{\hat{n}\sigma} - \mu))}{e^{\beta\epsilon} + 1}$$

$$\langle n_{\vec{k}\sigma}\rangle = \frac{1}{e^{\beta(\epsilon_{\vec{k}\sigma}-\mu)}+1} \longrightarrow \text{Fermi-Dirac distribution!}$$

$$\beta = \infty \quad (T = 0^+) \longrightarrow \langle n_{\vec{k}\sigma}\rangle = \Theta(\mu - \epsilon_{\vec{k}\sigma})$$



$\beta < \infty$

Metals $\quad k_B T \ll \mu$

Another observable: internal energy $\quad U = \langle H\rangle = \langle \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma} a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}\rangle = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma}\langle n_{\vec{k}\sigma}\rangle$

(done before for $T=0$)

Interacting systems are a different story...

Self-energy, Dyson's equation

Consider interacting fermions (bosons analogously up to "details")

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} + \frac{1}{2}\sum_{\vec{k}\vec{k}'\vec{q}}\sum_{\sigma\sigma'} V_{\vec{q}}\, a^\dagger_{\vec{k}+\vec{q}\sigma} a^\dagger_{\vec{k}'-\vec{q}\sigma'} a_{\vec{k}'\sigma'} a_{\vec{k}\sigma},$$

follow the previous path:

$$G^\alpha_{\vec{k}\sigma}(E) := \langle\langle a_{\vec{k}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle^\alpha_E \qquad (\alpha \in \text{Ret, Adv, c}) \quad \zeta = -1$$

e.o.m: $E G^{\alpha}_{\bar{k}\sigma}(E) = \hbar \langle [a_{\bar{k}\sigma}, a^{+}_{\bar{k}\sigma}]_{+} \rangle + \langle\langle [a_{\bar{k}\sigma}, H]_{-}, a^{+}_{\bar{k}\sigma} \rangle\rangle^{\alpha}_{E}$

{ Evaluate $[a_{\bar{k}\sigma}, H]_{-} = (\epsilon_{\bar{k}} - \mu) a_{\bar{k}\sigma} + \sum_{\bar{k}'\bar{q}} \sum_{\sigma'} V_{\bar{q}} \, a^{+}_{\bar{k}'+\bar{q},\sigma'} a_{\bar{k}'\sigma'} a_{\bar{k}+\bar{q}\sigma}$ ("mechanical" calculation – homework) }

and we obtain:

$$(E - (\epsilon_{\bar{k}} - \mu)) G^{\alpha}_{\bar{k}\sigma}(E) = \hbar + \underbrace{\sum_{\bar{k}'\bar{q}} \sum_{\sigma'} V_{\bar{q}} \langle\langle a^{+}_{\bar{k}'+\bar{q},\sigma'} a_{\bar{k}'\sigma'} a_{\bar{k}+\bar{q},\sigma}, a^{+}_{\bar{k}\sigma} \rangle\rangle^{\alpha}_{E}}_{:= {}^{\alpha}\Gamma^{\sigma\sigma'}_{\bar{k}',\bar{k},\bar{q}}(E)} \qquad (\otimes)$$

+ is ok here

(stuck..., not a closed equation...)

Last term is a function of $E, \bar{k}, \sigma$. Write it as $G^{\alpha}_{\bar{k}\sigma}(E) \cdot \Sigma^{\alpha}_{\sigma}(\bar{k}, E)$

The quantity $\Sigma^{\alpha}_{\sigma}(\bar{k}, E)$ – electronic self-energy

The "solution" to $\otimes$ is then $G^{\alpha}_{\bar{k}\sigma}(E) = \dfrac{\hbar}{E - (\epsilon_{\bar{k}} - \mu + \Sigma^{\alpha}_{\sigma}(\bar{k}, E))}$ $(\otimes\otimes)$

Comparing to the noninteracting case we see that the impact of interactions is contained in $\Sigma^{\alpha}_{\sigma}(\bar{k}, E)$