Total energy of the impurity model

$$H = \sum_{ks} \varepsilon_k C^+_{ks} C_{ks} + \sum_{ks} V_k C^+_{ks} d_s + V^*_k d^+_s C_{ks} + \sum_s \varepsilon_f d^+_s d_s + U n_\uparrow n_\downarrow$$

$$E = \langle H \rangle = \sum_{ks} \varepsilon_k n_{ks} + \sum_s \varepsilon_f n_s + U \langle n_\uparrow n_\downarrow \rangle + \sum_{ks} V_k \langle C^+_{ks} d_s \rangle + V^*_k \langle d^+_s C_{ks} \rangle$$

Using equations of motion we will prove below the following set of equations:

1) $$\langle T_\tau d^+_s(0) C_{ks}(\tau) \rangle = \frac{1}{\beta} \sum_{i\omega} e^{-i\omega\tau} \frac{V_k}{i\omega - \varepsilon_k} G_{imp}(i\omega)$$

2) $$\langle T_\tau C^+_{ks}(\tau) d_s(0) \rangle = \frac{1}{\beta} \sum_{i\omega} e^{i\omega\tau} \frac{V^*_k}{i\omega - \varepsilon_k} G_{imp}(i\omega)$$

3) $$G_{kk'}(i\omega) = \frac{\delta_{kk'}}{i\omega - \varepsilon_k} + \frac{V_k V^*_{k'}}{(i\omega - \varepsilon_k)(i\omega - \varepsilon_{k'})} G_{imp}(i\omega)$$

Then we have:

$$E = \underbrace{\frac{1}{\beta} \sum_{\substack{ks \\ i\omega}} \left(\varepsilon_k \delta_{kk'} G_{kk'}(i\omega) + V_k \langle C^+_{ks} d_s \rangle + V^*_k \langle d^+_s C_{ks} \rangle \right)}_{E_\Delta} + \sum_s \varepsilon_f n_s + U \langle n_\uparrow n_\downarrow \rangle$$

$$E_\Delta = \frac{1}{\beta} \sum_{\substack{ks \\ i\omega}} \left[\underbrace{\frac{\varepsilon_k}{i\omega - \varepsilon_k}} + \frac{\varepsilon_k |V_k|^2}{(i\omega - \varepsilon_k)^2} G_{imp}(i\omega) + \frac{|V_k|^2}{i\omega - \varepsilon_k} G_{imp}(i\omega) + \frac{|V_k|^2}{i\omega - \varepsilon_k} G_{imp}(i\omega) \right]$$

E^0 is the non-interacting energy

$$E_\Delta = E^0 + \frac{1}{\beta} \sum_{\substack{ks \\ i\omega}} G_{imp}(i\omega) \left[\frac{2 |V_k|^2}{i\omega - \varepsilon_k} + \frac{\varepsilon_k |V_k|^2}{(i\omega - \varepsilon_k)^2} \right]$$

$$\Delta(i\omega) = \sum_k \frac{|V_k|^2}{i\omega - \varepsilon_k} \qquad i\omega \frac{d\Delta}{di\omega} + \Delta = \sum_k - \frac{|V_k|^2 i\omega}{(i\omega - \varepsilon_k)^2} + \frac{|V_k|^2}{i\omega - \varepsilon_k} = \sum_k \frac{|V_k|^2}{(i\omega - \varepsilon_k)^2} (-i\omega + i\omega - \varepsilon_k) = - \sum_k \frac{|V_k|^2 \varepsilon_k}{(i\omega - \varepsilon_k)^2}$$

Finally: $$E_\Delta = E^0 + \frac{1}{\beta} \sum_{i\omega, s} G_{imp}(i\omega) \left[2\Delta(i\omega) - i\omega \frac{d\Delta}{di\omega} - \Delta(i\omega) \right] = E^0 + \mathrm{Tr}\left(G \left(\Delta - \omega_n \frac{d\Delta}{d\omega_n} \right) \right)$$

EOM for Eq. 1:

$$\frac{\partial}{\partial\tau}\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle = \langle T_\tau d_s^+(0)\, [H, c_{\vec{k}s}]_\tau\rangle$$

because: $c_{\vec{k}s}(\tau) = e^{H\tau} c_{\vec{k}s} e^{-H\tau}$

$$\frac{\partial c_{\vec{k}s}(\tau)}{\partial\tau} = e^{H\tau}[H, c_{\vec{k}s}]e^{-H\tau} = [H, c_{\vec{k}s}(\tau)]$$

Commutator is:

$$[H, c_{\vec{k}s}] = \sum_{\vec{k}'s'} \varepsilon_{\vec{k}'} \underbrace{[c_{\vec{k}'s'}^+ c_{\vec{k}'s'}, c_{\vec{k}s}]} + V_{\vec{k}'}[c_{\vec{k}'s'}^+ d_{s'}, c_{\vec{k}s}]$$

$$c_{\vec{k}'s'}^+ c_{\vec{k}'s'} c_{\vec{k}s} - c_{\vec{k}s} c_{\vec{k}'s'}^+ c_{\vec{k}'s'}$$

$$- c_{\vec{k}'s'}^+ c_{\vec{k}s} c_{\vec{k}'s'} - c_{\vec{k}s} c_{\vec{k}'s'}^+ c_{\vec{k}'s'}$$

$$- \delta_{\substack{\vec{k}\vec{k}'\\ss'}} c_{\vec{k}'s'} + c_{\vec{k}s} c_{\vec{k}'s'}^+ c_{\vec{k}'s'} - c_{\vec{k}s} c_{\vec{k}'s'}^+ c_{\vec{k}'s'} = -\delta_{\substack{\vec{k}\vec{k}'\\ss'}} c_{\vec{k}s}$$

Finally: $[H, c_{\vec{k}s}] = -\varepsilon_{\vec{k}} c_{\vec{k}s} - V_{\vec{k}} d_s$

Back to EOM:

$$\frac{\partial}{\partial\tau}\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle = -\varepsilon_{\vec{k}}\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle - V_{\vec{k}}\langle T_\tau d_s^+(0)\, d_s(\tau)\rangle$$

$$\left(\frac{\partial}{\partial\tau} + \varepsilon_{\vec{k}}\right)\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle = V_{\vec{k}}\langle T_\tau d_s(\tau)\, d_s^+(0)\rangle = -V_{\vec{k}}\, G_{imp}(\tau) \qquad \Big/ \int d\tau\, e^{i\omega\tau}$$

Note $G_{imp}(\tau) = -\langle T_\tau d_s(\tau)\, d_s^+(0)\rangle$

$$\int d\tau\, e^{i\omega\tau}\left[\left(\frac{\partial}{\partial\tau} + \varepsilon_{\vec{k}}\right)\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle\right] = -V_{\vec{k}}\int d\tau\, e^{i\omega\tau} G_{imp}(\tau) = -V_{\vec{k}}\, G_{imp}(i\omega)$$

$\frac{\partial}{\partial\tau}$ acts on the right, hence: $\int d\tau\, e^{i\omega\tau}\frac{\partial}{\partial\tau}A(\tau) \overset{by}{\underset{parts}{=}} -\int d\tau\left(\frac{\partial}{\partial\tau}e^{i\omega\tau}\right)A(\tau) = -i\omega\int d\tau\, e^{i\omega\tau}A(\tau)$

$$\int d\tau\, e^{i\omega\tau}\,(-i\omega + \varepsilon_{\vec{k}})\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle = -V_{\vec{k}}\, G_{imp}(i\omega)$$

$$\int d\tau\, e^{i\omega\tau}\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle = \frac{V_{\vec{k}}}{i\omega - \varepsilon_{\vec{k}}}\, G_{imp}(i\omega) \qquad \Big/ \frac{1}{\beta}\sum_{i\omega} e^{-i\omega\tau'}$$

and finally: $\langle T_\tau d_s^+(0)\, c_{\vec{k}s}(\tau)\rangle = \frac{1}{\beta}\sum_{i\omega} e^{-i\omega\tau}\frac{V_{\vec{k}}}{i\omega - \varepsilon_{\vec{k}}}\, G_{imp}(i\omega)$

Similarly $\quad \langle C_{2s}^{+} d_s \rangle = -\frac{1}{\beta} \sum_{i\omega} e^{i\omega 0^+} \frac{V_2^*}{i\omega - \varepsilon_2} G_{imp}(i\omega)$

The commutator is:

$$[H, C_{2s}] = \varepsilon_2 C_{2s}^{+} + V_2^* d_s^{+}$$

$$\frac{\partial}{\partial \tau} \langle T_\tau C_{2s}^{+}(\tau) d_s(0) \rangle = \langle T_\tau [H, C_{2s}^{+}]_\tau d_s(0) \rangle = \varepsilon_2 \langle T_\tau C_{2s}^{+}(\tau) d_s(0) \rangle + V_2^* \underbrace{\langle T_\tau d_s^{+}(\tau) d_s(0) \rangle}_{G_{imp}(-\tau)}$$

$$\left(\frac{\partial}{\partial \tau} - \varepsilon_2\right) \langle T_\tau C_{2s}^{+}(\tau) d_s(0) \rangle = V_2^* G_{imp}(-\tau) \quad \Big/ \int_0^\beta d\tau\, e^{-i\omega\tau}$$

$$\int d\tau\, e^{-i\omega\tau} \left[\left(\frac{\partial}{\partial \tau} - \varepsilon_2\right) \langle T_\tau C_{2s}^{+}(\tau) d_s(0) \rangle\right] = V_2^* G_{imp}(i\omega)$$

$$(i\omega - \varepsilon_2) \int d\tau\, e^{-i\omega\tau} \langle T_\tau C_{2s}^{+}(\tau) d_s(0) \rangle = V_2^* G_{imp}(i\omega)$$

Finally: $\quad \langle T_\tau C_{2s}^{+}(\tau) d_s(0) \rangle = \frac{1}{\beta} \sum_{i\omega} e^{i\omega\tau} \frac{V_2^*}{i\omega - \varepsilon_2} G_{imp}(i\omega)$

Impurity allows scattering from $k \to k'$ hence $G_{kk'}(\tau) = -\langle T_\tau c_k(\tau) c_{k'}(0)\rangle$ exists.

$$G_{kk'}(\tau-\tau') = -\langle T_\tau\, c_k(\tau)\, c_{k'}^+(\tau')\rangle = -\Theta(\tau-\tau')\langle c_k(\tau)\, c_{k'}^+(\tau')\rangle + \Theta(-\tau+\tau')\langle c_{k'}^+(\tau') c_k(\tau)\rangle$$

$$\frac{\partial}{\partial\tau} G_{kk'}(\tau-\tau') = -\delta(\tau-\tau')\langle c_k c_{k'}^+ + c_{k'}^+ c_k\rangle - \langle T_\tau [H, c_k(\tau)]\, c_{k'}^+(\tau')\rangle$$

$$\frac{\partial}{\partial\tau} G_{kk'}(\tau-\tau') = -\delta(\tau-\tau')\delta_{kk'} + \langle T_\tau (\varepsilon_k c_{k_s} + V_k d_s)_\tau\, c_{k'}^+(\tau')\rangle = -\delta(\tau-\tau')\delta_{kk'} - \varepsilon_k G_{kk'}(\tau-\tau') + V_k\langle T_\tau\, d_s(\tau)\, c_{k'}^+(\tau')\rangle$$

$$-\left(\frac{\partial}{\partial\tau} + \varepsilon_k\right) \underbrace{G_{kk'}(\tau-\tau')}_{= \frac{1}{\beta}\sum_{i\omega} e^{i\omega(\tau-\tau')} G_k(i\omega)} = \delta(\tau-\tau')\delta_{kk'} - V_k\langle T_\tau\, d_s(\tau)\, c_{k'}^+(\tau')\rangle$$

$$\frac{1}{\beta}\sum_{i\omega}(i\omega-\varepsilon_k) G_{kk'}(i\omega)\, e^{-i\omega(\tau-\tau')} = \delta(\tau-\tau')\delta_{kk'} - V_k\langle T_\tau\, d_s(\tau)\, c_{k'}^+(\tau')\rangle$$

$$(i\omega-\varepsilon_k) G_{kk'}(i\omega) = \delta_{kk'} - V_k \int d\tau\, e^{i\omega(\tau-\tau')}\langle T_\tau\, d_s(\tau)\, c_{k'}^+(\tau')\rangle$$

$$\frac{\partial}{\partial\tau'}\langle T_\tau\, d_s(\tau)\, c_{k'}^+(\tau')\rangle = \langle T_\tau\, d_s(\tau)\, [H, c_{k'}^+]_{\tau'}\rangle = \langle T_\tau\, d_s(\tau)(\varepsilon_{k'} c_{k'_s}^+(\tau') + V_{k'}^* d_s^+(\tau'))\rangle$$

$$\left(\frac{\partial}{\partial\tau'} - \varepsilon_{k'}\right)\langle T_\tau\, d_s(\tau)\, c_{k'}^+(\tau')\rangle = V_{k'}^*\langle T_\tau\, d_s(\tau)\, d_s^+(\tau')\rangle$$

$$\left(\frac{\partial}{\partial\tau'} - \varepsilon_{k'}\right)\langle T_\tau\, d_s(\tau)\, c_k^+(\tau')\rangle = V_{k'}^*\langle T_\tau\, d_s(\tau)\, d_s^+(\tau')\rangle$$

$$\int d\tau' e^{i\omega(\tau-\tau')}\cdot\left[\left(\frac{\partial}{\partial\tau'} - \varepsilon_{k'}\right)\langle T_\tau\, d_s(\tau)\, c_k^+(\tau')\rangle\right] = -V_{k'}^*\int d\tau'\, G_{imp}(\tau-\tau')\, e^{i\omega(\tau-\tau')}$$

by parts: $\int d\tau'\, e^{i\omega(\tau-\tau')}\left(\frac{\partial}{\partial\tau'} A(\tau')\right) = -\int d\tau'\, A(\tau')\left(\frac{\partial}{\partial\tau'} e^{i\omega(\tau-\tau')}\right) = +\int d\tau'\, A(\tau')\, i\omega\, e^{i\omega(\tau-\tau')}$

$$\int d\tau'\, e^{i\omega(\tau-\tau')}\left[(i\omega-\varepsilon_{k'})\langle T_\tau\, d_s(\tau)\, c_k^+(\tau')\rangle\right] = -V_{k'}^*\, G_{imp}(i\omega)$$

$$\int d\tau'\, e^{i\omega(\tau-\tau')}\langle T_\tau\, d_s(\tau)\, c_k^+(\tau')\rangle = -\frac{V_{k'}^*}{i\omega-\varepsilon_{k'}} G_{imp}(i\omega)$$

$$(i\omega-\varepsilon_k) G_{kk'}(i\omega) = \delta_{kk'} + \frac{V_k V_{k'}^*}{i\omega-\varepsilon_{k'}} G_{imp}(i\omega)$$

Finally: $$G_{kk'}(i\omega) = \frac{\delta_{kk'}}{i\omega-\varepsilon_k} + \frac{V_k V_{k'}^*}{(i\omega-\varepsilon_k)(i\omega-\varepsilon_{k'})} G_{imp}(i\omega)$$