Lecture 26

Equation's of motion for the Green's functions

The retarded Green's function of the system is (dropping "r") (and setting $\hbar = 1$)

$$G_{nm}(t) = -i\theta(t)\langle\{d_n(t), d_m^{+}(0)\}\rangle$$

$$i\frac{\partial}{\partial t}G_{nm}(t) = \delta(t)\delta_{nm} - i\theta(t)\langle\{[d_n(t), H], d_m^{+}(0)\}\rangle$$

$$H = H_{sys}^{(1)} + H_{leads} + H_T$$

$$[d_n, H_{leads}] = 0$$

$$[d_n, H_{sys}^{(1)}] = \sum_{n'}(H_{sys}^{(1)})_{nn'}\, d_{n'}$$

$$[d_n, H_T] = \sum_\alpha \sum_{k\in\alpha} \sum_n V_{nk}\, c_k$$

Define $\tilde{g}_{km}(t) = -i\theta(t)\left\langle \left\{ c_k(t), d_m^\dagger(0) \right\} \right\rangle$

$\Rightarrow$

$$\boxed{i\frac{\partial}{\partial t} G_{nm}(t) = \delta(t)\,\delta_{nm} + \sum_{n'} H^{(1)}_{nn'}\, G_{n'm}(t) + \sum_\alpha \sum_{k\in\alpha} V_{nk}\, \tilde{g}_{km}(t)}$$

<u>Eq. of motion for</u> $\tilde{g}(t)$:

$$i\frac{\partial}{\partial t}\tilde{g}_{km}(t) = -i\theta(t)\left\langle \left\{ [c_k(t), H], d_m^\dagger(0) \right\} \right\rangle$$

$$[c_k, H] = [c_k, H_T] + [c_k, H_{\text{leads}}]$$

$$= \sum_n V_{nk}^* d_n + \epsilon_k c_k$$

$$\Rightarrow \boxed{i \frac{\partial}{\partial t} \tilde{g}_{km}(t) = \epsilon_k \tilde{g}_{km}(t) + \sum_{n'} V^*_{n'k} G_{n'm}(t)}$$

Fourier transform:

$$(\omega - \epsilon_k + i0^+) \tilde{g}_{km}(\omega) = \sum_{n'} V^*_{n'k} G_{n'm}(\omega)$$

needed to generate $\theta(t)$ when Fourier transforming back to time domain

$$\omega G_{nm}(\omega) = \delta_{nm} + \sum_{n'} H^{(1)}_{nn'} G_{n'm}(\omega) + \sum_{\alpha} \sum_{k \in \alpha} V_{nk} \tilde{g}_{km}(\omega)$$

Inserting the solution for $\tilde{g}_{km}(\omega)$ from the upper equation into the lower equation gives a closed equation for G:

$$\boxed{\left(\mathbb{1}\omega - H^{(1)}_{sys} - \Sigma_T(\omega)\right) G(\omega) = \mathbb{1}}$$

Dyson's equation

where the "tunneling self-energy"

$$\left(\Sigma_T(\omega)\right)_{nn'} = \sum_\alpha \sum_{k\in\alpha} \frac{V_{nk} V^*_{n'k}}{\omega - \epsilon_k + i0^+}$$

Note

$$\mathrm{Im}\left(\Sigma_T(\omega)\right)_{nn'} = -\pi \sum_\alpha \sum_{k\in\alpha} V_{nk} V^*_{n'k}\, \delta(\omega - \epsilon_k)$$

$$\neq 0$$

(finite lifetime of particle in system)

Now we can solve for $G(\omega)$ by simple matrix inversion

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$$G(\omega) = \left(\mathbb{1}\omega - H^{(1)}_{sys} - \Sigma(\omega)\right)^{-1}$$

This result is more general.
We could also include
any other interactions in Σ:

$$\Sigma(\omega) = \underbrace{\Sigma_T(\omega)}_{\text{tunneling self-energy}} + \underbrace{\Sigma_C(\omega)}_{\text{coulomb self-energy}} + \underbrace{\Sigma_{e\text{-}ph}(\omega)}_{\text{electron-phonon self-energy}} + \cdots$$

Recalling

$$G_0(\omega) = \left(\mathbb{1}\omega - H^{(1)}_{sys} + i0^+\right)^{-1},$$

we can rewrite Dyson's equation as

$$G(\omega) = G_0(\omega) + G_0(\omega)\,\Sigma(\omega)\,G(\omega)$$

or simply

$$\boxed{G = G_0 + G_0 \Sigma G}$$

Dyson's equation

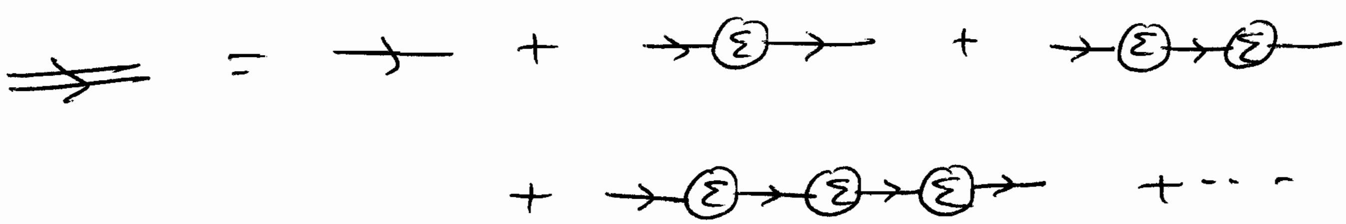
In the time domain (on the Keldysh contour):

$$\boxed{\begin{aligned} G(\tau_1,\tau_2) = {} & G_0(\tau_1,\tau_2) \\ & + \int d\tau_3 \int d\tau_4\; G_0(\tau_1,\tau_3)\,\Sigma(\tau_3,\tau_4) \\ & \times G(\tau_4,\tau_2) \end{aligned}}$$

Graphically, $G = \Rightarrow$, $G_0 = \rightarrow$

$$\boxed{\Rightarrow \;=\; \rightarrow \;+\; \rightarrow \Sigma \Rightarrow}$$

Iterative solution:



Relation to real-time GF's:

$$G^r = G_0^r + G_0^r \Sigma^r G^r$$

$$G^a = G_0^a + G_0^a \Sigma^a G^a$$

$$G^< = G_0^< + G_0^r \Sigma^r G^< + G_0^r \Sigma^< G^a + G_0^< \Sigma^a G^a$$

Replacing G_0^r in the lower equation with Σ^r and G^r using the upper equation leads to the Keldysh equation:

$$\boxed{G^< = G^r \Sigma^< G^a + \left(1 + G^r \Sigma^r\right) G_0^< \left(1 + \Sigma^a G^a\right)}$$

The last term in the Keldysh equation describes the effect of initial conditions. For a (finite) system coupled to a macroscopic environment, the initial conditions become irrelevant, at least for steady-state. They can be important to describe transient response.