Lecture 27

Transport theory

We derived the Green's functions of a system coupled to several (macroscopic) reservoirs out of equilibrium:

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

$$G^<(\omega) = G^r \Sigma^< G^a$$

where

$$\Sigma(\omega) = V g(\omega) V^\dagger$$

$$\left[\Sigma^r(\omega)\right]_{nm} = \sum_\alpha \sum_{k\in\alpha} \frac{V_{nk} V^*_{mk}}{\omega - \epsilon_k + i0^+}$$

$$\left[\Sigma^<(\omega)\right]_{nm} = i \sum_\alpha f_\alpha(\omega) \left[\Gamma^\alpha(\omega)\right]_{nm}$$

$$[\Gamma^\alpha(\omega)]_{nm} = 2\pi \sum_{k\in\alpha} V_{nk} V^*_{mk}\, \delta(\omega - \epsilon_k)$$

Γ^α = "tunneling-width matrix"

cf. Fermi's golden rule

1) <u>Electrical current</u>

The current flowing into lead α is

$$I_\alpha = -e \frac{d}{dt} \langle \hat{N}_\alpha \rangle ,$$

where

$$\hat{N}_\alpha = \sum_{k\in\alpha} c_k^\dagger c_k$$

$$I_\alpha = -e\left(-\frac{i}{\hbar}\right) \langle [\hat{N}_\alpha , \hat{H}] \rangle$$

$$H = H_{sys} + H_{leads} + H_T$$

$$[\hat{N}_\alpha, H_{sys}] = 0 = [\hat{N}_\alpha, H_{leads}]$$

$$[\hat{N}_\alpha, H_T] = -\sum_n \sum_{k\in\alpha} \Big[V_{nk} \langle d_n^\dagger c_k \rangle - V_{nk}^* \langle c_k^\dagger d_n \rangle \Big]$$

$$I_\alpha = -\frac{ie}{\hbar} \sum_{k\in\alpha} \sum_n \Big[V_{nk} \langle d_n^\dagger c_k \rangle - V_{nk}^* \langle c_k^\dagger d_n \rangle \Big]$$

$$\langle d_n^\dagger(t)\, c_k(t) \rangle = \tilde{g}^<_{kn}(t,t)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \tilde{g}^<_{kn}(\omega)$$

$\tilde{g}^{<}(\omega)$ can be expressed in terms of $G^{<}$ and $G^{r,a}$ using the equations of motion:

$$I_\alpha = \frac{ie}{h}\int_{-\infty}^{\infty} d\omega\, \mathrm{Tr}\Big\{\Gamma^\alpha(\omega)\Big(G^{<}(\omega) + f_\alpha(\omega)\big[G^{r}(\omega) - G^{a}(\omega)\big]\Big)\Big\}$$

Meir–Wingreen formula (1992)

Interpretation:

$-\frac{i}{2\pi} G^{<}(\omega)$ = electron source in system, injecting electrons into contact α at rate $\Gamma^\alpha(\omega)$

$-\frac{i}{2\pi}\left[G^{r}(\omega) - G^{a}(\omega)\right]$ = density of states of system

Lead α injects electrons into system at rate

$$f_\alpha(\omega)\, \Gamma^\alpha(\omega)\left(\frac{-i}{2\pi}\right)\left[G^r(\omega)-G^a(\omega)\right].$$

2) <u>Heat current</u> $(TdS = dE - \mu dN)$

$$I_\alpha^Q = T_\alpha \frac{dS_\alpha}{dt} = \frac{d}{dt}\langle H^{(\alpha)}_{\text{lead}}\rangle - \mu_\alpha \frac{d}{dt}\langle N_\alpha\rangle$$

$$I_\alpha^Q = -\frac{i}{h}\int_{-\infty}^{\infty} d\omega\,(\omega-\mu_\alpha)\,\mathrm{Tr}\Big\{\Gamma^\alpha(\omega)\Big(G^<(\omega) + f_\alpha(\omega)\left[G^r(\omega)-G^a(\omega)\right]\Big)\Big\}$$

<u>Bergfield - Stafford (2009)</u>

Using the identity (from Dyson equation)

$$i\left(G^r - G^a\right) = \sum_\beta G^r \Gamma^\beta G^a + i\, G^r\left(\Sigma_c^r - \Sigma_c^a\right) G^a$$

one can show

$$I_\alpha^{(\nu)} = I_\alpha^{(\nu)}\Big|_{el} + I_\alpha^{(\nu)}\Big|_{in} \quad , \text{where}$$

$$\boxed{I_\alpha^{(\nu)}\Big|_{el} = \frac{1}{h}\sum_\beta \int dE\,(E-\mu_\alpha)^\nu\,(f_\beta - f_\alpha) \times \mathrm{Tr}\left\{\Gamma^\alpha G^r \Gamma^\beta G^a\right\}}$$

$$I_\alpha^{(\nu)}\Big|_{in} = -\frac{i}{h}\int dE\,(E-\mu_\alpha)^\nu\,\mathrm{Tr}\left\{\Gamma^\alpha G^r\left[(1-f_\alpha)\Sigma_c^< + f_\alpha \Sigma_c^>\right] G^a\right\}$$

$$T_{\alpha\beta}(E) = \mathrm{Tr}\left\{\Gamma^\alpha(E)\, G^r(E)\, \Gamma^\beta(E)\, G^a(E)\right\}$$

⇒ Landauer formula

$$\Sigma_c^{<}(\mu) \sim \max\{(k_B T)^2, (\Delta\mu)^2\}$$

⇒ At low temperatures and bias voltages, we recover Landauer formula for the current.

Bulk systems

$$G^{<}(\vec{p},\omega,\vec{R},T) = i\, A(\vec{p},\omega,\vec{R},T)\, f(\vec{p},\vec{R},T)$$

$$\vec{r} = \vec{x}_1 - \vec{x}_2 \leftrightarrow \vec{p}\,, \quad \vec{R} = \frac{1}{2}(\vec{x}_1 + \vec{x}_2)$$

$$t = t_1 - t_2 \leftrightarrow \omega\,, \quad T = \frac{1}{2}(t_1 + t_2)$$

A = "spectral function"

Eq. of motion for

$G^<$ $\Longrightarrow$ quantum Boltzmann equation