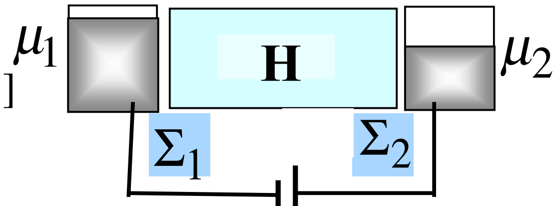
Useful Results

Basic equations of coherent transport



$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^{+}], \Gamma_2 = i[\Sigma_2 - \Sigma_2^{+}]$$

$$G(E) = [EI - H - \Sigma_1 - \Sigma_2]^{-1},$$

$$A(E) = i[G - G^{+}] = G\Gamma_1 G^{+} + G\Gamma_2 G^{+}$$ ***Density of states***

$$[G^{n}(E)] = [G\Gamma_1 G^{+}]\, f_1 + [G\Gamma_2 G^{+}]\, f_2$$ ***Electron density***

$$I_i(E) = (q/h)\,((Trace[\Gamma_i A]) f_i - Trace[\Gamma_i G^{n}])$$ ***Current/energy***

$$I(E) = (q/h)\;\; Trace[\Gamma_1 G \Gamma_2 G^{+}](f_1(E) - f_2(E))$$ ***2-terminal current***

Simpler version $n(E) \;=\; D(E)\,\dfrac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1 + \gamma_2}$ ***Electron density***

$$I_i(E) \;=\; (q\,\gamma_i/\hbar)\big(D(E) f_i(E) - n(E)\big)$$ ***Current/energy***

$$I(E) = \frac{q}{\hbar}\;\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}\, D(E)\,(f_1(E) - f_2(E))$$ ***2-terminal current***

Ballistic transport: $\gamma_1 = \gamma_2 = \hbar v_x / L$. In diffusive regime $dI^{+}/dx = dI^{-}/dx = -I/mfp$, leading to a reduction in the current $I = I^{+} - I^{-}$ by a factor ***mfp / (mfp+L) .***

In general H has to be replaced with H+U, and D(E) with D(E-U) where U has to be calculated self-consistently from an appropriate "Poisson"-like equation.

Other useful relations: $f(E) = \dfrac{1}{1 + \exp(E - \mu)/kT}$ *Fermi function*

$$P_\alpha = (1/Z)\exp(-(E_\alpha - \mu N_\alpha)/kT)$$ *Law of equilibrium*

$$[h(\vec{k})] = \sum_m [H_{nm}]\exp(i\vec{k}.(\vec{d}_m - \vec{d}_n))$$ *Bandstructure*

$$D(E) = \sum_{\vec{k}} \delta(E - \varepsilon(\vec{k}))$$ *Density of states*

$$M(E) = \sum_{\vec{k}} \delta(E - \varepsilon(\vec{k}))\,\frac{\pi\hbar\,\left|v_x(\vec{k})\right|}{L}$$ *Density of modes*