Quantum thermoelectricity - a few exercises

1. Show that the Onsager reciprocal relation $\Pi = TS$ between Peltier coefficient Π and Seebeck coefficient S (T is the temperature) is valid, for a two-terminal system described by Landauer scattering theory, also when a generic magnetic field $\mathbf{B}$ is applied, that is, $\Pi(\mathbf{B}) = TS(\mathbf{B})$ (which is different from the Onsager-Casimir relation $\Pi(\mathbf{B}) = TS(-\mathbf{B})$).

2. Given a scatterer connected to two reservoirs (L, R), in the steady-state the entropy of the scatterer does not change in time, while the rate of change of entropy in the reservoirs is $\dot{\mathscr{S}}_i = -J_{h,i}/T_i$, with $i = L, R$, and $J_{h,i}$ heat current out of reservoir i (at temperature T_i) into the scatterer. Show that, within linear response, the total entropy production reduces to $\dot{\mathscr{S}} = \mathcal{F}_e J_e + \mathcal{F}_h J_h$. Here J_h and J_e are the heat and electric currents, while the thermodynamic forces are $\mathcal{F}_e = \Delta V/T$ (where ΔV is the applied voltage) and $\mathcal{F}_h = \Delta T/T^2$ ($\Delta T \equiv T_L - T_R$). Discuss generalization of this problem to N reservoirs.

3. Compute the transmission probabilities $\mathcal{T}_{ij}$ ($i, j = 1, 2, 3$) for a system made of two dots in series, each with a single energy level, described by the Hamiltonian:

$$H = \begin{bmatrix} E_L & -t \\ -t & E_R \end{bmatrix}. \tag{1}$$

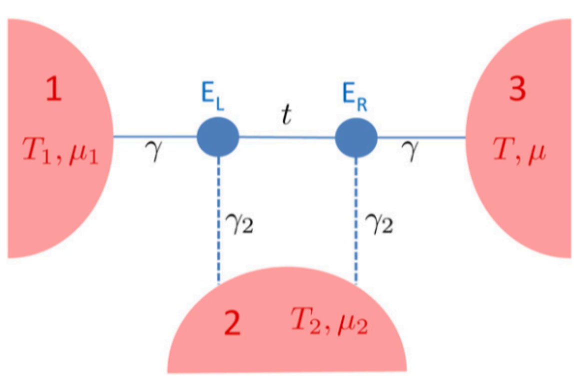
In the wide-band approximation the self-energies may be written as

$$\Sigma_1 = \begin{bmatrix} -i\frac{\gamma_1}{2} & 0 \\ 0 & 0 \end{bmatrix}, \quad \Sigma_3 = \begin{bmatrix} 0 & 0 \\ 0 & -i\frac{\gamma_3}{2} \end{bmatrix},$$
$$\Sigma_2 = \begin{bmatrix} -i\frac{\gamma_2}{2} & 0 \\ 0 & -i\frac{\gamma_2}{2} \end{bmatrix}. \tag{2}$$

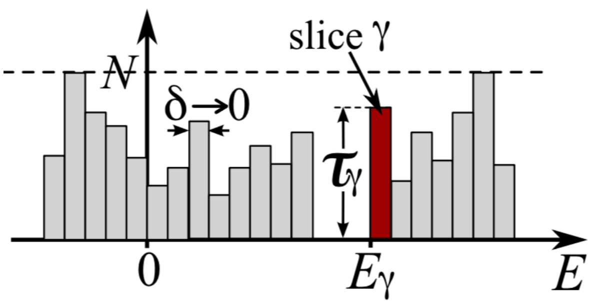
Suggestion: use the Fisher-Lee formula:

$$\mathcal{T}_{ij} = \mathrm{Tr}\left[\Gamma_i\, G\, \Gamma_j\, G^\dagger\right], \tag{3}$$

where the broadening matrices $\Gamma_i = i(\Sigma_i - \Sigma_i^\dagger)$ and G the retarded Green's function of the system.



4. Find the optimal transmission function which maximizes the thermoelectric figure of merit ZT in the case when thermal conductivity is dominated by phonons. Suggestion: consider the transmission function as an infinite set of slices each of width $\delta \to 0$, where we define τ_γ as the transmission of slice γ, which sits at energy E_γ.



5. Consider a quantum dot coupled to left (L) and right (R) reservoirs. The simplest case is that in which we neglect spin and assume the charging energy for double-occupancy, U, is much bigger than all other energy scales (temperatures, biases, etc.). Then we only have two system states 0 (dot-level empty) and 1 (dot-level singly occupied), with energies $E_0 = 0$ and $E_1 = \epsilon_1$, respectively. Then, the rate equation for the dot's dynamics is

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} P_0(t) \\ P_1(t) \end{pmatrix} = \begin{pmatrix} -\Gamma_{10} & \Gamma_{01} \\ \Gamma_{10} & -\Gamma_{01} \end{pmatrix} \begin{pmatrix} P_0(t) \\ P_1(t) \end{pmatrix}, \tag{4}$$

where $\Gamma_{ba} = \Gamma_{ba}^{(\mathrm{L})} + \Gamma_{ba}^{(\mathrm{R})}$. Here $P_i(t)$ is the probability to find the dot in state i at time t. Moreover, the rates obey the local detailed balance condition

$$\Gamma_{ab}^{(i)} = \Gamma_{ba}^{(i)} \exp\left[-\Delta\mathscr{S}_{ba}^{(i)} \Big/ k_\mathrm{B}\right], \tag{5}$$

where $\Delta\mathscr{S}_{ba}^{(i)}$ is the change in entropy in reservoir i when it induces a system transition from a to b. This entropy change is given by the Clausius relation

$$\Delta\mathscr{S}_{ba}^{(i)} = \frac{\Delta Q_{ba}^{(i)}}{T_i} = \frac{E_a - E_b - (N_a - N_b)\mu_i}{T_i}, \tag{6}$$

where E_a and N_a are the energy and electron-number for system state a and μ_i is the electrochemical potential of reservoir i. Here $\Delta Q_{ba}^{(i)}$ is the change in heat in reservoir i associated with the transition $a \to b$.

Compute the steady state, the efficiency (for power production and for refrigeration), and the value of the electrochemical potential difference $\mu = \mu_R - \mu_L$ (for simplicity, set $\mu_L = 0$) such that the Carnot efficiency is achieved.

Note: the particle current into the system from reservoir i is

$$J_{\rho,i}(t) = \tfrac{1}{2}\sum_{ab}(N_b - N_a)\,\mathcal{I}_{ba}^{(i)}(t), \tag{7}$$

where the probability current for the transition from state a to state b at time t due to reservoir i is

$$\mathcal{I}_{ba}^{(i)}(t) \;=\; -\mathcal{I}_{ab}^{(i)}(t) \;=\; \Gamma_{ba}^{(i)}\,P_a(t) - \Gamma_{ab}^{(i)}\,P_b(t)\;, \tag{8}$$

and the factor of $\frac{1}{2}$ is due to the fact that the sum over a and b counts each transition twice. By analogy, the energy current out of reservoir i into the system is

$$J_{u,i}(t) = \tfrac{1}{2}\sum_{ab}(E_b - E_a)\,\mathcal{I}_{ba}^{(i)}(t). \tag{9}$$

At steady state,

$$\mathcal{I}_{ba}^{(i)\mathrm{steady}}(t) \;=\; -\mathcal{I}_{ab}^{(i)\mathrm{steady}}(t) \;=\; \Gamma_{ba}^{(i)}\,P_a^{\mathrm{steady}} - \Gamma_{ab}^{(i)}\,P_b^{\mathrm{steady}}\;. \tag{10}$$