ECE 659 EXAM V

Monday May 4, 2015, EE 117 8A-10A

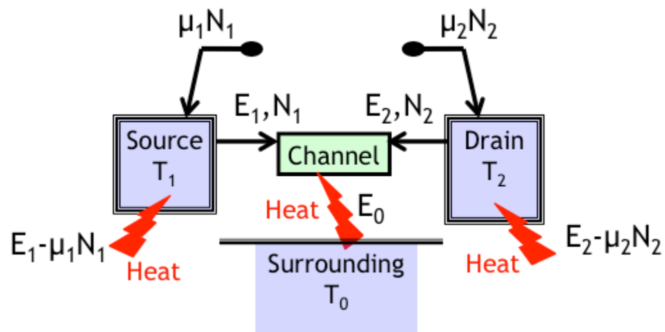
NAME : SOLUTION

CLOSED BOOK

All five questions carry equal weight

Please show all work.
No credit for just writing down the answer, even if correct.

5.1.



Consider a channel exchanging electrons and energies with three reservoirs as shown.

(a) What relationship among the different quantities (N_1, N_2, E_1, E_2, E_0) is required by
(i) Conservation of number of electrons
(ii) Conservation of energy
(iii) Second law of thermodynamics:

(b) Two materials A and B have different density of states D_A and D_B for electrons in a certain energy range. If these materials are in equilibrium with electrons flowing freely between them, will the number of electrons in this energy range in the two materials n_A and n_B be equal? If not, what will be the ratio $\frac{n_A}{n_B}$? Explain.

SOLUTION:

(a)

$$N_1 + N_2 = 0$$

$$E_1 + E_2 + E_0 = 0$$

$$\frac{E_1 - \mu_1 N_1}{T_1} + \frac{E_2 - \mu_2 N_2}{T_2} + \frac{E_0}{T_0} \leq 0$$

(b)

$\frac{n_A}{n_B} = \frac{D_A}{D_B}$ so that the same fraction of states is occupied in either case.

5.2. Consider a quantum dot with 4 degenerate levels, all with the same energy ε, in equilibrium with a reservoir with electrochemical potential μ and temperature T. If there were no interactions, the average number of electrons at equilibrium would be given by

$$< n >= \frac{4}{1+e^{(\varepsilon-\mu)/kT}}$$

Obtain an expression for the average number of electrons if the electron-electron interaction is so large that no more than one of the 4 levels can be occupied at the same time.

SOLUTION:

There is one zero-electron state with probability

$$P_0 = \frac{1}{Z}$$

and 4 one-electron states each with a probability

$$P_1 = \frac{e^{-x}}{Z}\,, \quad x \equiv \frac{\varepsilon-\mu}{kT}$$

$$< n >= \frac{\sum_n nP_n}{\sum_n P_n} = \frac{4P_1}{P_0+4P_1}$$

$$< n >= \frac{4e^{-x}}{1+4e^{-x}} = \frac{4}{4+e^{x}} = \frac{4}{4+e^{(\varepsilon-\mu)/kT}}$$

5.3. Consider a single quantum dot with ***just one level*** with energy ε. We wish to find the current as a function of the electrochemical potential $\mu_2 = \mu_1 + qV$ (keeping μ_1 fixed) using the Fock space picture by writing

$$\frac{d}{dt}\begin{Bmatrix} P_0 \\ P_1 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} = [W_1 + W_2]\begin{Bmatrix} P_0 \\ P_1 \end{Bmatrix}$$

where the W_1 and W_2 matrices describe the transition rates between the different states due to electron exchange with contacts 1 and 2 respectively which are held in equilibrium with electrochemical potentials μ_1 and μ_2.

(a) Write down the matrices W_1 and W_2 is terms of the Fermi functions in contacts 1, 2.
(b) Obtain the steady-state probabilities P_0 and P_1.
(c) Obtain the steady-state current.

SOLUTION:

(a)

$$W_1 = \gamma_1 \begin{bmatrix} -f_1 & 1-f_1 \\ +f_1 & -(1-f_1) \end{bmatrix} \qquad W_2 = \gamma_2 \begin{bmatrix} -f_2 & 1-f_2 \\ +f_2 & -(1-f_2) \end{bmatrix}$$

(b)

$$\begin{Bmatrix} 0 \\ 0 \end{Bmatrix} = \begin{bmatrix} -\gamma_1 f_1 - \gamma_2 f_2 & \gamma_1(1-f_1)+\gamma_2(1-f_2) \\ \gamma_1 f_1 + \gamma_2 f_2 & -\gamma_1(1-f_1)-\gamma_2(1-f_2) \end{bmatrix}\begin{Bmatrix} P_0 \\ P_1 \end{Bmatrix}$$

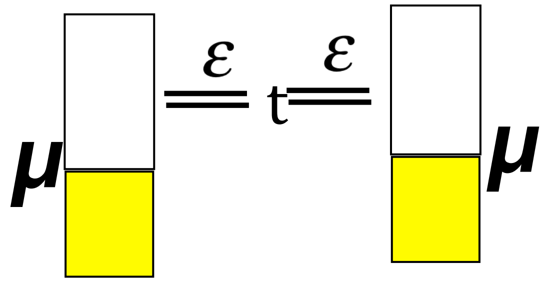
$$\frac{P_1}{P_0} = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1(1-f_1)+\gamma_2(1-f_2)} \rightarrow P_1 = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}, \quad P_0 = 1 - P_1$$

(c)

$$I = q\gamma_1 \{0 \quad 1\}\begin{bmatrix} -f_1 & 1-f_1 \\ +f_1 & -(1-f_1) \end{bmatrix}\begin{Bmatrix} P_0 \\ P_1 \end{Bmatrix} = q\gamma_1\left(f_1 P_0 - (1-f_1)P_1\right) = \gamma_1(f_1 - P_1)$$

$$= q\gamma_1\left(f_1 - \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right) = q\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}(f_1 - f_2)$$

5.4. Consider two coupled quantum dots each with two spin-degenerate levels, described by the one-electron Hamiltonian,



$$h = \begin{array}{c} \begin{matrix} u_1 & u_2 & d_1 & d_2 \end{matrix} \\ \begin{bmatrix} \varepsilon & t & 0 & 0 \\ t & \varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon & t \\ 0 & 0 & t & \varepsilon \end{bmatrix} \end{array}$$

having an intra-dot interaction energy U and zero inter-dot interaction energy.

Useful result: Eigenvalues of $\begin{bmatrix} a & 0 & t & t \\ 0 & a & t & t \\ t & t & b & 0 \\ t & t & 0 & b \end{bmatrix}$ *are*

a, b and $\dfrac{(a+b) \pm \sqrt{(a-b)^2 + 16t^2}}{2}$

(a) At what value of μ does the total number of electrons change from N = 2 to 3?

(b) At what value of μ does the total number of electrons change from N = 3 to 4?

SOLUTION:

Two-electron states

$$H_2 = \begin{array}{c} \begin{matrix} u_1d_1 & u_2d_2 & u_1d_2 & u_2d_1 & u_1u_2 & d_1d_2 \end{matrix} \\ \begin{bmatrix} 2\varepsilon+U & 0 & t & t & 0 & 0 \\ 0 & 2\varepsilon+U & t & t & 0 & 0 \\ t & t & 2\varepsilon & 0 & 0 & 0 \\ t & t & 0 & 2\varepsilon & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\varepsilon & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\varepsilon \end{bmatrix} \end{array}$$

$$\min(E-\mu N)= \quad \frac{2\varepsilon+2\varepsilon+U-\sqrt{U^2+16t^2}}{2}-2\mu \quad = \quad 2\varepsilon-2\mu+\frac{U}{2}-\sqrt{\left(\frac{U}{2}\right)^2+4t^2}$$

Three-electron states

$$H_3 = \begin{array}{cccc} u_2d_1d_2 & u_1d_1d_2 & u_1u_2d_2 & u_1u_2d_1 \\ \left[\begin{matrix} 3\varepsilon+U & t & 0 & 0 \\ t & 3\varepsilon+U & 0 & 0 \\ 0 & 0 & 3\varepsilon+U & t \\ 0 & 0 & t & 3\varepsilon+U \end{matrix}\right. & & & \left.\right] \end{array}$$

$$\min(E-\mu N)= \quad 3\varepsilon+U-|t|-3\mu \qquad = \quad 2\varepsilon-2\mu+\frac{U}{2}-\sqrt{\left(\frac{U}{2}\right)^2+4t^2}$$

Four-electron states

$$u_1u_2d_1d_2$$

$$\left[2\varepsilon+2U\right]$$

$$\min(E-\mu N)= \quad 4\varepsilon+2U-4\mu$$

(a) N=2 to N=3:

$$2\varepsilon-2\mu+\frac{U}{2}-\sqrt{\left(\frac{U}{2}\right)^2+4t^2} \quad = \quad 3\varepsilon+U-|t|-3\mu$$

$$\mu(2\to 3) \quad = \quad \varepsilon+\frac{U}{2}-|t|+\sqrt{\left(\frac{U}{2}\right)^2+4t^2}$$

(a) N=3 to N=4:

$$3\varepsilon+U-|t|-3\mu \quad = \quad 4\varepsilon+2U-4\mu$$

$$\mu(3\to 4) \quad = \quad \varepsilon+|t|+U$$

5.5. What is the entropy per spin (ρ : density matrix)

$$S \;=\; -k\ Trace[\rho\ \ell n\ \rho]$$

corresponding to each of these three collections of spins

a) All pointing along +z

b) All pointing along +y

c) 50% pointing along +x, 50% along -x

Please write down the density matrix in each case, in ± z basis

SOLUTION:

(a)

$$\rho \;=\; \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$S \;=-k\ Trace\ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \ell n1 & 0 \\ 0 & \ell n0 \end{bmatrix} \;=\; 0$$

(b)

$$\rho \;=\; \frac{1}{2}\begin{pmatrix} 1 \\ i \end{pmatrix}\begin{pmatrix} 1 & -i \end{pmatrix} = \;\frac{1}{2}\begin{bmatrix} 1 & -i \\ +i & 1 \end{bmatrix}$$

Diagonalizing

$$\rho \;=\; \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$S \;=-k\ Trace\ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \ell n1 & 0 \\ 0 & \ell n0 \end{bmatrix} \;=\; 0$$

(c)

$$\rho \;=\; 0.5 * \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + 0.5 * \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \;=\; \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

Hence

$$S \;=-k\ Trace\ \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}\begin{bmatrix} \ell n1/2 & 0 \\ 0 & \ell n1/2 \end{bmatrix} \;=\; k\ \ell n2$$

Have a great summer !!