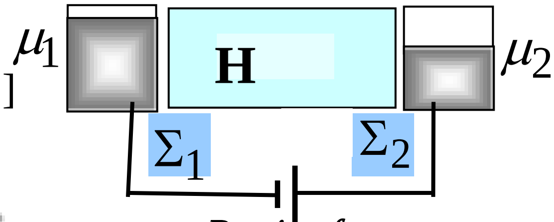
ECE 495N, Fall'08 Fundamentals of Nanoelectronics

Final examination: Friday 12/19/08, 7-9 pm in LYNN G167.

Cumulative, closed book. Equations listed on this page will be provided.

Basic equations of coherent transport



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

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

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

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

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

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

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

$$I_i(E) = (q\gamma_i/\hbar)\left(D(E)\, f_i(E) - n(E)\right) \qquad \textit{Current/energy}$$

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

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*

$$P_\alpha = (1/Z)\exp(-(E_\alpha - \mu N_\alpha)/kT) \qquad \textit{Law of equilibrium}$$

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

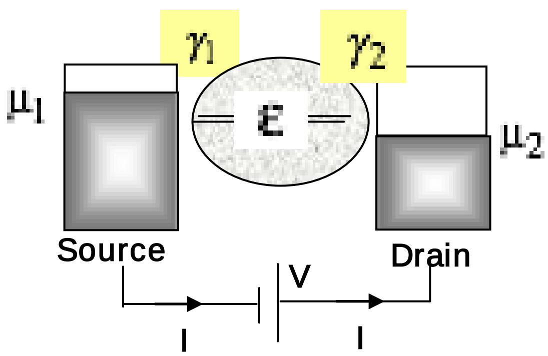
$$D(E) = \sum_{\vec{k}} \delta(E - \varepsilon(\vec{k})) \qquad \textit{Density of states}$$

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

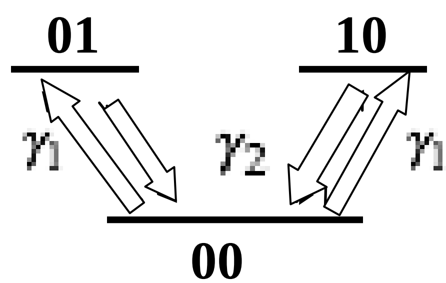
Problem 1 (Simple model for conduction): Suppose a material has a density of states (per unit energy), $D(E) = AE^{\alpha}$ and a density of modes (dimensionless), $M(E) = BE^{\beta}$, where A, B, α and β are constants. Assuming ballistic transport, obtain an expression for the conductance as a function of the total number of electrons N at T=0K. Hint: First, obtain separate expressions for N and the conductance as a function of the equilibrium electrochemical potential μ.

Problem 2 (Multi-electron picture):

One-electron picture



Multi-electron picture
(state 11 excluded because
it is energetically inaccessible)



(a) A box has two degenerate energy levels both having energy ε. Use the multielectron picture to derive the correct expression for the maximum current if the electron-electron interaction energy is so high that no more than one electron can be inside the box at the same time. Your answer should be in terms of γ_1, γ_2, q *and* $\hbar$, assuming a bias polarity such that $\mu_1 > \mu_2$, as shown.
(b) Assuming $\gamma_1 = 10\gamma_2$. if we reverse the polarity of the applied bias so that $\mu_1 < \mu_2$. will the current change? By what factor ?

Problem 3 (Bandstructure): Consider an infinitely long linear 1-D lattice (lattice constant: a) with one s-orbital per atom (assumed orthogonal) and having a site energy of E_0, so that the Hamiltonian looks like (t is real)

$$H = \begin{bmatrix} \varepsilon & te^{i\varphi} & 0 & 0 & \cdots \\ te^{-i\varphi} & \varepsilon & te^{i\varphi} & 0 & \cdots \\ 0 & te^{-i\varphi} & \varepsilon & te^{i\varphi} & \cdots \\ \cdots & \cdots & \cdots & & \end{bmatrix}$$

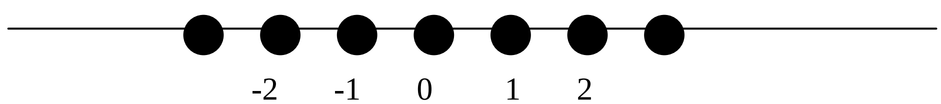
Impose periodic boundary conditions and assume a solution of the form $\phi_n = \phi_0 \, e^{ik\,na}$ to find the dispersion relation E(k).

Problem 4 (Density of states): A ***three-dimensional*** conductor (S: cross-sectional area, L: Length) has an E(k) relationship $E = Bk^2$. Find the density of states (per unit energy), D(E) and the density of modes (dimensionless), M(E).

Problem 5 (spin): Consider a device with two spin-degenerate levels, described by a (2x2) Hamiltonian $[H] = \begin{bmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix}$. A magnetic field B is applied along an arbitrary direction $\hat{n} = \hat{x}\sin\theta\cos\varphi + \hat{y}\sin\theta\sin\varphi + \hat{z}\cos\theta$.

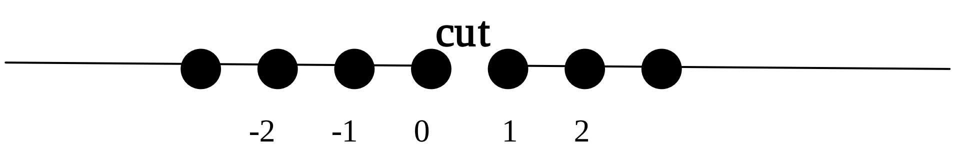
This gives rise to an additional term in [H] that can be written as $[H_B] = \mu_B B \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}$ ***if we use up- and down-spins along $\hat{n}$ as our basis.*** Transform bases to up and down spins along $\hat{z}$, to show that $[H_B]$ can be written in the form $[H_B] = \mu_B B_x [\sigma_x] + \mu_B B_y [\sigma_y] + \mu_B B_z [\sigma_z]$. Find the matrices $[\sigma_x]$, $[\sigma_y]$ and $[\sigma_z]$.

Problem 6 (Matrix model for conduction): (a) Consider an infinite wire modeled as a discrete lattice with points spaced by 'a'



having a Hamiltonian with $H_{n,n} = 2t_0$ and $H_{n,n+1} = -t_0 = H_{n,n-1}$ (all other elements are zero), such that the dispersion relation is given by $E = 2t_0(1-\cos ka)$. What is the local density of states at the point "0", D(0,E) ?

(b) Suppose we cut the wire in Problem 2 into two separate semi-infinite wires as shown so that $H_{01} = H_{10} = 0$ (other elements of the H-matrix remain unchanged).



What is the local density of states at the point "0", D(0,E) ?

Useful Relations: **1.** $\sin\theta = 2\sin(\theta/2)\cos(\theta/2)$,

$$1+\cos\theta = 2\cos^2(\theta/2),\ 1-\cos\theta = 2\sin^2(\theta/2)$$

2. Spins along $+\hat{n} : \{c \quad s\}^T$, $-\hat{n} : \{-s^* \quad c^*\}^T$ **(T:transpose)**

where $c \equiv \cos(\theta/2)\, e^{-i\varphi/2}$ **and** $s \equiv \sin(\theta/2)\, e^{+i\varphi/2}$