ECE 659, EXAM III

Friday, March 10, 2017, ME 1012, 330-420PM

NAME : SOLUTION

CLOSED BOOK

One page of notes provided, please see last page

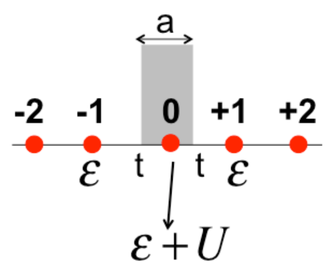
All four questions carry equal weight

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

3.1. Calculate the transmission through a single scatterer of height U in a 1D wire (t < 0) using the expression

$$\bar{T}(E) = \quad Trace[\Gamma_1 G^R \Gamma_2 G^A]$$

in terms of E, t, U and ϵ



SOLUTION:

Treat site "0" as device described by (1x1) [H] matrix and rest as contacts.

$$[H] = \varepsilon + U$$
$$[\Sigma_1] = [\Sigma_2] = te^{ika}$$
$$[\Gamma_1] = [\Gamma_2] = i(te^{ika} - te^{-ika}) = -2t\sin ka$$

$$\bar{T}(E) = \quad [\Gamma_1 G^R \Gamma_2 G^A]$$
$$= (2t\sin ka)^2 \frac{1}{E-\varepsilon-U-2te^{ika}} \frac{1}{E-\varepsilon-U-2te^{-ika}}$$

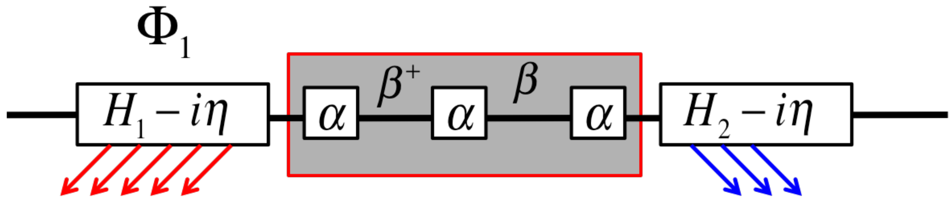
$$= (2t\sin ka)^2 \frac{1}{2t\cos ka-U-2te^{ika}} \frac{1}{2t\cos ka-U-2te^{-ika}}$$

$$= (2t\sin ka)^2 \frac{1}{-U-2it\sin ka} \frac{1}{-U+2it\sin ka}$$

$$= \frac{(2t\sin ka)^2}{U^2+(2t\sin ka)^2}$$

$$\text{where } \cos(ka) = (E-\epsilon)/2t$$

3.2.



Starting from

$$\begin{bmatrix} E+i\eta-H_1 & -\tau_1^+ & 0 \\ -\tau_1 & E-H & -\tau_2 \\ 0 & -\tau_2^+ & E+i\eta-H_2 \end{bmatrix} \begin{Bmatrix} \Phi_1+\chi_1 \\ 0+\ \psi \\ 0\ +\chi_2 \end{Bmatrix} = \begin{Bmatrix} \tilde{s}_1 \\ 0 \\ 0 \end{Bmatrix}$$

Obtain the result

$$E\psi = H\psi + \ (\Sigma_1+\Sigma_2)\psi + \quad s_1$$

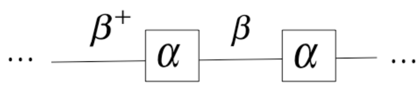
Stating clearly how Σ_1, Σ_2, s_1 *are related to the quantities appearing in the original equation*

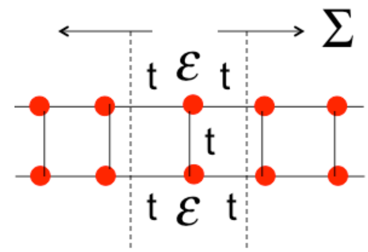
SOLUTION:

Please see **video lecture 3-L3.3 on course website.**
https://www.youtube.com/watch?v=YPMgw9nL74g **after 06:30**

3.3. Consider a conductor described by a tight-binding model two lattice sites along the width as shown below. We wish to find the self-energy Σ.

We can represent it by a 1-D chain of the form





where $\alpha = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$, $\beta = \begin{bmatrix} t & 0 \\ 0 & t \end{bmatrix}$

The matrix α has eigenvalues ($\varepsilon + t$) and ($\varepsilon - t$)

with eigenvectors $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ respectively.

We can use these eigenvectors as the basis, to diagonalize the matrix α.

(a) Write down the matrices α, β. And Σ(E) in this eigenvector basis (the one that diagonalizes α).

(b) Write down the matrix Σ(E) in the original basis.

SOLUTION:

(a)

$$\alpha = \begin{bmatrix} \varepsilon + t & 0 \\ 0 & \varepsilon - t \end{bmatrix}, \ \beta = \begin{bmatrix} t & 0 \\ 0 & t \end{bmatrix}$$

$$\Sigma(E) = \begin{bmatrix} te^{ik_1 a} & 0 \\ 0 & te^{ik_2 a} \end{bmatrix} \equiv \begin{bmatrix} p & 0 \\ 0 & q \end{bmatrix}$$

where k_1 and k_2 are given by

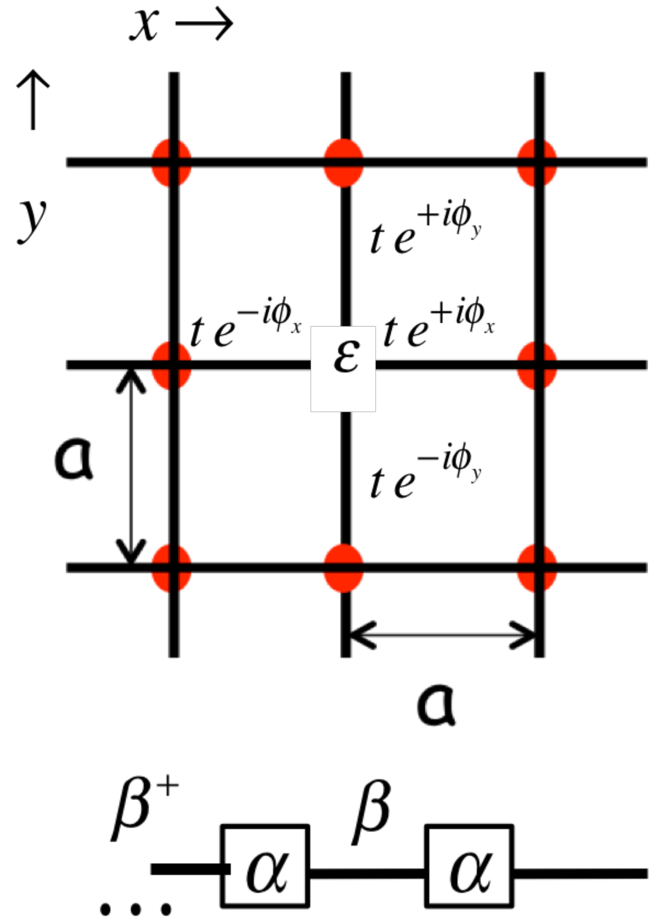
$$\begin{aligned} E &= \varepsilon + t + 2t\cos k_1 a \quad \rightarrow \quad \cos k_1 a = (E - \varepsilon - t)/2t \\ &= \varepsilon - t + 2t\cos k_2 a \quad \rightarrow \quad \cos k_2 a = (E - \varepsilon + t)/2t \end{aligned}$$

(b) $$\Sigma(E) = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} p & 0 \\ 0 & q \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} p & p \\ q & -q \end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix} p+q & p-q \\ p-q & p+q \end{bmatrix}$$

3.4.

$$\phi_x = \frac{qA_x a}{\hbar}, \ \phi_y = \frac{qA_y a}{\hbar}$$



A conductor in a magnetic field B can be modeled with a 2D square lattice using nearest neighbor couplings as shown where **A_x = By.**

Do you think you can split the 2D conductor into independent conductors **by transforming the basis so as to diagonalize** α

as we do when B=0 ?

Explain why or why not.

SOLUTION:

With B=0, $$\beta = \begin{bmatrix} t & 0 & 0 \\ 0 & t & 0 \\ 0 & 0 & t \end{bmatrix}$$

which is t times the identity matrix, so that it is unchanged byany basis transformation.

But in this case

$$\beta = \begin{bmatrix} te^{i\phi_{n+1}} & 0 & 0 \\ 0 & te^{i\phi_n} & 0 \\ 0 & 0 & te^{i\phi_{n-1}} \end{bmatrix}$$

where

$$\phi_n = qBay_n/\hbar$$

so that it is not a number times an identity matrix.

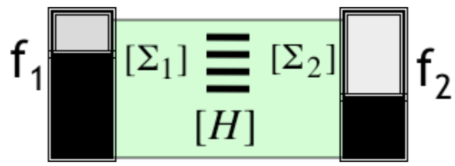
We will not get independent 1D conductors, because

$$\textit{If we diagonalize } \alpha$$
$$\textit{it will un-diagonalize } \beta$$

This can be proved by showing that the two matrices do not commute:

$$\alpha\beta \neq \beta\alpha$$

NEGF Equations



$$G^R = [EI - H - \Sigma]^{-1}$$

$$G^n = G^R \; \Sigma^{in} \; G^A$$

$$A = G^R \Gamma G^A = G^A \Gamma G^R$$

$$= i[G^R - G^A]$$

$$\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_0$$

$$\Gamma_{0,1,2} = i[\Sigma_{0,1,2} - \Sigma_{0,1,2}^{+}]$$

$$\tilde{I}_p = \frac{q}{h} Trace[\Sigma_p^{in} A - \Gamma_p G^n]$$

$$\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_0$$

$$\Sigma^{in} = \underbrace{f_1 \Gamma_1}_{\Sigma_1^{in}} + \underbrace{f_2 \Gamma_2}_{\Sigma_2^{in}} + \Sigma_0^{in}$$

Coherent transport

$$I = \frac{q}{h} \int_{-\infty}^{+\infty} dE \; (f_1(E) - f_2(E)) \, \bar{T}(E)$$

$$\bar{T}(E) \equiv \frac{G(E)}{q^2 / h} = Trace[\Gamma_1 G^R \Gamma_2 G^A]$$

Device with multiple terminals "r"

$$\Gamma = \sum_r \Gamma_r$$

$$\Sigma^{in} = \sum_r \Sigma_r^{in} = \sum_r \Gamma_r f_r$$

Surface Green's function $\quad g_N^{-1} = E + i\eta - \alpha - \beta^{+} g_{N-1} \beta$

Self-energy $\quad \Sigma_1 = \tau_1 \; \overbrace{[E + i\eta - H_1]^{-1}}^{g_1} \; \tau_1^{+}$

This integral may be useful: $\displaystyle\int_{-\infty}^{+\infty} \frac{dx}{x^2 + a^2} = \frac{\pi}{a}$