ECE 659, PRACTICE EXAM III

Actual Exam

Friday, Mar.14, 2014, FRNY B124, 330-420PM

NAME : ____

CLOSED BOOK

One page of notes provided, please see last page

Actual Exam will have five questions.

The following questions have been chosen to stress what I consider the most important concepts / skills that you should be clear on.

3.1. NEGF treatment of one-level device
3.2. NEGF from Schrodinger
3.3. Important NEGF related identity
3.4. Sum rule for coherent transport
3.5. 1D self-energy and scattering theory
3.6. 1D scattering from NEGF
3.7. Dephasing processes in NEGF
3.8. Potential drop across a scatterer**
3.9. 2D self-energy using basis transformation
3.10. Conductance quantization**

** It may be instructive to try out MATLAB-based numerical examples, please see "MATLAB-based homework" posted on website.

Text: *Lecture 19-21, LNE*

Reference: *Chapters 8-9, QTAT*

3.1. A one-level device is described by a (1x1) Hamiltonian and contact self-energies

$$[H]=[\varepsilon] \qquad [\Sigma_1]=-i\,[\gamma_1/2] \quad , \quad [\Sigma_2]=-i\,[\gamma_2/2]$$

Obtain an expression for the ***current*** and the ***correlation function*** (or the "electron density") $G^n(E)$ in terms of $\varepsilon, \gamma_1, \gamma_2$ and the Fermi functions $f_1(E)$, $f_2(E)$.

SOLUTION:

$$G^R = \left(E-\varepsilon+i\gamma/2\right)^{-1} \qquad \gamma=\gamma_1+\gamma_2$$

$$\Gamma_1 = i\left(-\frac{i\gamma_1}{2}-i\frac{\gamma_1}{2}\right)=\gamma_1$$

$$\Gamma_2 = \gamma_2$$

$$G^n = G^R\left(\Gamma_1 f_1+\Gamma_2 f_2\right)G^A$$

$$= \frac{\gamma_1 f_1+\gamma_2 f_2}{(E-\varepsilon)^2+(\gamma/2)^2}$$

$$A = \quad i\,[G^R-G^A] = \quad i\left[\frac{1}{E-\varepsilon+i\gamma/2}-\frac{1}{E-\varepsilon-i\gamma/2}\right]$$

$$= \frac{\gamma}{(E-\varepsilon)^2+(\gamma/2)^2}$$

$$\tilde{I}_1 = \frac{q}{h}Trace[\Sigma_1^{in}A-\Gamma_1 G^n] \quad = \quad \frac{q}{h}[\gamma_1 f_1 A-\gamma_1 G^n]$$

$$= \frac{q}{h}\frac{\gamma\,\gamma_1 f_1-\gamma_1(\gamma_1 f_1+\gamma_2 f_2)}{(E-\varepsilon)^2+(\gamma/2)^2} = \frac{q}{h}\frac{\gamma_1\gamma_2\,(f_1-f_2)}{(E-\varepsilon)^2+(\gamma/2)^2}$$

$$I_1 = \int_{-\infty}^{+\infty} dE\,\tilde{I}_1 = \frac{q}{h}\int_{-\infty}^{+\infty} dE\,\underbrace{\frac{\gamma_1\gamma_2}{(E-\varepsilon)^2+(\gamma/2)^2}}_{\equiv\ \bar{T}(E)}\,(f_1-f_2)$$

3.2. Starting from the modified Schrodinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi = [H+\Sigma]\psi + S$$

show how you obtain the NEGF equations for the matrix electron density [G^n], the matrix density of states [A],

$$G^n = G^R\,\Sigma^{in}\,G^A \quad , \quad A = G^R\,\Gamma\,G^A$$

and the current

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

SOLUTION: Please see Section 19.2 of LNE.

3.3. Starting from the relations

$$G^R = [EI - H - \Sigma]^{-1}, G^A \equiv \left[G^R\right]^+ \quad and \quad \Gamma = i\left[\Sigma - \Sigma^+\right]$$

show that

$$A \equiv G^R\Gamma G^A = G^A\Gamma G^R = i[G^R - G^A]$$

SOLUTION:

$$(G^R)^{-1} = EI - H - \Sigma$$

$$((G^R)^{-1})^\dagger = (G^A)^{-1} = EI - H - \Sigma^\dagger$$

$$(G^R)^{-1} - (G^A)^{-1} = \Sigma^\dagger - \Sigma = i\Gamma$$

- Multiply by G^R from left and G^A from right

$$G^A - G^R = i\,G^R\Gamma G^A$$

- Multiply by G^A from left and G^R from right

$$G^A - G^R = i\,G^A\Gamma G^R$$

Hence $\quad i\,(G^R - G^A) = G^R\Gamma G^A = G^A\Gamma G^R$

3.4. Starting from $\tilde{I}_p \;=\; \frac{q}{h} Trace\left[\Sigma_p^{in} A - \Gamma_p G^n\right]$

show that for a multiterminal device

(a) $\tilde{I}_p = \frac{q}{h} \sum_r \left(f_p(E) - f_r(E)\right) \bar{T}_{pr}(E) \qquad \bar{T}_{pr}(E) \equiv Trace[\Gamma_p G^R \Gamma_r G^A]$

(b) $\sum_p \bar{T}_{pr} \;=\; \sum_p \bar{T}_{rp}$

SOLUTION:

$$\tilde{I}_p = \frac{q}{h} \, Trace \; f_p \Gamma_p \underset{\substack{\uparrow \\ G^R \underset{\substack{\uparrow \\ \sum_r \Gamma_r}}{\Gamma} G^A}}{A} - \Gamma_p \underset{\substack{\nwarrow \\ G^R \underset{\substack{\uparrow \\ \sum_r \Gamma_r f_r}}{\Sigma^{in}} G^A}}{G^n}$$

$$= \frac{q}{h} \sum_r Trace \; f_p \, \Gamma_p G^R \Gamma_r G^A - \Gamma_p G^R \Gamma_r f_r \, G^A$$

$$= \frac{q}{h} \sum_r (f_p - f_r) \underbrace{Trace\left[\Gamma_p G^R \Gamma_r G^A\right]}_{\equiv \, \bar{T}_{pr}}$$

(b)

$$\sum_p \bar{T}_{pr} \;=\; Trace\, \Gamma G^R \Gamma_r G^A = \; Trace\, \Gamma_r G^A \Gamma G^R = \; Trace\, \Gamma_r A$$

$$\sum_p \bar{T}_{rp} \;=\; Trace\, \Gamma_r G^R \Gamma G^A = \; Trace\, \Gamma_r A$$

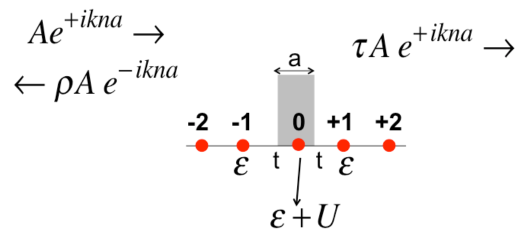
3.5. Consider a 1D wire with a potential at site "0".

Assume that the solution for $n \le 0$ can be written as a sum of incident and reflected waves as shown while the solution for $n \ge 0$ can be written as a transmitted wave.
We can then write the wavefunctions at n= -1, 0 and +1 as

$$\psi_{-1} = A\, e^{-ika} + \rho A\, e^{+ika} \qquad (1)$$

$$\psi_0 = A + \rho A = \tau A \qquad (2)$$

$$\psi_{+1} = \tau A\, e^{+ika} \qquad (3)$$



Starting from $E\psi_0 = \quad (\varepsilon + U)\psi_0 + t\psi_{-1} + t\psi_{+1} \qquad (4)$
use Eqs.(1), (2) and (3) from above to show that $E\psi_0 = \quad (\varepsilon + U + 2\sigma)\psi_0 + s$
and obtain an expression for σ and s in terms of ε, t, ka, A
Also find the transmission coefficient.

SOLUTION:

From (3) and (2), $\qquad \psi_{+1} = e^{ika}\,\psi_0$

From (1) and (2), $\qquad \psi_{-1} = e^{ika}\,\psi_0 + Ae^{-ika} - Ae^{+ika}$

Substituting into (4)

$$E\psi_0 = \quad (\varepsilon + U + \underbrace{2te^{ika}}_{2\sigma})\psi_0 + \underbrace{tA(e^{-ika} - e^{+ika})}_{s}$$

$$\sigma = \quad te^{ika}, \qquad s = \quad -2it\,A \sin ka$$

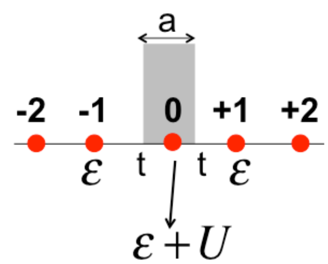
$$\psi_0 = \quad \frac{tA(e^{-ika} - e^{+ika})}{E - \varepsilon - U - 2te^{ika}}$$

$$\tau = \frac{\psi_0}{A} = \quad \frac{-2it \sin ka}{2t\cos ka - U - 2te^{ika}}$$

$$= \quad \frac{-2it \sin ka}{-U - 2it \sin ka}$$

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

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



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

and compare with the result in Prob.3.5 from scattering theory.

SOLUTION:

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

$$[H] = \varepsilon + U$$

$$[\Sigma_1] = [\Sigma_2] = te^{ika}$$

$$[\Gamma_1] = [\Gamma_2] = i(te^{ika} - te^{-ika}) = -2t \sin ka$$

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

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

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

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

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

3.7. Suppose ***elastic*** dephasing processes are included in the NEGF model by adding extra self-energy terms $\Sigma_0 = D_1 G$ and $\Sigma_0^{in} = D_2 G^n$
Does D_1 have to equal D_2? Explain why or why not.

SOLUTION:

D_1 must equal D_2 in order to ensure current conservation.

The current into the "contact" described by $\Sigma_0 = D_1 G$ and $\Sigma_0^{in} = D_2 G^n$ is given by

$$\tilde{I}_0 = \frac{q}{h} Trace[\Sigma_0^{in} A - \Gamma_0 G^n] \qquad (1)$$

$$\Gamma_0 = i[\Sigma_0 - \Sigma_0^+] = D_1 i[G - G^+] = D_1 A \qquad (2)$$

Substituting (2) into (1),

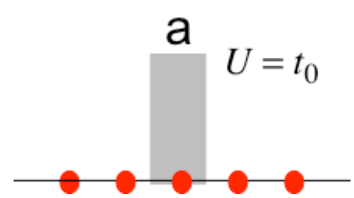
$$\tilde{I}_0 = \frac{q}{h} Trace[D_1 G^n A - D_2 A G^n] \quad = \quad \frac{q}{h}(D_1 - D_2) Trace[G^n A]$$

For current conservation, $\tilde{I}_0 = 0$

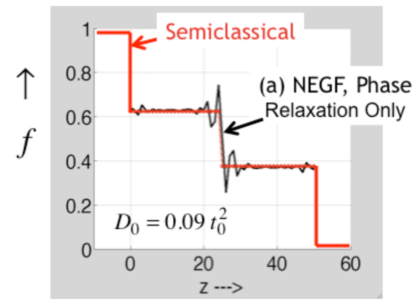
Hence, $D_1 = D_2$.

3.8. Shown below is the occupation factor defined as

$$f(p) = \frac{G^n(p,p)}{A(p,p)}$$



calculated for a 1D wire with one scatterer U=t_0 for D_0 = 0.09 t_0^2, (momentum conserving,). An energy E = t_0 is used.



The semiclassical curve shows a drop of
0.375 at each end
and 0.25 at the scatterer.

How would these figures change if the scatterer potential were $U = \sqrt{3}\, t_0$ instead of $U = t_0$?

SOLUTION:

1. $$T = \frac{(2t_0 \sin ka)^2}{U^2 + (2t_0 \sin ka)^2}$$

$$E = t_0 = 2t_0(1 - \cos ka) \quad \rightarrow \quad \cos ka = \frac{1}{2} \quad \rightarrow \quad \sin ka = \frac{\sqrt{3}}{2}$$

2. $$T = \frac{3}{3+3} \quad \rightarrow \quad \frac{1-T}{T} = 1$$

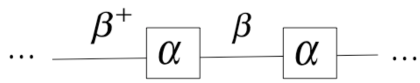
3. The normalized resistances are $\frac{1}{2} : 1 : \frac{1}{2}$

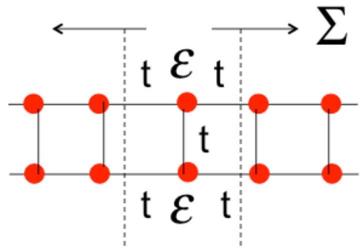
and so the potential drops are also in the same ratio

$$1:2:1 \quad = \quad \frac{1}{4} : \frac{2}{4} : \frac{1}{4} \quad = \quad 0.25 \ : \ 0.5 \ : \ 0.25$$

3.9. 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

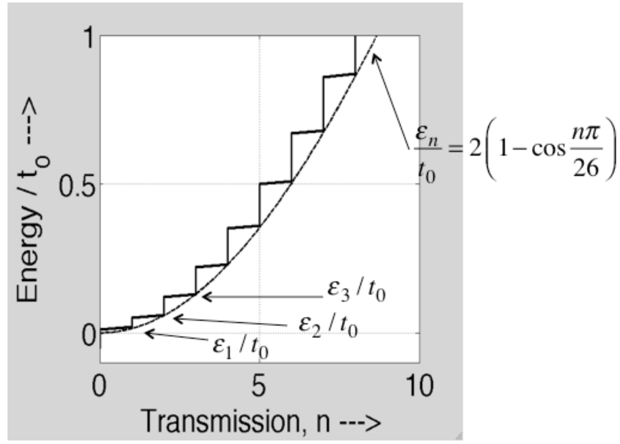
$$\begin{aligned} E &= \varepsilon + t + 2t\cos k_1 a \quad \rightarrow \quad \cos k_1 a = (\varepsilon + t)/2t \\ &= \varepsilon - t + 2t\cos k_2 a \quad \rightarrow \quad \cos k_2 a = (\varepsilon - t)/2t \end{aligned}$$

(b)

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

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

3.10. The plot shows the transmission T(E) over the energy range $-0.05t_0 < E < +1.05t_0$ for a ballistic conductor of width W = 26*a (25 points along width).



The model uses a 2D square lattice model with onsite elements $\varepsilon = 4t_0$, $t = -t_0$, having a dispersion relation

$$E(\vec{k}) = \ \ 2t_0(1-\cos k_x a) + 2t_0(1-\cos k_y a)$$

(a) The transmission shows a series of steps occurring at energies which are desribed well by the relation

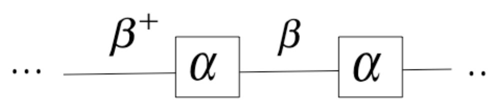
$$\varepsilon_n = 2t_0\left(1-\cos\frac{n\pi}{26}\right) \qquad (1)$$

such that $\quad \varepsilon_n < E < \varepsilon_{n+1}, \ \ \bar{T}(E) = n$

Explain why.

(b) Suppose the same conductor is assumed to be rolled up along the width in the form of a cylinder, corresponding to imposing periodic boundary conditions along the width. What would the steps in transmission look like?

SOLUTION: Please see Section 21.1.



The 2-D model can be represented by a 1-D chain of the form shown above.

(a) The eigenvalues α_n of the matrix [α] are given by

$$\alpha_n \ = \ \varepsilon - 2t_0 \cos k_y a \ = \ 4t_0 - 2t_0 \cos k_y a, \quad k_y a = \frac{n\pi a}{W} = \frac{n\pi}{26}$$

Each eigenvalue is related to a separate subabnd with a dispersion relation

$$E_n(k_x) \ = \ \alpha_n - 2t_0 \cos k_x a$$

The energies ε_n in Eq.(1) above are given by

$$\varepsilon_n \ = \ \min(E) \ = \ \alpha_n - 2t_0 \quad \mathit{for}\ k_x = 0$$

$$= \ 2t_0 - 2t_0 \cos\frac{n\pi}{26}$$

(b) For periodic boundary conditions, the eigenvalues α_n of the matrix [α] are given by

$$\alpha_n = \varepsilon - 2t_0 \cos k_y a = 4t_0 - 2t_0 \cos k_y a, \quad k_y a = \frac{2n\pi a}{W} = \frac{2n\pi}{25}$$

$$E_n(k_x) = \alpha_n - 2t_0 \cos k_x a$$

$$\varepsilon_n = \min(E) = \alpha_n - 2t_0 \quad \textit{for } k_x = 0$$

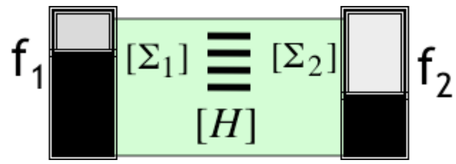
$$= 2t_0 - 2t_0 \cos\frac{2n\pi}{25}$$

The transmission is given by

$$\varepsilon_n < E < \varepsilon_{n+1}, \quad \bar{T}(E) = 2n+1$$

Lowest step occurs at n=0 and subsequent steps are of height two because of two degenerate levels.

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"

$$\Gamma = \sum_r \Gamma_r$$

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

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