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

\[ [H] = [\epsilon] \quad [\Sigma_1] = -i \left[ \frac{\gamma_1}{2} \right] \quad [\Sigma_2] = -i \left[ \frac{\gamma_2}{2} \right] \]

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

**SOLUTION:**

\[
G_{\text{R}}^n = \left( E - \epsilon + i \frac{\gamma_1}{2} \right)^{-1} \quad \gamma = \gamma_1 + \gamma_2
\]

\[
T_1 = i \left( -\frac{i \gamma_1}{2} - \frac{\gamma_1}{2} \right) = \gamma_1
\]

\[
T_2 = \gamma_2
\]

\[
G_{\text{A}} = \left( T_1 f_1 + T_2 f_2 \right) G_{\text{A}}
\]

\[
A = i [G^R - G^A] = i \left[ \frac{1}{E - \epsilon + i \gamma / 2} - \frac{1}{E - \epsilon - i \gamma / 2} \right] = \frac{\gamma}{(E - \epsilon)^2 + (\gamma / 2)^2}
\]

\[
\tilde{I}_1 = \frac{q}{h} \text{Trace} \left[ \Sigma_1 \text{Tr} \left[ A - \Gamma_1 G^n \right] \right] = \frac{q}{h} \left[ \gamma_1 f_1 A - \gamma_1 G^n \right]
\]

\[
= \frac{q}{h} \frac{\gamma_1 f_1 - \gamma_1 (\gamma_1 f_1 + \gamma_2 f_2)}{(E - \epsilon)^2 + (\gamma / 2)^2} = \frac{q}{h} \frac{\gamma_1 \gamma_2 (f_1 - f_2)}{(E - \epsilon)^2 + (\gamma / 2)^2}
\]

\[
I_1 = \int_{-\infty}^{+\infty} dE \tilde{I}_1 = \frac{q}{h} \int_{-\infty}^{+\infty} dE \frac{\gamma_1 \gamma_2}{(E - \epsilon)^2 + (\gamma / 2)^2} (f_1 - f_2) \equiv \tilde{T}(E)
\]
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 \([G^\text{n}]\), the matrix density of states \([A]\),
\[ G^\text{n} = G^R \Sigma^\text{in} G^A, \quad A = G^R \Gamma G^A \]
and the current
\[ \bar{I}_p = \frac{q}{\hbar} \text{Trace}[\Sigma^\text{in} A - \Gamma \rho G^R] \]

**SOLUTION:** Please see Section 19.2 of LNE.

3.3. Starting from the relations
\[ G^R = [EI - H - \Sigma]^{-1}, G^A \equiv [G^R]^+ \quad \text{and} \quad \Gamma = i [\Sigma - \Sigma^+] \]
show that
\[ A \equiv G^R \Gamma G^A = G^A \Gamma G^R = i[G^R - G^A] \]

**SOLUTION:**
\[ (G^R)^{-1} = EI - H - \Sigma \]
\[ (G^A)^{-1} = EI - H - \Sigma^+ \]
\[ (G^R)^{-1} - (G^A)^{-1} = \Sigma^+ - \Sigma = i \Gamma \]
- 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
\[ i (G^R - G^A) = G^R \Gamma G^A = G^A \Gamma G^R \]
3.4. Starting from \( \tilde{I}_p = \frac{q}{h} \text{Trace} \left[ \Sigma_p^A - \Gamma_p G^A \right] \)

show that for a multiterminal device

(a) \( \tilde{I}_p = \frac{q}{h} \sum_r (f_p(E) - f_r(E)) T_{pr}(E) \quad T_{pr}(E) \equiv \text{Trace}[\Gamma_p G^R \Gamma_r G^A] \)

(b) \( \sum_p \tilde{T}_{pr} = \sum_p \tilde{T}_{rp} \)

SOLUTION:

\[
\tilde{I}_p = \frac{q}{h} \text{Trace} \left[ f_p \Gamma_p A - \Gamma_p G^A \right]^R \Gamma_r G^A \sum_r \Gamma_r f_r \]

\[
= \frac{q}{h} \sum_r \text{Trace} \left[ f_p \Gamma_p G^R \Gamma_r G^A - \Gamma_p G^R \Gamma_r f_r G^A \right]
\]

\[
= \frac{q}{h} \sum_r (f_p - f_r) \text{Trace} \left[ \Gamma_p G^R \Gamma_r G^A \right]
\]

\( \equiv \tilde{T}_{pr} \)

(b)

\[
\sum_p \tilde{T}_{pr} = \text{Trace} \Gamma G^R \Gamma_r G^A = \text{Trace} \Gamma_r G^A \Gamma G^R = \text{Trace} \Gamma_r A
\]

\[
\sum_p \tilde{T}_{rp} = \text{Trace} \Gamma_r G^R \Gamma G^A = \text{Trace} \Gamma_r A
\]
3.5. Consider a 1D wire with a potential at site “0”.

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

\[
\psi_{-1} = A e^{-ika} + \rho A e^{+ika} \tag{1}
\]

\[
\psi_0 = A + \rho A = \tau A \tag{2}
\]

\[
\psi_{+1} = \tau A e^{+ika} \tag{3}
\]

Starting from \( E\psi_0 = (\epsilon + U)\psi_0 + t\psi_{-1} + t\psi_{+1} \tag{4} \) use Eqs.(1), (2) and (3) from above to show that \( E\psi_0 = (\epsilon + U + 2\sigma)\psi_0 + s \) and obtain an expression for \( \sigma \) and \( s \) in terms of \( \epsilon, t, ka, A \).

Also find the transmission coefficient.

**SOLUTION:**

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

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

Substituting into (4)

\[
E\psi_0 = (\epsilon + U + \frac{2te^{ika}}{2\sigma})\psi_0 + tA(e^{-ika} - e^{+ika})
\]

\[
\sigma = te^{ika}, \quad s = -2itA \sin ka
\]

\[
\psi_0 = \frac{tA(e^{-ika} - e^{+ika})}{E - \epsilon - U - 2te^{ika}}
\]

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

\[
= \frac{-2it \sin ka}{-U - 2it \sin ka}
\]

\[
\tau^* \tau = \frac{(2t \sin ka)^2}{U^2 + (2t \sin ka)^2}
\]
3.6. Calculate the transmission through a single scatterer of height U in a 1D wire (t < 0) using the expression

\[ \mathcal{T}(E) = \text{Trace}[\Gamma_1 G^R \Gamma_2 G^A] \]

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.

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

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

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

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

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

\[ = \frac{(2t \sin ka)^2}{U^2 + (2t \sin ka)^2} \]
Suppose elastic dephasing processes are included in the NEGF model by adding extra self-energy terms \( \Sigma_0 = D_1 G \) and \( \Sigma^{in}_0 = D_2 G^n \).

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 \( \Sigma^{in}_0 = D_2 G^n \) is given by

\[
\tilde{I}_0 = \frac{q}{h} \text{Trace}[\Sigma^{in} A - \Gamma_0 G^n]
\]

(1)

\[
\Gamma_0 = i[\Sigma_0 - \Sigma_0^+] = D_1 i[G - G^+] = D_1 A
\]

(2)

Substituting (2) into (1),

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

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
- 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

\[ 1:2:1 = \frac{1}{4} : \frac{2}{4} : \frac{1}{4} = 0.25 : 0.5 : 0.25 \]
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 $\Sigma$.

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

$$\begin{array}{c}
\ldots & \beta^+ & \alpha & \beta & \alpha & \ldots \\
\end{array}$$

where

$$\alpha = \begin{bmatrix} \epsilon & t \\ t & \epsilon \end{bmatrix}, \quad \beta = \begin{bmatrix} t & 0 \\ 0 & t \end{bmatrix}$$

The matrix $\alpha$ has eigenvalues $(\epsilon + t)$ and $(\epsilon - t)$ with eigenvectors $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ respectively.

We can use these eigenvectors as the basis, to diagonalize the matrix $\alpha$.

(a) Write down the matrices $\alpha$, $\beta$. And $\Sigma(E)$ in this eigenvector basis (the one that diagonalizes $\alpha$).

(b) Write down the matrix $\Sigma(E)$ in the original basis.

**SOLUTION:**

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

$$\Sigma(E) = \begin{bmatrix} te^{ik_1a} & 0 \\ 0 & te^{ik_2a} \end{bmatrix} \equiv \begin{bmatrix} p & 0 \\ 0 & q \end{bmatrix}$$

where $k_1$ and $k_2$ are given by

$$E = \epsilon + t + 2t \cos k_1a \rightarrow \cos k_1a = (\epsilon + t)/2t$$
$$= \epsilon - t + 2t \cos k_2a \rightarrow \cos k_2a = (\epsilon - t)/2t$$

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

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

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

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

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

such that $\varepsilon_n < E < \varepsilon_{n+1}$, $T(E) = n$ 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 $\alpha_n$ of the matrix $[\alpha]$ are given by

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

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

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

The energies $\varepsilon_n$ in Eq.(1) above are given by

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

$$= 2t_0 - 2t_0 \cos \frac{n\pi}{26}$$
(b) For periodic boundary conditions, the eigenvalues $\alpha_n$ of the matrix $[\alpha]$ are given by

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

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

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

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

The transmission is given by

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

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

\[ G^R = (Ei - H - \Sigma)^{-1} \]

\[ G^n = G^R \Sigma^{in} G^A \]

\[ A = G^R \Gamma G^A = G^A \Gamma G^R \]

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

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

**Coherent transport**

\[ I = \frac{q}{\hbar} \int_{-\infty}^{\infty} dE \left( f_1(E) - f_2(E) \right) \bar{T}(E) \]

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

This integral may be useful:

\[ \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{x^2 + a^2}} = \frac{\pi}{a} \]

**Device with multiple terminals “r”**

\[ \Sigma = \Sigma_1 + \Sigma_2 + \Sigma_0 \]

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

\[ \Gamma = \Gamma_1 + \Gamma_2 + \Gamma_0 \]

\[ \Sigma^{in} = \frac{f_1 \Gamma_1}{\Sigma_{1}} + \frac{f_2 \Gamma_2}{\Sigma_{2}} + \Sigma^{in}_0 \]

\[ \Sigma^{in} = \sum_r \Sigma^{in}_r = \sum_r \Gamma_r f_r \]