ECE 659 EXAM IV Friday, Apr.10, 2015 230-320PM, EE117

NAME:	SOLUTION	

CLOSED BOOK

One page of notes provided, please see last page

All five questions carry equal weight

Please show all work.

No credit for just writing down the answer, even if correct.

4.1. A channel with two levels connected to TWO contacts is described by

$$H = \begin{bmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix} \qquad \Sigma_1 = -\frac{i}{2} \gamma \left(I + P \, \vec{\sigma} . \hat{n} \right) \qquad \qquad \Sigma_2 = -\frac{i}{2} \gamma \left(I - P \, \vec{\sigma} . \hat{n} \right)$$

Calculate the transmission $\overline{T}_{21}(E) = Trace[\Gamma_2 G^R \Gamma_1 G^A]$ in terms of E, ε, γ, P .

Solution:

$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+] = \gamma \left(I + P \vec{\sigma} . \hat{n} \right)$$

$$\Gamma_2 = i[\Sigma_2 - \Sigma_2^+] = \gamma \left(I - P \vec{\sigma} . \hat{n} \right)$$

$$\begin{split} [G^R]^{-1} &= EI - \varepsilon I + i \gamma I \quad \rightarrow \quad [G^R] = \quad \frac{1}{E - \varepsilon + i \gamma} [I] \\ \overline{T}_{21} &= Trace [\Gamma_2 G^R \Gamma_1 G^A] \\ &= \quad \frac{\gamma^2}{(E - \varepsilon)^2 + \gamma^2} Trace [I + P \vec{\sigma}. \hat{n}] [I - P \vec{\sigma}. \hat{n}] \\ &= \quad \frac{\gamma^2}{(E - \varepsilon)^2 + \gamma^2} Trace [I - P^2 (\vec{\sigma}. \hat{n}) (\vec{\sigma}. \hat{n})] \\ &= \quad \frac{\gamma^2}{(E - \varepsilon)^2 + \gamma^2} Trace [I - P^2 I] = \quad \frac{2\gamma^2 (1 - P^2)}{(E - \varepsilon)^2 + \gamma^2} \end{split}$$

4.2. A contact pointing along +z is described by $\Gamma = \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix}$. What is the Γ for an identical contact pointing along +x?

Solution:

Given:
$$\Gamma = \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} = \frac{\alpha + \beta}{2} [I] + \frac{\alpha - \beta}{2} [\sigma_z]$$

If contact points along x

$$\Gamma = \frac{\alpha + \beta}{2} [I] + \frac{\alpha - \beta}{2} [\sigma_x]$$
$$= \frac{1}{2} \begin{bmatrix} \alpha + \beta & \alpha - \beta \\ \alpha - \beta & \alpha + \beta \end{bmatrix}$$

Can obtain this result directly through basis transformation as well.

$$\Gamma = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$
$$= \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \alpha & \alpha \\ \beta & -\beta \end{bmatrix}$$
$$= \frac{1}{2} \begin{bmatrix} \alpha + \beta & \alpha - \beta \\ \alpha - \beta & \alpha + \beta \end{bmatrix}$$

4.3. An electron has a spinor wavefunction given by $\frac{1}{2} \begin{Bmatrix} 1-i \\ 1+i \end{Bmatrix}$ What are the x, y and z components of its spin \vec{S} .

Solution:

$$\psi \psi^{+} = \frac{1}{4} \begin{cases} 1-i \\ 1+i \end{cases} \left\{ 1+i \quad 1-i \right\}$$
$$= \frac{1}{4} \begin{bmatrix} 2 & -2i \\ 2i & 2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix}$$

Compare

$$\frac{G^n}{2\pi} = \frac{1}{2} \begin{bmatrix} N + S_z & S_x - iS_y \\ S_x + iS_y & N - S_z \end{bmatrix}$$

Clearly,
$$N+S_z=1$$
 , $N-S_z=1$ \rightarrow $N=1$, $S_z=0$
$$S_x=0$$
 , $S_y=1$

(Can do this more formally by taking traces too)

$$\vec{S} = \hat{y}$$

4.4. The Dirac equation for relativistic electrons is written as

$$E\{\psi\} = \begin{bmatrix} mc^2 I_2 & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^2 I_2 \end{bmatrix} \{\psi\}$$

where I_2 is the (2x2) identity matrix. It follows that

$$E^{2}\{\psi\} = \begin{bmatrix} mc^{2}I_{2} & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^{2}I_{2} \end{bmatrix} \begin{bmatrix} mc^{2}I_{2} & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^{2}I_{2} \end{bmatrix} \{\psi\}$$

Show that

$$\begin{bmatrix} mc^2I_2 & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^2I_2 \end{bmatrix} \begin{bmatrix} mc^2I_2 & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^2I_2 \end{bmatrix} = K[I_4]$$

where I_4 is the (4x4) identity matrix. What is K?

Solution:
$$\begin{bmatrix} mc^2I_2 & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^2I_2 \end{bmatrix} \begin{bmatrix} mc^2I_2 & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^2I_2 \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

$$A = m^2 c^4 I_2 + c^2 [\vec{\sigma}.\vec{p}] [\vec{\sigma}.\vec{p}] = m^2 c^4 I_2 + c^2 (\vec{p}.\vec{p}) I_2 = (m^2 c^4 + c^2 p^2) I_2$$

$$B = mc^{3}([\vec{\sigma}.\vec{p}] - [\vec{\sigma}.\vec{p}]) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \equiv Z_{2}$$

$$C = mc^{3}([\vec{\sigma}.\vec{p}] - [\vec{\sigma}.\vec{p}]) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} = Z_{2}$$

$$D = c^2(\vec{p}.\vec{p})I_2 + m^2c^4I_2 = (m^2c^4 + c^2p^2)I_2$$

Hence

$$\begin{bmatrix} mc^2I_2 & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^2I_2 \end{bmatrix} \begin{bmatrix} mc^2I_2 & c\vec{\sigma}.\vec{p} \\ c\vec{\sigma}.\vec{p} & -mc^2I_2 \end{bmatrix}$$

$$= (m^2c^4 + c^2p^2) \begin{bmatrix} I_2 & Z_2 \\ Z_2 & I_2 \end{bmatrix} = (m^2c^4 + c^2p^2) [I_4]$$

4.5. Suppose an electron with a 2x1 wavefunction $\{\psi\}$ in an x-directed B-field is described by

$$i\hbar \frac{d}{dt} \{ \psi \} = \mu_B B_x [\sigma_x] \{ \psi \}$$
 (1)

and we define its spin \vec{s} any direction "j" as $s_j \equiv \{\psi\}^+ [\sigma_j] \{\psi\}$ (2)

Starting from (1) and (2), find an expression for $\frac{d s_y}{d t}$ in terms of $\mu_B B_x$ and the components of \vec{s} (that is, s_x , s_y , s_z).

SOLUTION:

$$i\hbar \frac{d}{dt} \psi = \mu_B B_x \ \sigma_x \psi$$

$$i\hbar \frac{d}{dt} \psi^+ = -\mu_B B_x \ \psi^+ \sigma_x$$

$$\frac{ds_y}{dt} = \frac{d}{dt} \psi^+ \sigma_y \psi$$

$$i\hbar \frac{ds_y}{dt} = \left[i\hbar \frac{d}{dt} \psi^+ \right] \sigma_y \psi + \psi^+ \sigma_y \left[i\hbar \frac{d}{dt} \psi \right]$$

$$= \mu_B B_x \left[-\psi^+ \sigma_x \sigma_y \psi + \psi^+ \sigma_y \sigma_x \psi \right]$$

$$= \mu_B B_x \psi^+ \left[-\sigma_x \sigma_y + \sigma_y \sigma_x \right] \psi$$

$$= -2i \mu_B B_x \psi^+ \sigma_z \psi = -2i \mu_B B_x s_z$$

$$\frac{d s_y}{d t} = -\frac{2\mu_B B_x}{\hbar} s_z \implies \frac{2\mu_B}{\hbar} (\vec{s} \times \vec{B})_y$$

NEGF Equations

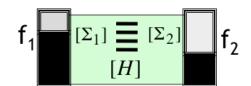
$$G^{R} = [EI - H - \Sigma]^{-1}$$

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

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

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

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



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

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

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

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

Coherent transport

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

$$\Gamma = \sum_r \Gamma_r$$

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

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

Device with multiple terminals "r"

$$\Gamma = \sum_{r} \Gamma_r$$

$$\Sigma^{in} = \sum_{r} \Sigma_{r}^{in} = \sum_{r} \Gamma_{r} f_{r}$$

Useful Identities:
$$\left(\vec{a} \times \vec{b}\right)_m = \sum_{n,p} \varepsilon_{mnp} a_n b_p$$

$$\sum_{i,j} \varepsilon_{ijk} \varepsilon_{ijn} = 2\delta_{kn}$$

$$\sum_{i,j} \varepsilon_{ijk} \varepsilon_{ijn} = 2\delta_{kn} \qquad \sum_{i} \varepsilon_{ijk} \varepsilon_{imn} = \delta_{jm} \delta_{kn} - \delta_{jn} \delta_{km}$$
prin matrices:

(2x2) Identity matrix:

Pauli spin matrices:

(2x2) Identity matrix:

$$\sigma_{x} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_{y} = \begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix}, \sigma_{z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\begin{split} \sigma_m \sigma_n &= \delta_{mn} \, I + i \, \sum_p \varepsilon_{mnp} \, \sigma_p \\ [\vec{\sigma}.\vec{V}_1] [\vec{\sigma}.\vec{V}_2] &= (\vec{V}_1.\vec{V}_2) \, [I] + i \, [\vec{\sigma}.(\vec{V}_1 \times \vec{V}_2) \,] \end{split}$$

Eigenvectors of $\vec{\sigma} \cdot \hat{n} = \sigma_x \sin \theta \cos \phi + \sigma_y \sin \theta \sin \phi + \sigma_z \cos \theta$

corresponding to eigenvalues +1 and -1 can be written as

$$\begin{cases} c \\ s \end{cases}, \begin{cases} -s^* \\ c^* \end{cases}$$
 respectively,

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