ECE 659 EXAM IV

Friday, Apr.11, 2014 330-420PM, FRNY B124

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

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

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

Solution:

$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+] = \gamma\left(I + P\,\vec{\sigma}.\hat{n}\right)$$
$$\Gamma_2 = i[\Sigma_2 - \Sigma_2^+] = \gamma\left(I - P\,\vec{\sigma}.\hat{n}\right)$$

$$[G^R]^{-1} = EI - \varepsilon I + i\gamma I \quad \rightarrow \quad [G^R] = \frac{1}{E - \varepsilon + i\gamma}[I]$$

$$\bar{T}_{21} = Trace[\Gamma_2 G^R \Gamma_1 G^A]$$

$$= \frac{\gamma^2}{(E-\varepsilon)^2 + \gamma^2} Trace[I + P\vec{\sigma}.\hat{n}][I - P\vec{\sigma}.\hat{n}]$$

$$= \frac{\gamma^2}{(E-\varepsilon)^2 + \gamma^2} Trace[I - P^2(\vec{\sigma}.\hat{n})\,(\vec{\sigma}.\hat{n})]$$

$$= \frac{\gamma^2}{(E-\varepsilon)^2 + \gamma^2} Trace[I - P^2\, I] = \frac{2\gamma^2(1-P^2)}{(E-\varepsilon)^2 + \gamma^2}$$

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 +y ?

Solution:

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

If contact points along y

$$\Gamma = \frac{\alpha+\beta}{2}[I] + \frac{\alpha-\beta}{2}[\sigma_y]$$

$$= \frac{1}{2}\begin{bmatrix} \alpha+\beta & -i(\alpha-\beta) \\ +i(\alpha-\beta) & \alpha+\beta \end{bmatrix}$$

Can obtain this result directly through basis transformation as well.

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

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

$$= \frac{1}{2}\begin{bmatrix} \alpha+\beta & -i(\alpha-\beta) \\ i(\alpha-\beta) & \alpha+\beta \end{bmatrix}$$

4.3. An electron has a spinor wavefunction given by $\frac{1}{\sqrt{11}}\begin{Bmatrix}1-3i\\1\end{Bmatrix}$
What are the x, y and z components of its spin $\vec{S}$.

Solution:

$$\psi\psi^{+}=\frac{1}{11}\begin{Bmatrix}1-3i\\1\end{Bmatrix}\{1+3i \quad 1\}$$

$$=\frac{1}{11}\begin{bmatrix}10 & 1-3i\\1+3i & 1\end{bmatrix}$$

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, $N+S_z=\frac{20}{11}$, $N-S_z=\frac{2}{11}$ $\rightarrow$ $N=1, S_z=\frac{9}{11}$

$$S_x=\frac{2}{11}\ ,\ S_y=\frac{6}{11}$$

(Can do this more formally by taking traces too)

$$\vec{S}=\frac{2}{11}\hat{x}+\frac{6}{11}\hat{y}+\frac{9}{11}\hat{z}$$

4.4. An electron is described by a 2D Hamiltonian of the form

$$h(\vec{k}) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)[I] + \eta\vec{\sigma}.\vec{k}$$

(a) What is the dispersion relation ?
(b) What are the (2x1) eigenspinors corresponding to each of the two branches of the dispersion relation for a specific wavevector given by

$$\vec{k} = \frac{k}{\sqrt{2}}(\hat{x} + \hat{y})$$

SOLUTION:

(a)

$$E = \frac{\hbar^2 k^2}{2m} \pm \eta k$$

(b)

Eigenspinors point up and down along k which is described by

$$\theta = \frac{\pi}{2}, \varphi = \frac{\pi}{4}$$

So eigenspinors are given by

$$\frac{1}{\sqrt{2}}\begin{Bmatrix} e^{-i\pi/8} \\ e^{+i\pi/8} \end{Bmatrix} \quad and \quad \frac{1}{\sqrt{2}}\begin{Bmatrix} -e^{-i\pi/8} \\ e^{+i\pi/8} \end{Bmatrix}$$

OR equivalently

$$\frac{1}{\sqrt{2}}\begin{Bmatrix} e^{-i\pi/4} \\ 1 \end{Bmatrix} \quad and \quad \frac{1}{\sqrt{2}}\begin{Bmatrix} -e^{-i\pi/4} \\ 1 \end{Bmatrix}$$

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

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

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

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

SOLUTION:

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

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

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

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

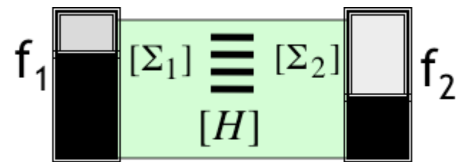
$$= \mu_B B_x \left[-\psi^+ \sigma_x \sigma_y \psi \;+\; \psi^+ \sigma_y \sigma_x \psi\right]$$

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

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

$$\frac{d s_y}{dt} = -\frac{2\mu_B B_x}{\hbar} s_z \;\Rightarrow\; \frac{2\mu_B}{\hbar}\left(\vec{s} \times \vec{B}\right)_y$$

NEGF Equations



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

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

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

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

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

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

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

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

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

Coherent transport

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

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

Device with multiple terminals "r"

$$\Gamma = \sum_r \Gamma_r$$

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

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

$$\sum_{i,j} \varepsilon_{ijk} \varepsilon_{ijn} = 2\delta_{kn} \quad , \quad \sum_i \varepsilon_{ijk} \varepsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$$

Pauli spin matrices:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = \begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix}, \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

(2x2) Identity matrix:

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

$$\sigma_m \sigma_n = \delta_{mn} \, I + i \sum_p \varepsilon_{mnp} \, \sigma_p$$

$$[\vec{\sigma}.\vec{V}_1] [\vec{\sigma}.\vec{V}_2] = (\vec{V}_1.\vec{V}_2) [I] + i [\vec{\sigma}.(\vec{V}_1 \times \vec{V}_2)$$

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

corresponding to eigenvalues +1 and -1 can be written as $\begin{Bmatrix} c \\ s \end{Bmatrix}, \begin{Bmatrix} -s^* \\ c^* \end{Bmatrix}$ respectively,

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