ECE 659 PRACTICE EXAM IV

Actual Exam IV

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

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.

4.1. NEGF for device with one spin degenerate level
4.2. Transforming contacts
4.3. Function of a matrix
4.4. Interpreting G^n
4.5. Interpreting G^n
4.6. Vector potential in Schrodinger equation
4.7. Pauli equation
4.8. Rashba Hamiltonian
4.9. Energy dispersion and eigenspinors of Rashba Hamiltonian
4.10. Spin Precession**

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

Text: *Lecture 14, 22, 24.1-24.2, LNE*

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

$$H = \begin{bmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix} \qquad \Sigma_1 = -\frac{i}{2}\gamma_1\left(I + P_1\,\vec{\sigma}.\hat{n}_1\right) \qquad \Sigma_{\bar{1}} = -\frac{i}{2}\gamma_1\left(I - P_1\,\vec{\sigma}.\hat{n}_1\right)$$

$$\Sigma_2 = -\frac{i}{2}\gamma_2\left(I + P_2\,\vec{\sigma}.\hat{n}_2\right) \qquad \Sigma_{\bar{2}} = -\frac{i}{2}\gamma_2\left(I - P_2\,\vec{\sigma}.\hat{n}_2\right)$$

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

Solution:

$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+] = \gamma_1\left(I + P_1\,\vec{\sigma}.\hat{n}_1\right)$$
$$\Gamma_2 = i[\Sigma_2 - \Sigma_2^+] = \gamma_2\left(I + P_2\,\vec{\sigma}.\hat{n}_2\right)$$

$$[G^R]^{-1} = EI - \varepsilon I + i\gamma_1 I + i\gamma_2 I \quad \rightarrow \quad [G^R] = \frac{1}{E - \varepsilon + i\gamma_1 + i\gamma_2}[I]$$

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

$$= \frac{\gamma_1\gamma_2}{(E-\varepsilon)^2 + (\gamma_1+\gamma_2)^2} Trace[I + P_1\,\vec{\sigma}.\hat{n}_1][I + P_2\,\vec{\sigma}.\hat{n}_2]$$

$$= \frac{\gamma_1\gamma_2}{(E-\varepsilon)^2 + (\gamma_1+\gamma_2)^2} Trace[I + P_1\,\vec{\sigma}.\hat{n}_1 + P_2\,\vec{\sigma}.\hat{n}_2 + P_1P_2\,(\vec{\sigma}.\hat{n}_1)\,(\vec{\sigma}.\hat{n}_2)]$$

$$= \frac{\gamma_1\gamma_2}{(E-\varepsilon)^2 + (\gamma_1+\gamma_2)^2} Trace[I + P_1\,\vec{\sigma}.\hat{n}_1 + P_2\,\vec{\sigma}.\hat{n}_2 + P_1P_2\,\hat{n}_1.\hat{n}_2 + iP_1P_2\,\vec{\sigma}.(\hat{n}_1 \times \hat{n}_2)]$$

$$= \frac{2\gamma_1\gamma_2}{(E-\varepsilon)^2 + (\gamma_1+\gamma_2)^2}\,(1 + P_1P_2\,\hat{n}_1.\hat{n}_2)$$

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 +x ?

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 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. Evaluate the matrix $\exp\left[i\alpha\sigma_y\right]$.

Solution:

If we use $\pm$ y as our basis, $\exp\left[i\alpha\sigma_y\right]$ will be given by

$$\exp i\alpha\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = \begin{bmatrix}e^{i\alpha} & 0\\ 0 & e^{-i\alpha}\end{bmatrix}$$

Transforming from $\pm$ y to $\pm$ z ,

$$\exp[i\alpha\sigma_y] = \frac{1}{2}\begin{bmatrix}1 & i\\ i & 1\end{bmatrix}\begin{bmatrix}e^{i\alpha} & 0\\ 0 & e^{-i\alpha}\end{bmatrix}\begin{bmatrix}1 & -i\\ -i & 1\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1 & i\\ i & 1\end{bmatrix}\begin{bmatrix}e^{i\alpha} & -ie^{i\alpha}\\ -ie^{-i\alpha} & e^{-i\alpha}\end{bmatrix} = \begin{bmatrix}\cos\alpha & \sin\alpha\\ -\sin\alpha & \cos\alpha\end{bmatrix}$$

4.4. An electron has a spinor wavefunction given by $\frac{1}{\sqrt{14}}\begin{Bmatrix}-1i \\ 2+3i\end{Bmatrix}$

What are the x, y and z components of its spin $\vec{S}$.

Solution:

$$\psi\psi^{+} = \frac{1}{14}\begin{Bmatrix}-1i \\ 2+3i\end{Bmatrix}\{1i \quad 2-3i\}$$

$$= \frac{1}{14}\begin{bmatrix}1 & -3-2i \\ -3+2i & 13\end{bmatrix}$$

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, $N+S_z = \frac{1}{7}$, $N-S_z = \frac{13}{7} \quad \rightarrow \quad N=1\,, S_z = -\frac{6}{7}$

$$S_x = -\frac{3}{7} \;,\; S_y = \frac{2}{7}$$

(Can do this more formally by taking traces too)

$$\vec{S} = -\frac{3}{7}\hat{x} + \frac{2}{7}\hat{y} - \frac{6}{7}\hat{z}$$

4.5. At a point in a channel the correlation matrix [G^n] is given by

(e) $\frac{G^n}{2\pi} = \begin{bmatrix} 50 & +i10 \\ -i10 & 50 \end{bmatrix}$

(a) What is the number of electrons ?
(b) What is the number of spins and in what direction do they point ?

Solution:

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

Clearly, $N+S_z = 100 = N-S_z \quad \rightarrow \quad N = 100 \,, S_z = 0$
$S_x = 0 \,, S_y = -20$

More formally we can multiply by Pauli matrices and take traces.

$$N = Trace\begin{bmatrix} 50 & +i10 \\ -i10 & 50 \end{bmatrix} = 100$$

$$S_x = Trace\begin{bmatrix} 50 & +i10 \\ -i10 & 50 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = Trace\begin{bmatrix} +i10 & \cdots \\ \ldots & -i10 \end{bmatrix} = 0$$

$$S_y = Trace\begin{bmatrix} 50 & +i10 \\ -i10 & 50 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = Trace\begin{bmatrix} -10 & \cdots \\ \ldots & -10 \end{bmatrix} = -20$$

$$S_z = Trace\begin{bmatrix} 50 & +i10 \\ -i10 & 50 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = Trace\begin{bmatrix} 50 & \cdots \\ \ldots & -50 \end{bmatrix} = 0$$

100 electrons with net spin of 20 pointing along negative y.

4.6. The energy in a magnetic field is written in the form (**A** is the vector potential)

$$E(\vec{x},\vec{p}) = \sum_j \frac{(p_j + qA_j(\vec{x}))^2}{2m} + U(\vec{x})$$

Starting from the semiclassical equations of motion

$$\frac{d\vec{x}}{dt} = \vec{\nabla}_p E \qquad \frac{d\vec{p}}{dt} = -\vec{\nabla} E$$

show that

$$\frac{d\vec{x}}{dt} = \frac{\vec{p} + q\vec{A}(\vec{x})}{m} \equiv \frac{\vec{p}\,'}{m}$$

$$\frac{d\vec{p}\,'}{dt} = -q(\vec{F} + \vec{v}\ x\ \vec{B})$$

where

$$q\vec{F} = \vec{\nabla} U \quad and \quad \vec{B} = \vec{\nabla} \times \vec{A}$$

SOLUTION:

$$E(\vec{x},\vec{p}) = \sum_j \frac{(p_j + qA_j(\vec{x}))^2}{2m} + U(\vec{x})$$

$$\rightarrow \quad v_i \equiv \frac{dx_i}{dt} = \frac{p_i + qA_i(\vec{x})}{m}, \quad \rightarrow \quad \vec{v} = \frac{\vec{p} + q\vec{A}(\vec{x})}{m},$$

$$\rightarrow \quad \frac{dp_i}{dt} = -\frac{\partial U}{\partial x_i} - q\sum_j v_j \frac{\partial A_j}{\partial x_i}$$

$$\frac{d}{dt}(p_i + qA_i(\vec{x})) = -\frac{\partial U}{\partial x_i} - q\sum_j v_j \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right)$$

$$= -\frac{\partial U}{\partial x_i} - q\sum_{j,n} v_j\, \varepsilon_{ijn} \left(\vec{\nabla}\, x\, \vec{A} \right)_n$$

$$\rightarrow \quad \frac{d(\vec{p} + q\vec{A})}{dt} = -q(\vec{F} + \vec{v}\ x\ \vec{B}) \qquad \text{where } q\vec{F} = \vec{\nabla} U \text{ and } \vec{B} = \vec{\nabla}\, x\, \vec{A}$$

4.7. The Pauli equation for electrons in a magnetic field is written as (assuming U=0 for simplicity)

$$E\{\psi\} = \frac{[\vec{\sigma}.(\vec{p}+q\vec{A})]^2}{2m}\{\psi\}$$

where the wavefunction $\{\psi\}$ is a (2x1) spinor.

Show that this equation can be rewritten in the form

$$E\{\psi\} = \left(\frac{(\vec{p}+q\vec{A})^2}{2m}[I] + i\frac{q}{2m}[\vec{\sigma}.\vec{Q}_{op}]\right)\{\psi\}$$

where $\vec{Q}_{op}$ is an operator involving the momentum operator $\vec{p}$ and the vector potential $\vec{A}$

(a) What is $\vec{Q}_{op}$?

(b) Show that for any function ϕ, $\vec{Q}_{op}\phi = -i\hbar\,\vec{B}\phi\,, \quad where\ \vec{B} = \vec{\nabla}\times\vec{A}$

Solution:

$$[\vec{\sigma}.(\vec{p}+q\vec{A})]^2 = (\vec{p}+q\vec{A})^2[I] + i\,\vec{\sigma}.(\vec{p}+q\vec{A})\times(\vec{p}+q\vec{A})$$

Hence,

$$E\{\psi\} = \left(\frac{(\vec{p}+q\vec{A})^2}{2m}[I] + i\frac{q}{2m}[\vec{\sigma}.\vec{Q}_{op}]\right)\{\psi\}$$

where

$$\vec{Q}_{op} = \frac{1}{q}(\vec{p}+q\vec{A})\times(\vec{p}+q\vec{A}) = \vec{A}\times\vec{p}+\vec{p}\times\vec{A}$$

For any function ϕ,

$$\vec{Q}_{op}\phi = -i\hbar\,(\vec{A}\times\vec{\nabla}\phi + \vec{\nabla}\times\vec{A}\phi) = -i\hbar\,\phi\,(\vec{\nabla}\times\vec{A})$$

$$= -i\hbar\,\vec{B}\phi\,, \quad where\ \vec{B} = \vec{\nabla}\times\vec{A}$$

Hence,

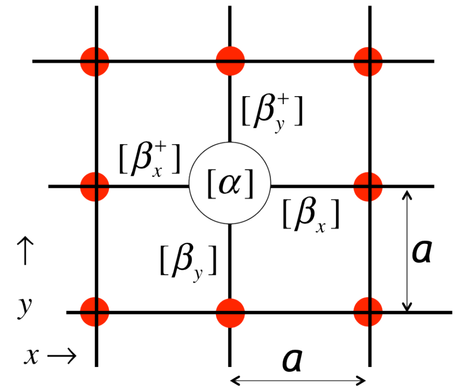
$$E\{\psi\} = \left(\frac{(\vec{p}+q\vec{A})^2}{2m}[I] + \mu_B\,[\vec{\sigma}.\vec{B}]\right)\{\psi\}$$

where $\mu_B \equiv \dfrac{q\hbar}{2m}$ and $\vec{B} \equiv \vec{\nabla}\times\vec{A}$.

4.8. An electron is described by a Hamiltonian of the form

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

Approximate it with cosines and sines to obtain the appropriate tight-binding matrices $[\alpha]$ and $[\beta]$.



SOLUTION:

Please see Section 22.3.2 of LNE.

4.9. Show that (a) the dispersion relation corresponding to $h(\vec{k})$ in Problem 4.7 can be written as

$$E = E_0 + \frac{\hbar^2 (k \pm k_0)^2}{2m}$$

$$\text{where} \quad E_0 = -\frac{m\eta^2}{2\hbar^2}, \qquad k_0 = \frac{m\eta}{\hbar^2}$$

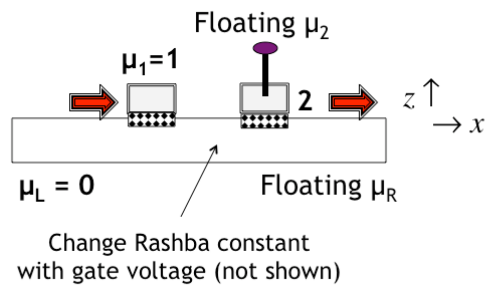
and (b) the eigenspinors for any given $\vec{k}$ have spins that are perpendicular to $\vec{k}$.

SOLUTION:

Please see HW Problem 4

4.10. The output voltage is measured by the floating probe as a function of the Rashba constant η that determines the spin-orbit term

$$H_R = \eta(\sigma_x k_y - \sigma_y k_x)$$



(a) Explain why the output voltage is expected to oscillate periodically as a function of η

(b) Find the period of the oscillation in the output voltage as η is changed noting that in a magnetic field the spin precesses around it with an angular velocity of $\omega = \dfrac{2\mu_B B_{eff}}{\hbar}$.

(c) Would there be oscillations if the magnets pointed ***along z ,*** instead of along x as shown?

Solution:

(a) Electrons traveling along +x have non-zero k_x and feel an effective magnetic field along –y. So their spins rotate around the y axis as they propagate.

The output magnet registers a voltage proportional to the x-component of the spin which equals $\cos\alpha$, α being the angle by which the spin has rotated in propagating from the injecting to the detecting contact.

Since α is proportional to the effective magnetic field and hence to η the output is expected to oscillate as a function of η

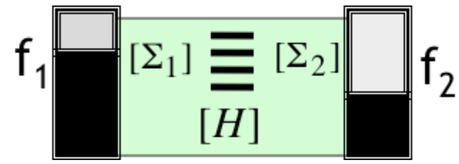
(b)

$$\alpha = \frac{2\mu_B B_{eff}}{\hbar} t = \frac{2\eta k}{\hbar} \frac{L}{v} = \frac{2mL\eta}{\hbar^2}$$

Period is obtained by setting

$$\frac{2mL}{\hbar^2} \Delta\eta = 2\pi \quad \rightarrow \quad \Delta\eta = \frac{\pi\hbar^2}{mL}$$

(c) Yes, oscillations are expected if the magnets point along z, since the injected spins will point along z and rotate around the effective B-field pointing along 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

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

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

Device with multiple terminals "r"

$$\Gamma = \sum_r \Gamma_r$$

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

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

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

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,

where

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