ECE 659, EXAM IV

Friday, Apr.7, 2017, ME 1012, 330-420PM

NAME : SOLUTION

CLOSED BOOK

Notes provided on last page

All four questions carry equal weight

Please show all work.
No credit for just writing down the answer, even if correct.

4.1. 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

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

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

4.2. An electron has a spinor wavefunction given by $\frac{1}{\sqrt{29}}\begin{Bmatrix} 2 \\ 3-4i \end{Bmatrix}$

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

SOLUTION:

$$\psi\psi^{+} = \frac{1}{29}\begin{Bmatrix} 2 \\ 3-4i \end{Bmatrix}\begin{Bmatrix} 2 & 3+4i \end{Bmatrix}$$

$$= \frac{1}{29}\begin{bmatrix} 4 & 6+8i \\ 6-8i & 25 \end{bmatrix}$$

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, $\frac{N+S_z}{2} = \frac{4}{29}, \frac{N-S_z}{2} = \frac{25}{29} \rightarrow N = 1, S_z = -\frac{21}{29}$

$$S_x = \frac{12}{29}, S_y = \frac{16}{29}$$

(Can do this more formally by taking traces too)

$$\vec{S} = \frac{12}{29}\hat{x} + \frac{16}{29}\hat{y} - \frac{21}{29}\hat{z}$$

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

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

(a) What is the dispersion relation, E(**k**) ?

(b) What are the (2x1) eigenspinors corresponding to each of the two branches of the dispersion relation for a specific wavevector $\vec{k} = k\,\hat{y}$ pointing along positive y ?

SOLUTION:

Rewrite h(k) as $$h(\vec{k}) = \frac{\hbar^2 k^2}{2m}[I] + \eta k\,\sigma.\hat{n}$$

where $$\hat{n} = \frac{k_y\hat{x} - k_x\hat{y}}{k}$$ and $$k = \sqrt{k_x^2 + k_y^2}$$

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

(b) ***Eigenspinors point up and down along the "effective field" which points along***

$$\hat{n} = \frac{k_y\hat{x} - k_x\hat{y}}{k}$$

With $\vec{k} = k\,\hat{y}$

We have

$$\hat{n} = \hat{x} \rightarrow \theta = \frac{\pi}{2}, \phi = 0$$

So eigenspinors are given by

$$\frac{1}{\sqrt{2}}\begin{bmatrix} +1 \\ +1 \end{bmatrix} \quad and \quad \frac{1}{\sqrt{2}}\begin{bmatrix} +1 \\ -1 \end{bmatrix}$$

4.4. The time evolution of a single electron spin in a magnetic field is described by

$$i\hbar\frac{d\psi}{dt} = \mu_B[\vec{\sigma}.\vec{B}]\,\psi \qquad \textbf{(1)}$$

The expectation value of the spin **s** along a direction **n** is given by

$$\vec{s}.\hat{n} = \psi^{+}[\vec{\sigma}.\hat{n}]\,\psi \qquad \textbf{(2)}$$

so that we can write

$$i\hbar\frac{d}{dt}\vec{s}.\hat{n} = \left(i\hbar\frac{d}{dt}\psi^{+}\right)[\vec{\sigma}.\hat{n}]\,\psi + \psi^{+}[\vec{\sigma}.\hat{n}]\left(i\hbar\frac{d}{dt}\psi\right) \qquad \textbf{(3)}$$

Using Eqs.(1) and (2) show from (3) that

$$\frac{d}{dt}\vec{s}.\hat{n} = K(\vec{B}\times\vec{s}).\hat{n}$$

Or equivalently $\quad \dfrac{d}{dt}\vec{s} = K(\vec{B}\times\vec{s})$

What is the constant K?

SOLUTION:

Using Eq.(1) we can rewrite Eq.(2) as

$$i\hbar\frac{d}{dt}\vec{s}.\hat{n} = -\psi^{+}\mu_B[\vec{\sigma}.\vec{B}][\vec{\sigma}.\hat{n}]\psi + \psi^{+}[\vec{\sigma}.\hat{n}]\mu_B[\vec{\sigma}.\vec{B}]\psi$$

$$= -\mu_B\psi^{+}\big([\vec{\sigma}.\vec{B}][\vec{\sigma}.\hat{n}] - [\vec{\sigma}.\hat{n}][\vec{\sigma}.\vec{B}]\big)\psi$$

$$= -\mu_B\psi^{+}\big(2i[\vec{\sigma}.(\vec{B}\times\hat{n})]\big)\psi$$

$$= -2i\mu_B\,\vec{s}.(\vec{B}\times\hat{n}) \qquad \text{Using Eq.(2)}$$

$$= 2i\mu_B\,(\vec{B}\times\vec{s}).\hat{n}$$

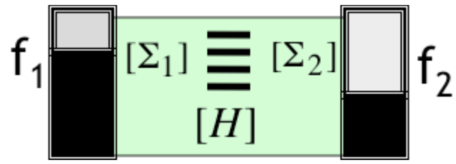
Hence $\dfrac{d}{dt}\vec{s}.\hat{n} = K(\vec{B}\times\vec{s}).\hat{n}$ or $\dfrac{d}{dt}\vec{s} = K(\vec{B}\times\vec{s})$

where

$$K = \frac{2\mu_B}{\hbar}$$

NEGF Equations

$$G^R \;=\; [EI - H - \Sigma]^{-1}$$
$$G^n \;=\; G^R\,\Sigma^{in}\,G^A$$
$$A = \;G^R \Gamma G^A = \;G^A \Gamma G^R$$
$$= \;i[G^R - G^A]$$
$$\Gamma = \;\Gamma_1 + \Gamma_2 + \Gamma_0$$
$$\tilde{I}_p = \;\frac{q}{h} Trace[\Sigma_p^{in} A - \Gamma_p G^n]$$



$$\Sigma = \;\Sigma_1 + \Sigma_2 + \Sigma_0$$
$$\Gamma_{0,1,2} = i[\Sigma_{0,1,2} - \Sigma_{0,1,2}^{+}]$$
$$\Sigma^{in} = \;\underbrace{f_1 \Gamma_1}_{\Sigma_1^{in}} \;+\; \underbrace{f_2 \Gamma_2}_{\Sigma_2^{in}} \;+\; \Sigma_0^{in}$$

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"

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

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

Useful Identities:

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

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,

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