FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

1. Schrodinger Equation
2. Contact-ing Schrodinger
3. More Examples
4. Spin Transport

4.1. Introduction

4.2. Magnetic contacts

4.3. Rotating contacts

4.4. Vectors and spinors

4.5. Spin-orbit coupling

4.6. Spin Hamiltonian

4.7. Spin density/current

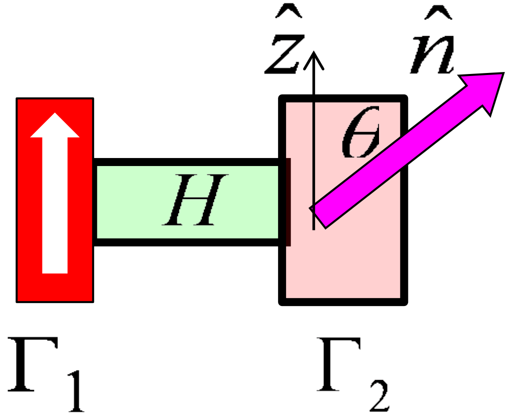
4.8. Spin voltage

4.9. Spin circuits

4.10. Summing up ..

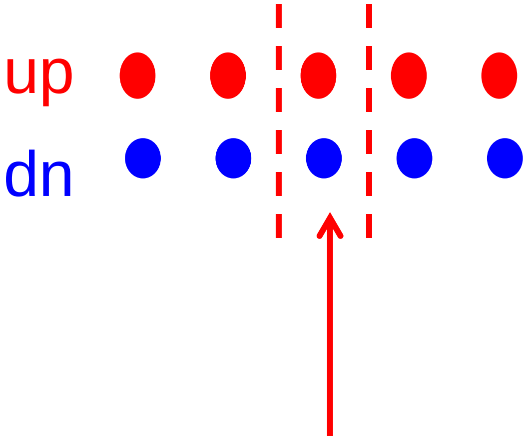
Supriyo Datta

4.7a Spin density/current



$$\frac{A}{2\pi} \leftrightarrow D$$

$$\frac{G^n}{2\pi} \leftrightarrow N$$



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

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

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

NEGF Equations

$$I^{op} = \frac{\Sigma G^n - G^n \Sigma^+}{i\hbar} + \frac{\Sigma^{in} G^A - G^R \Sigma^{in}}{i\hbar}$$

Current Operator

4.7b Spin density/current

$$\frac{G^n}{2\pi} \rightarrow \quad \psi\psi^+ = \begin{Bmatrix} c \\ s \end{Bmatrix} \begin{Bmatrix} c^* & s^* \end{Bmatrix} = \begin{bmatrix} cc^* & cs^* \\ sc^* & ss^* \end{bmatrix}$$

$$c \equiv \cos\theta/2\ e^{-i\varphi/2}$$

$$s \equiv \sin\theta/2\ e^{+i\varphi/2}$$

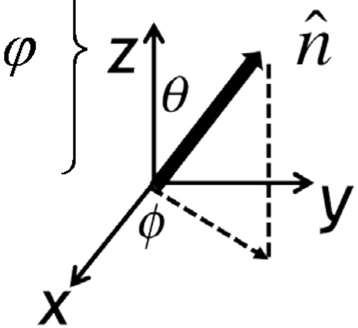
$$= \begin{bmatrix} \cos^2\frac{\theta}{2} & \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{-i\varphi} \\ \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{+i\varphi} & \sin^2\frac{\theta}{2} \end{bmatrix}$$

$$+\hat{n}: \begin{Bmatrix} c \\ s \end{Bmatrix} \qquad -\hat{n}: \begin{Bmatrix} -s^* \\ c^* \end{Bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix} 1+\cos\theta & \sin\theta\, e^{-i\varphi} \\ \sin\theta\, e^{+i\varphi} & 1-\cos\theta \end{bmatrix}$$

$$= \frac{1}{2}\underbrace{\begin{bmatrix} 1+n_z & n_x - in_y \\ n_x + in_y & 1-n_z \end{bmatrix}} = \frac{1}{2}\left(I + \vec{\sigma}.\hat{n}\right)$$

$$\begin{Bmatrix} x : \sin\theta\cos\varphi \\ y : \sin\theta\sin\varphi \\ z : \cos\theta \end{Bmatrix}$$



$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + n_z\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + n_x\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + n_y\begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix}$$

4.7c Spin density/current

$$\frac{G^n}{2\pi} \rightarrow \quad \psi\psi^+ = \begin{Bmatrix} c \\ s \end{Bmatrix} \begin{Bmatrix} c^* & s^* \end{Bmatrix}$$

$$= \underbrace{\frac{1}{2} \begin{bmatrix} 1+n_z & n_x - in_y \\ n_x + in_y & 1-n_z \end{bmatrix}}$$

$$= \frac{1}{2}\left(I + \vec{\sigma}.\hat{n}\right)$$

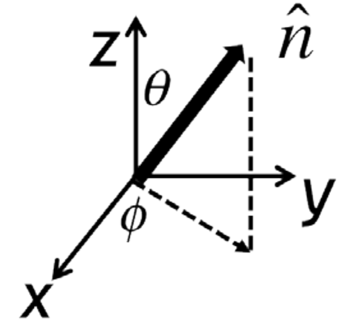
$\theta = 0$	$\theta = \pi$	*Unpolarized*	$\theta = \pi/2$
$+\hat{z}$	$-\hat{z}$		$+\hat{x}$
$\begin{Bmatrix} 1 \\ 0 \end{Bmatrix}\begin{Bmatrix} 1 & 0 \end{Bmatrix}$	$\begin{Bmatrix} 0 \\ 1 \end{Bmatrix}\begin{Bmatrix} 0 & 1 \end{Bmatrix}$	??	$\frac{1}{\sqrt{2}}\begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \frac{\begin{Bmatrix} 1 & 1 \end{Bmatrix}}{\sqrt{2}}$
$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$

$$\frac{G^n}{2\pi} = \frac{1}{2}\left(NI + \vec{\sigma}.\vec{S}\right)$$

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

$$c \equiv \cos\theta/2 \; e^{-i\varphi/2}$$

$$s \equiv \sin\theta/2 \; e^{+i\varphi/2}$$



4.7d Spin density/current

$$\frac{G^n}{2\pi} = \frac{1}{2}\left(NI + \vec{\sigma}.\vec{S}\right) = \frac{1}{2}\begin{bmatrix} N+S_z & S_x - iS_y \\ S_x + iS_y & N - S_z \end{bmatrix}$$

$$= \frac{1}{2}\left(NI + \sigma_x S_x + \sigma_y S_y + \sigma_z S_z\right)$$

$$Trace\left[\frac{G^n}{2\pi}\right] = N$$

$$\frac{G^n \sigma_x}{2\pi} = \frac{1}{2}\left(N\sigma_x + S_x I - i\,S_y \sigma_z + i\,S_z \sigma_y\right)$$

$$Trace\left[\frac{G^n \sigma_x}{2\pi}\right] = S_x$$

$$Trace\left[\frac{G^n \sigma_y}{2\pi}\right] = S_y \ , \ Trace\left[\frac{G^n \sigma_z}{2\pi}\right] = S_z$$

$$\sigma_x^2 = I \ , \sigma_y \sigma_x = -i\,\sigma_z \ , \sigma_z \sigma_x = +i\,\sigma_y$$

$$[\vec{\sigma}.\vec{V}_1][\vec{\sigma}.\vec{V}_2] =$$

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

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

4.7e Spin density/current

$$\frac{G^n}{2\pi} = \frac{1}{2}\left(NI + \vec{\sigma}.\vec{S}\right) = \frac{1}{2}\begin{bmatrix} N+S_z & S_x - iS_y \\ S_x + iS_y & N - S_z \end{bmatrix}$$

$$= \frac{1}{2}\left(NI + \sigma_x S_x + \sigma_y S_y + \sigma_z S_z\right)$$

$$Trace\left[\frac{G^n}{2\pi}\right] = N$$

$$Trace\left[\frac{G^n \sigma_i}{2\pi}\right] = S_i$$

$$Trace\left[\frac{G^n}{2\pi}\,\vec{\sigma}.\hat{n}\right] = \vec{S}.\hat{n}$$

$$\downarrow$$

$$Trace\left[\psi\psi^{+}\,\vec{\sigma}.\hat{n}\right]$$

$$\downarrow$$

$$Trace\left[\psi^{+}\,[\vec{\sigma}.\hat{n}]\;\psi\right]$$

Spin Operator

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

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

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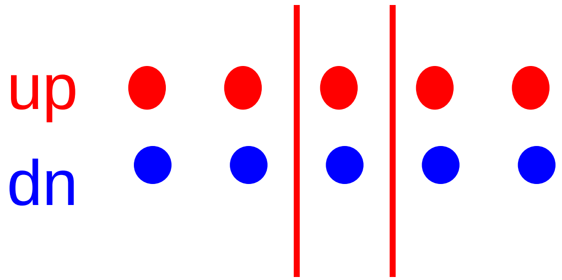
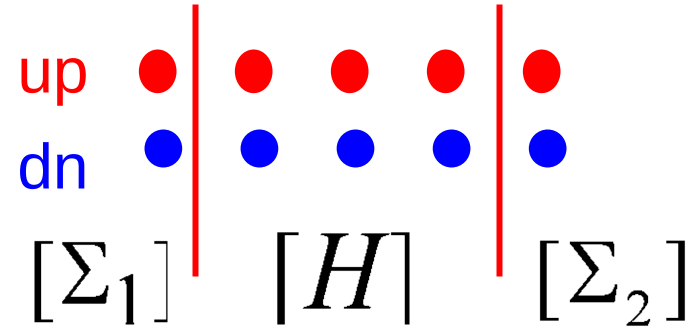
4.7f Spin density/current

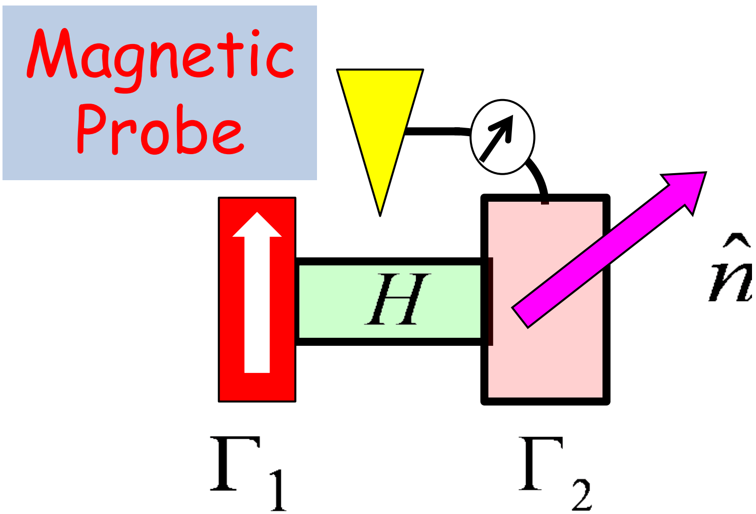
$$Trace\left[\frac{G^n}{2\pi}\,\vec{\sigma}.\hat{n}\right] = \vec{S}.\hat{n}$$

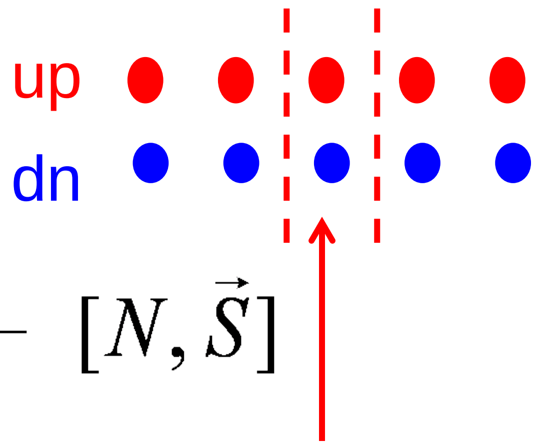


$$Trace\left[I_{op}\,\vec{\sigma}.\hat{n}\right] = \vec{I}_s.\hat{n}$$



$$\begin{array}{c|cccccc} & 1up & 1dn & 2up & 2dn & 3up & 3dn \\ \hline 1up & \multicolumn{2}{c}{\multirow{2}{*}{$[N_1, \vec{S}_1]$}} & & & & \\ 1dn & & & & & & \\ 2up & & & \multicolumn{2}{c}{\multirow{2}{*}{$[N_2, \vec{S}_2]$}} & & \\ 2dn & & & & & & \\ 3up & & & & & \multicolumn{2}{c}{\multirow{2}{*}{$[N_3, \vec{S}_3]$}} \\ 3dn & & & & & & \end{array}$$





$$\begin{Bmatrix} V \\ \vec{V}_s \end{Bmatrix} \leftarrow \quad [N, \vec{S}]$$

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

Coming up next ..

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