Spintronics and Nanomagnetics

ECS 521/641

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Quantum mechanics of spin

How to include spin?

- 1920s: OLD quantum theory → NEW quantum theory
- OLD quantum theory
  - Bohr's model
  - Quantization of energy levels and spacing
- NEW quantum theory
  - Schrodinger's **wave mechanics**
  - Heisenberg's **matrix mechanics**
  - A physical quantity can be described by a matrix or by a linear operator
  - **Schrodinger** and **Eckart** have independently showed the equivalence between the two theories
  - 1926: Dirac's **transformation theory** for unification
  - **Profound implication to treat spin in quantum theory**

Dirac's transformation theory

- Hilbert and Neumann introduced the notion of linear space
  - Matrices and vectors
  - Linear operators and functions
- State vector in Hilbert space, ψ_n or $\psi(q)$
  - The magnitude squared is the probability amplitude
- Dirac's transformation theory: The state vector
  - evolves in time according to a unitary transformation
  - satisfies a **first order** differential equation

Schrodinger

$$\psi(\boldsymbol{r}) = \psi(x, y, z, t) \qquad i\,\hbar \frac{\partial \psi(\boldsymbol{r})}{\partial t} = H_0 \psi(\boldsymbol{r})$$

$$H_0 = \frac{|\boldsymbol{p}|^2}{2m} + V(\boldsymbol{r}) \qquad \boldsymbol{p} = p_x \hat{\boldsymbol{x}} + p_y \hat{\boldsymbol{y}} + p_z \hat{\boldsymbol{z}} \qquad p_r = -i\,\hbar \frac{\partial}{\partial r}$$

$$\boldsymbol{r} = [x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}}], t$$

Pauli's spin matrices

- Pauli's approach
  - Measurement of spin angular momentum along any axis $\pm \hbar/2$
  - Commutation rules like orbital angular momentum

$$L_x L_y - L_y L_x = i\hbar L_z$$
$$L_y L_z - L_z L_y = i\hbar L_x$$
$$L_z L_x - L_x L_z = i\hbar L_y$$

$$S_x S_y - S_y S_x = i\hbar S_z$$
$$S_y S_z - S_z S_y = i\hbar S_x$$
$$S_z S_x - S_x S_z = i\hbar S_y$$

$$S_x = \frac{\hbar}{2}\sigma_x$$
$$S_y = \frac{\hbar}{2}\sigma_y$$
$$S_z = \frac{\hbar}{2}\sigma_z$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_x \sigma_y - \sigma_y \sigma_x = 2i\sigma_z$$
$$\sigma_y \sigma_z - \sigma_z \sigma_y = 2i\sigma_x$$
$$\sigma_z \sigma_x - \sigma_x \sigma_z = 2i\sigma_y$$

Exercise

DERIVE σ_x and σ_y

Deriving σ_x and σ_y

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Hermitian
- Have off-diagonal terms only (assume)

$$\sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z$$
$$\sigma_y\sigma_z - \sigma_z\sigma_y = 2i\sigma_x$$
$$\sigma_z\sigma_x - \sigma_x\sigma_z = 2i\sigma_y$$

$$\sigma_x = \begin{pmatrix} 0 & a \\ a^* & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & b \\ b^* & 0 \end{pmatrix}$$

- Eigenvalues of $\sigma_x = \pm 1$ and $\sigma_y = \pm 1$
- $|a|^2 = |b|^2 = 1$
- $a \; and \; b = \pm 1 \; or \; \pm i$
- Commutation relation: $Im(ab^*) = 1$
- Select $a = 1, b = -i$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Square of the Pauli matrices

Exercise

DERIVE $|S|^2 = S_x^2 + S_y^2 + S_z^2 = s(s+1)\hbar^2[I]$

Similar to $|L|^2 = m(m+1)\hbar^2[I]$

$$|S|^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2[I] = s(s+1)\hbar^2[I]$$

$$s = \frac{1}{2}$$

Pauli equation

$$[H] = [H_0] + [H_B] + [H_{SO}]$$

- $[H_0] = H_0[I]$ is the spin-**independent** Hamiltonian
- $[H_B] = -\left(\frac{g}{2}\right)\mu_B \boldsymbol{B}\cdot\boldsymbol{\sigma},$ $\boldsymbol{B}$ is the external field
  - Two eigenvalues and eigenenergies are not same
  - Spin-splitting, lifts the degeneracy between the two spin states
  - Zeeman splitting
- $[H_{SO}]$ is associated with spin-orbit interaction which also lifts the spin degeneracy

$$\left[\frac{\hbar}{i}\frac{\partial}{\partial t}[I] + [H_0] + [H_B] + [H_{SO}]\right][\psi(x,y,z,t)] = [0]$$

2-component wavefunction

Einstein-De Broglie equation

- Pauli equation is non-relativistic
- **Schrodinger** and **Klein/Gordon** have independently derived relativistic equivalent

Einstein's special theory of relativity $\bar{E}^2 = p^2c^2 + m_0^2c^4$

De Broglie

$$\bar{E} = h\nu$$

$$p = \frac{h}{\lambda}$$

Einstein-De Broglie equation

$$\nu^2 - \left(\frac{c}{\lambda}\right)^2 = \left(\frac{m_0 c^2}{h}\right)^2$$

$$\left[\left(\frac{i\,\hbar}{c}\frac{\partial}{\partial t}\right)^2 - \sum_{r=1}^{3}\left(-i\,\hbar\frac{\partial}{\partial x_r}\right)^2 - m_0^2c^2\right]\psi(x,y,z,t) = 0$$

Einstein-De Broglie equation

$$\left[\left(\frac{i\,\hbar}{c}\frac{\partial}{\partial t}\right)^2 - \sum_{r=1}^{3}\left(-i\,\hbar\frac{\partial}{\partial x_r}\right)^2 - m_0^2c^2\right]\psi(x,y,z,t) = 0$$

$$\psi(x,y,z,t) = e^{i(\boldsymbol{k}.\boldsymbol{r}-\omega t)}$$

$$\omega = 2\pi\nu$$

$$k = \frac{2\pi}{\lambda}$$

Einstein-De Broglie equation

$$\nu^2 - \left(\frac{c}{\lambda}\right)^2 = \left(\frac{m_0c^2}{h}\right)^2$$

Exercise

DERIVE Einstein-De Broglie equation

Klein-Gordon equation

$$\left[\left(\frac{i\hbar}{c}\frac{\partial}{\partial t}\right)^2 - \sum_{r=1}^{3}\left(-i\hbar\frac{\partial}{\partial x_r}\right)^2 - m_0^2c^2\right]\psi(x,y,z,t) = 0$$

$$\boldsymbol{A} = \left(A_0, A_x, A_y, A_z\right)$$

$$\left[\left(\frac{i\hbar}{c}\frac{\partial}{\partial t} + eA_0\right)^2 - \sum_{r=1}^{3}\left(-i\hbar\frac{\partial}{\partial x_r} + eA_r\right)^2 - m_0^2c^2\right]\psi(x,y,z,t) = 0$$

Dirac equation

Klein-Gordon equation

$$\left[\left(\frac{i\hbar}{c}\frac{\partial}{\partial t}+eA_0\right)^2-\sum_{r=1}^{3}\left(-i\hbar\frac{\partial}{\partial x_r}+eA_r\right)^2-m_0^2c^2\right]\psi(x,y,z,t)=0$$

Dirac: Equation must be of **first order**

$$\left[\left(\frac{i\hbar}{c}\frac{\partial}{\partial t}+eA_0\right)-\sum_{r=1}^{3}\alpha_r\left(-i\hbar\frac{\partial}{\partial x_r}+eA_r\right)-\alpha_0 m_0 c\right]\psi(x,y,z,t)=0$$

Must satisfy

Einstein-De Broglie equation

$$\nu^2-\left(\frac{c}{\lambda}\right)^2=\left(\frac{m_0c^2}{h}\right)^2$$

$\boldsymbol{A}=(A_0,A_x,A_y,A_z)$ will be omitted for brevity

Dirac equation

$$\left[\left(\frac{i\,\hbar}{c}\frac{\partial}{\partial t}\right)-\sum_{r=1}^{3}\alpha_r\left(-i\,\hbar\frac{\partial}{\partial x_r}\right)-\alpha_0 m_0 c\right]\psi(x,y,z,t)=0$$

Apply operator

$$\left[\left(\frac{i\,\hbar}{c}\frac{\partial}{\partial t}\right)+\sum_{r=1}^{3}\alpha_r\left(-i\,\hbar\frac{\partial}{\partial x_r}\right)+\alpha_0 m_0 c\right]$$

$$\left[\left(\frac{i\,\hbar}{c}\frac{\partial}{\partial t}\right)^2-\sum_{r=1}^{3}\{\alpha_r\}^2\left(-i\,\hbar\frac{\partial}{\partial x_r}\right)^2\right.$$

$$\left.-\sum_{m<n}(\{\alpha_m\}\{\alpha_n\}+\{\alpha_n\}\{\alpha_m\})\frac{\partial^2}{\partial x_m\partial x_n}-\{\alpha_0\}^2 m_0^2 c^2\right]\psi(x,y,z,t)=0$$

Dirac equation

$$\left[\left(\frac{i\,\hbar}{c}\frac{\partial}{\partial t}\right)^2 - \sum_{r=1}^{3}\{\alpha_r\}^2\left(-i\,\hbar\frac{\partial}{\partial x_r}\right)^2 - \sum_{m<n}(\{\alpha_m\}\{\alpha_n\}+\{\alpha_n\}\{\alpha_m\})\frac{\partial^2}{\partial x_m \partial x_n} - \{\alpha_0\}^2 m_0^2 c^2\right]\psi(x,y,z,t) = 0$$

$$\{\alpha_m\}^2 = [I] \quad (m = 0,1,2,3)$$

$$\{\alpha_m\}\{\alpha_n\}+\{\alpha_n\}\{\alpha_m\} = [0] \quad (m \neq n, m, n = 0,1,2,3)$$

To match

Einstein-De Broglie equation

$$\left[\left(\frac{i\,\hbar}{c}\frac{\partial}{\partial t}\right)^2 - \sum_{r=1}^{3}\left(-i\,\hbar\frac{\partial}{\partial x_r}\right)^2 - m_0^2 c^2\right]\psi(x,y,z,t) = 0$$

Dirac equation

$$\{\alpha_m\}^2 = [I] \quad (m = 0,1,2,3)$$

$$\{\alpha_m\}\{\alpha_n\} + \{\alpha_n\}\{\alpha_m\} = [0] \quad (m \neq n, m, n = 0,1,2,3)$$

$$\alpha_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad \alpha_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\alpha_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \quad \alpha_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

$$\alpha_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

$$\alpha_1 = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$$

$$\alpha_2 = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}$$

$$\alpha_3 = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}$$

- ✓ Total (**orbital + spin**) angular momentum is conserved
- ✓ Spin **quantization**, electron's self-rotation model cannot explain

Time-independent Dirac equation

$$\left[\sum_{r=1}^{3} c\,\alpha_r(p_r + eA_r) + \alpha_0 m_0 c^2\right]\psi(x,y,z) = \bar{E}\,\psi(x,y,z)$$

$$\alpha_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} \quad \alpha_1 = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \quad \alpha_2 = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} \quad \alpha_3 = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}$$

$$p_r = -i\,\hbar\frac{\partial}{\partial x_r}$$

$$\bar{E} = i\,\hbar\frac{\partial}{\partial t} + ceA_0$$

$$\begin{bmatrix} A & 0 & C & D^* \\ 0 & A & D & -C \\ C & D^* & B & 0 \\ D & -C & 0 & B \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \bar{E}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

$$A = m_0c^2 + V$$

$$B = -m_0c^2 + V$$

V is scalar potential

$$C = c(p_z + eA_z)$$

$$D = c\left[(p_x + eA_x) + i(p_y + eA_y)\right]$$

Time-independent Dirac equation

$$\begin{bmatrix} A & 0 & C & D^* \\ 0 & A & D & -C \\ C & D^* & B & 0 \\ D & -C & 0 & B \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \bar{E} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

$$A = m_0 c^2 + V$$

$$B = -m_0 c^2 + V$$

$$C = c(p_z + eA_z)$$

$$D = c\left[(p_x + eA_x) + i(p_y + eA_y)\right]$$

$$\begin{bmatrix} (m_0 c^2 + V)[I] & c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A}) \\ c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A}) & (-m_0 c^2 + V)[I] \end{bmatrix} \begin{bmatrix} \psi \\ \phi \end{bmatrix} = \bar{E} \begin{bmatrix} \psi \\ \phi \end{bmatrix}$$

$$\{\psi\} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \qquad \{\phi\} = \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix}$$

Time-independent Dirac equation

$$\begin{bmatrix} (m_0c^2 + V)[I] & c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A}) \\ c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A}) & (-m_0c^2 + V)[I] \end{bmatrix} \begin{bmatrix} \psi \\ \phi \end{bmatrix} = \bar{E} \begin{bmatrix} \psi \\ \phi \end{bmatrix}$$

$$\left\{(m_0c^2 + V)[I] + c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A}) \; \frac{[I]}{\bar{E} + m_0c^2 - V} c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})\right\}[\psi] = \bar{E}[\psi]$$

$$\left\{(-m_0c^2 + V)[I] + c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A}) \; \frac{[I]}{\bar{E} - m_0c^2 - V} c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})\right\}[\phi] = \bar{E}[\phi]$$

Non-relativistic approximation

$$\left\{(m_0c^2 + V)[I] + c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})\ \frac{[I]}{\bar{E} + m_0c^2 - V} c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})\right\}[\psi] = \bar{E}[\psi]$$

$$\left\{(-m_0c^2 + V)[I] + c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})\ \frac{[I]}{\bar{E} - m_0c^2 - V} c\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})\right\}[\phi] = \bar{E}[\phi]$$

$$\bar{E} \approx m_0c^2 \qquad \left\{(m_0c^2 + V)[I] + \frac{[\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})]^2}{2m_0}\right\}[\psi] = \bar{E}[\psi]$$

$$E[\psi] = (\bar{E} - m_0c^2)[\psi] = \left(\frac{(\boldsymbol{p}+e\boldsymbol{A})^2}{2m_0}[I] + \mu_B\boldsymbol{B}\cdot\boldsymbol{\sigma} + V[I]\right)[\psi]$$
$$= ([H_0] + [H_B])[\psi]$$

$$[\boldsymbol{\sigma}.(\boldsymbol{p} + e\boldsymbol{A})]^2 = (\boldsymbol{p} + e\boldsymbol{A})^2[I] + 2m_0\,\mu_B\boldsymbol{B}.\boldsymbol{\sigma}$$

- ✓ Pauli equation **without spin-orbit term** (physics not included yet)
- ✓ Zeeman interaction term appears **automatically**

Anti-matter

$$\left\{(m_0c^2+V)[I]+c\boldsymbol{\sigma}.(\boldsymbol{p}+e\boldsymbol{A})\ \frac{[I]}{\bar{E}+m_0c^2-V}c\boldsymbol{\sigma}.(\boldsymbol{p}+e\boldsymbol{A})\right\}[\psi]=\bar{E}[\psi]$$

$$\left\{(-m_0c^2+V)[I]+c\boldsymbol{\sigma}.(\boldsymbol{p}+e\boldsymbol{A})\ \frac{[I]}{\bar{E}-m_0c^2-V}c\boldsymbol{\sigma}.(\boldsymbol{p}+e\boldsymbol{A})\right\}[\phi]=\bar{E}[\phi]$$

$$\bar{E}\approx -m_0c^2 \qquad \left\{(m_0c^2+V)[I]+\frac{[\boldsymbol{\sigma}.(\boldsymbol{p}+e\boldsymbol{A})]^2}{-2m_0}\right\}[\phi]=\bar{E}[\phi]$$

- ✓ Second equation, $m_0 \rightarrow -m_0$
- ✓ $\bar{E}^2=p^2c^2+m_0^2c^4$ gives **two** dispersions
- ✓ Positive curvature → Positive mass
- ✓ Negative curvature → Negative mass
- ✓ Energy separation between the two curves $2m_0c^2\ \sim 1\ MeV$
- ✓ Energy scale for **high energy physics**