Homework 3 Koichiro Takahashi

Kane-Mele Hamiltonian

tight-binding

$$\mathcal{H} = t\sum_{\langle ij\rangle} c_i^\dagger c_j + \lambda_{so}\sum_{\langle\langle ij\rangle\rangle} \nu_{ij} c_i^\dagger s^z c_j$$

spin-orbit coupling

$$+ i\lambda_R \sum_{\langle ij\rangle} c_i^\dagger (\vec{s}\times\vec{d}_{ij})_z c_j$$

Rashba effect

$$+ \lambda_\nu \sum_i \xi_i c_i^\dagger c_i$$

staggered sublattice potential

Here, the label i specifies each point on lattice,

$\therefore$ Crystal lattice points

$$\vec{R}_i = i_x\vec{a}_1 + i_y\vec{a}_2 + \{\vec{\tau}_1, \vec{\tau}_2\}$$

$\Rightarrow$ The creation/anhilation operators are labeled by 3 indices (i_x, i_y, τ)

$$c_i \equiv c_{i_x i_y \tau}, \quad c_i^\dagger \equiv c_{i_x i_y \tau}^\dagger$$

where
$$\begin{cases} i_x = 1, 2, \cdots, L \\ i_y = 1, 2, \cdots, L \\ \tau = A, B \end{cases}$$

Periodic boundary condition for $\vec{a}_1$ direction

$\Rightarrow$ Discrete Fourier Transform (Bloch states)

$$\begin{cases} C_{i_y\tau}(k_x) = \sum_{i_x} e^{-ik_x a_1 i_x} C_{i_x i_y \tau} \\ C^\dagger_{i_y\tau}(k_x) = \sum_{i_x} e^{ik_x a_1 i_x} C^\dagger_{i_x i_y \tau} \end{cases}$$

$\Leftrightarrow$ Inverse transformation

$$\begin{cases} C_{i_x i_y \tau} = \sum_{k_x} e^{ik_x a_1 i_x} C_{i_y\tau}(k_x) \\ C^\dagger_{i_x i_y \tau} = \sum_{k_x} e^{-ik_x a_1 i_x} C^\dagger_{i_y\tau}(k_x) \end{cases}$$

putting into this equations into the Hamiltonian,

$$\mathcal{H} = t \sum_{k_x k_x'} \sum_{n.n.} e^{ia_1(k_x i_x - k_x' j_x)} c^\dagger_{i_y \tau}(k_x) c_{j_y \tau'}(k_x')$$

$$+ \lambda_{SO} \sum_{k_x k_x'} \sum_{s.n.n.} e^{ia_1(k_x i_x - k_x' j_x)} \nu_{(i_y, j_y)} c^\dagger_{i_y \tau}(k_x) S_z c_{j_y \tau'}(k_x')$$

$$+ i \lambda_R \sum_{k_x k_x'} \sum_{n.n.} e^{ia_1(k_x i_x - k_x' j_x)} c^\dagger_{i_y \tau}(k_x) (\vec{S} \times \vec{d}_{ij})_z c_{j_y \tau'}(k_x')$$

$$+ \lambda_\nu \sum_{k_x} \sum_{i_y} \xi_{i_y} c^\dagger_{i_y \tau}(k_x) c_{i_y \tau}(k_x)$$

Here, $\displaystyle\sum_{k_x k_x'} \sum_{\langle i_x j_x \rangle} e^{ia_1(k_x i_x - k_x' j_x)} f(k_x) g(k_x')$

$$= \sum_{k_x k_x'} \sum_{\langle i_x j_x \rangle} e^{ia_1(k_x i_x - k_x' j_x \underbrace{+ k_x' i_x - k_x' i_x}_{=0})} f(k_x) g(k_x')$$

$$= \sum_{k_x k_x'} \sum_{\langle i_x, j_x \rangle} e^{ia_1(k_x - k_x') i_x} e^{-ia_1 k_x' (i_x - j_x)} f(k_x) g(k_x')$$

$(i_x, j_x) \mapsto (i_x, i_x' = i_x - j_x)$ where, $\underline{i_x' = 0, \pm 1}$ for. n.n. & s.n.n.

different sublattices

$$= \sum_{k_x k_x'} \sum_{i_x, i_x'} e^{ia_1(k_x - k_x') i_x} e^{-ia_1 k_x' i_x'} f(k_x) g(k_x')$$

$$= \sum_{k_x k_x'} \sum_{i_x'} \underbrace{\left(\sum_{i_x} e^{ia_1(k_x - k_x') i_x} \right)}_{= \delta_{k_x - k_x', G_x}} f(k_x) g(k_x')$$

$\rightarrow$ choose $G_x = 0$

$$= \sum_{k_x} \sum_{i_x'} e^{-ia_1 k_x i_x'} f(k_x) g(k_x)$$

$\therefore$

$$\mathcal{H} = t \sum_{k_x} \sum_{n.n.} \sum_{i_x'} e^{-ia_1 k_x i_x'} C^\dagger_{i_y\tau}(k_x) C_{j_y\tau'}(k_x)$$

$$+ \lambda_{SO} \sum_{k_x} \sum_{s.n.n} \sum_{i_x'} e^{-ia_1 k_x i_x'} \nu_{(i_y, j_y)} C^\dagger_{i_y\tau}(k_x) S_z C_{j_y\tau'}(k_x)$$

$$+ i\lambda_R \sum_{k_x} \sum_{n.n.} \sum_{i_x'} e^{-ia_1 k_x i_x'} C^\dagger_{i_y\tau}(k_x) (\vec{S} \times \vec{d}_{ij})_z C_{j_y\tau'}(k_x)$$

$$+ \lambda_\nu \sum_{k_x} \sum_{i_y} \xi_{i_y} C^\dagger_{i_y\tau}(k_x) C_{i_y\tau}(k_x)$$

$$\Rightarrow \quad \mathcal{H} = \sum_{k_x} \mathcal{H}(k_x)$$

where

$$\mathcal{H}(k_x) = t \sum_{n.n.} \sum_{i_x'} e^{-ia_1 k_x i_x'} C^\dagger_{i_y\tau} C_{j_y\tau'}$$

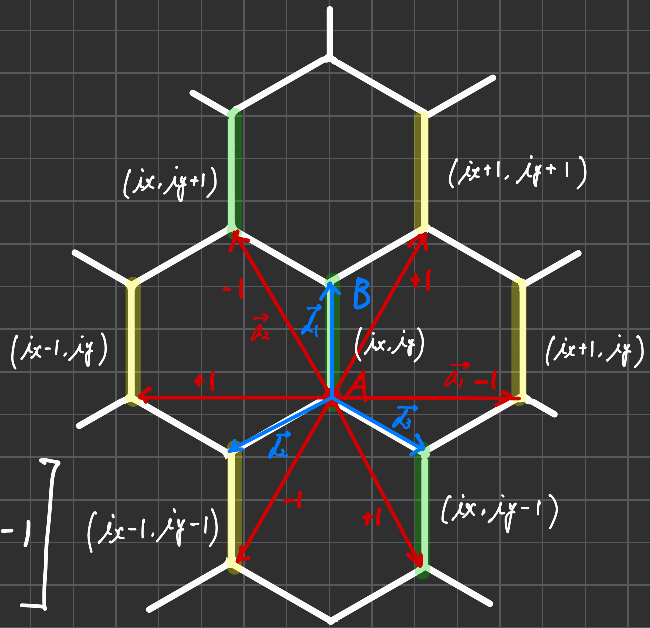
$$+ \lambda_{SO} \sum_{s.n.n.} \sum_{i_x'} e^{-ia_1 k_x i_x'} \nu_{(i_y, j_y)} C^\dagger_{i_y\tau} S_z C_{j_y\tau'}$$

$$+ i\lambda_R \sum_{n.n.} \sum_{i_x'} e^{-ia_1 k_x i_x'} C^\dagger_{i_y\tau} (\vec{S} \times \vec{d}_{ij})_z C_{j_y\tau'}$$

$$+ \lambda_\nu \sum_{i_y} \underbrace{\xi_{i_y}}_{= \begin{cases} +1 & (\tau = A) \\ -1 & (\tau = B) \end{cases}} C^\dagger_{i_y\tau} C_{i_y\tau}$$

The bulk $i_y \neq 1$ or L

$$
\langle i_y | \mathcal{H}(k_x) | j_y \rangle \overset{(4\times 4)}{=} \begin{array}{c|cc} & A & B \\ \hline A & \sim & \sim \\ B & \sim & \sim \end{array}
$$



$$
= \Big\{ \underbrace{\delta_{\tau B}\delta_{\tau' A}}_{B \leftarrow A} \times \Big[1\cdot\delta_{j_y, i_y} + e^{+ik_x a_1}\delta_{j_y, i_y-1} + 1\cdot\delta_{j_y, i_y-1} \Big]
$$

$$
\underbrace{+ \underbrace{\delta_{\tau A}\delta_{\tau' B}}_{A \leftarrow B} \Big[1\cdot\delta_{j_y, i_y} + e^{-ik_x a_1}\delta_{j_y, i_y+1} + \delta_{j_y, i_y+1} \Big] \Big\} \times t \times \mathbb{1}}_{\text{tight-binding}}
$$

$$
+ \Big\{ \delta_{\tau A}\delta_{\tau' A} \times \Big[1\cdot(\delta_{j_y, i_y-1} - \delta_{j_y, i_y+1})
$$

$$
+ e^{-ik_x a_1}\cdot(\delta_{j_y, i_y+1} - \delta_{j_y, i_y}) + e^{+ik_x a_1}(\delta_{j_y, i_y} - \delta_{j_y, i_y-1}) \Big]
$$

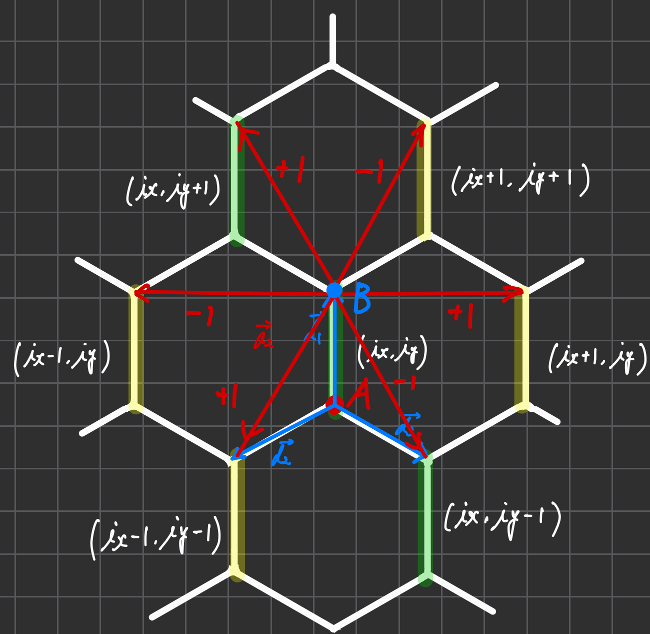
$$
+ \delta_{\tau B}\delta_{\tau' B} \times \Big[1\cdot(\delta_{j_y, i_y+1} - \delta_{j_y, i_y-1})
$$

the sign of ν_{ij} is flipped

$$
+ e^{-ik_x a_1}\cdot(\delta_{j_y, i_y} - \delta_{j_y, i_y+1})
$$

$$
+ e^{+ik_x a_1}\cdot(\delta_{j_y, i_y-1} - \delta_{j_y, i_y}) \Big] \Big\}
$$

$$
\underbrace{\times i \lambda_{SO} S_z}_{\text{spin-orbit}}
$$



$$+\Big\{\delta_{\tau A}\delta_{\tau' A}\times\Big[1\cdot\Big(\big(\vec{s}\times(-\vec{d}_1+\vec{d}_3)\big)_z\,\delta_{jy,iy-1}+\big(\vec{s}\times(-\vec{d}_3+\vec{d}_1)\big)_z\,\delta_{jy,iy+1}\Big)$$

$$+e^{-ik_x a_1}\cdot\Big(\big(\vec{s}\times(-\vec{d}_2+\vec{d}_1)\big)_z\,\delta_{jy,iy+1}+\big(\vec{s}\times(-\vec{d}_2+\vec{d}_3)\big)_z\,\delta_{jy,iy}\Big)$$

$$+e^{+ik_x a_1}\Big(\big(\vec{s}\times(-\vec{d}_3+\vec{d}_2)\big)_z\,\delta_{jy,iy}+\big(\vec{s}\times(-\vec{d}_1+\vec{d}_2)\big)_z\,\delta_{jy,iy-1}\Big)\Big]$$

$$+\delta_{\tau B}\delta_{\tau' B}\times\Big[1\cdot\Big(\big(\vec{s}\times(\vec{d}_1-\vec{d}_3)\big)_z\,\delta_{jy,iy+1}+\big(\vec{s}\times(\vec{d}_3-\vec{d}_1)\big)_z\,\delta_{jy,iy-1}\Big)$$

$$+e^{-ik_x a_1}\cdot\Big(\big(\vec{s}\times(\vec{d}_3-\vec{d}_2)\big)_z\,\delta_{jy,iy}+\big(\vec{s}\times(\vec{d}_1-\vec{d}_2)\big)_z\,\delta_{jy,iy+1}\Big)$$

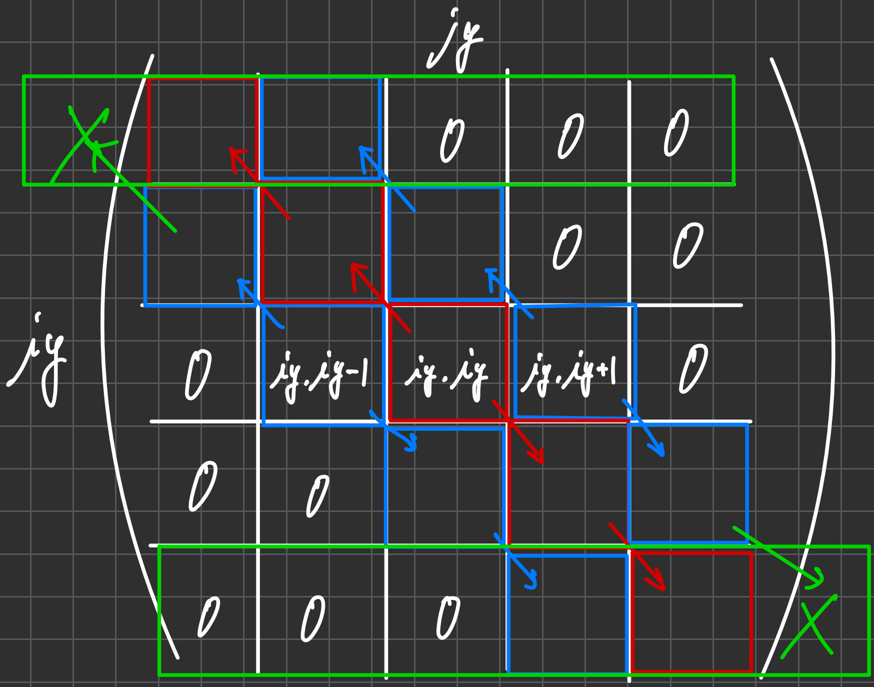
$$+e^{+ik_x a_1}\cdot\Big(\big(\vec{s}\times(\vec{d}_2-\vec{d}_1)\big)_z\,\delta_{jy,iy-1}+\big(\vec{s}\times(\vec{d}_2-\vec{d}_3)_z\big)\,\delta_{jy,iy}\Big)\Big]\Big\}$$

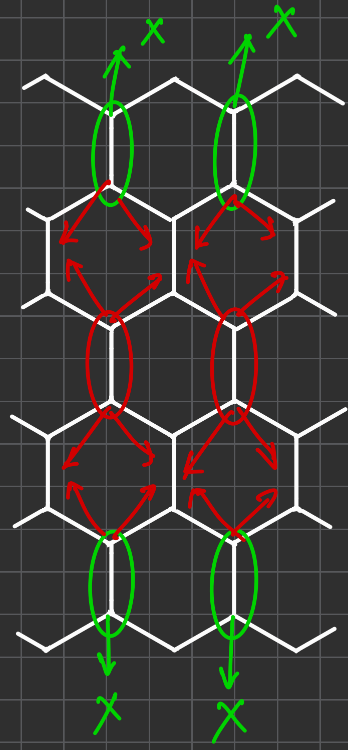
$$\times\, i\lambda_R$$

Rashba

$$+\delta_{iy,jy}\cdot\big[+1\,\delta_{\tau A}\delta_{\tau' A}-\delta_{\tau B}\delta_{\tau' B}\big]\times\lambda_v$$

Staggered potential





At boundary $j_y = 0$, you don't have $\langle j_y | \mathcal{H} | j_y - 1 \rangle$

j_y ''

$j_y = L$, you don't have $\langle j_y | \mathcal{H} | j_y + 1 \rangle$

$$\langle j_y | \mathcal{H} | j_y \rangle = \mathcal{H}^0 = \begin{array}{c|cc} & A & B \\ \hline A & \mathcal{H}^0_{AA} & \mathcal{H}^0_{AB} \\ B & \mathcal{H}^0_{BA} & \mathcal{H}^0_{BB} \end{array}$$

Hermitian ??

$$\mathcal{H}^0_{AA} = \lambda_{SO}\,\nu S_z \left(e^{ik_x a_1} - e^{-ik_x a_1}\right) + i\lambda_R\left(\nu\vec{s}\times(\vec{d}_2-\vec{d}_3)\right)_z\left(e^{ik_x a_1} - e^{-ik_x a_1}\right) + \lambda_\nu$$

$$\mathcal{H}_{BB}^{0} = -\lambda_{SO} S_z \left(e^{ik_x a_1} - e^{-ik_x a_1}\right)$$

$$-i\lambda_R \left(\vec{S}\times(\vec{d}_2-\vec{d}_3)\right)_z \left(e^{ik_x a_1} - e^{-ik_x a_1}\right)$$

$$-\lambda_v$$

$$\mathcal{H}_k \vec{\psi}_k = \varepsilon_k \vec{\psi}_k$$

$\psi_k(\vec{r})$

$$\vec{\psi}_k = \begin{pmatrix} \psi_k^{\uparrow} \\ \psi_k^{\downarrow} \end{pmatrix}$$

$$S_z \vec{\psi}_k = \begin{pmatrix} \frac{\hbar}{2} \\ -\frac{\hbar}{2} \end{pmatrix}$$

$$\mathcal{H}_{AB}^{0} = t \ , \ \mathcal{H}_{BA}^{0} = t$$

$$\langle i_y | \mathcal{H} | i_y - 1 \rangle$$

$$= \mathcal{H}^{-1} = \begin{array}{c|cc} & A & B \\ \hline A & \mathcal{H}_{AA}^{-1} & \mathcal{H}_{AB}^{-1} \\ B & \mathcal{H}_{BA}^{-1} & \mathcal{H}_{BB}^{-1} \end{array}$$

$$\mathcal{H}_{AA}^{-1} = \lambda_{SO} S_z \left(1 - e^{ik_x a_1}\right)$$

$$+ i\lambda_R \left[1 \cdot \left(\vec{S}\times(\vec{d}_3-\vec{d}_1)\right)_z + e^{ik_x a_1}\left(\vec{S}\times(\vec{d}_2-\vec{d}_1)\right)_z\right]$$

$$\mathcal{H}_{BB}^{-1} = -\lambda_{SO} S_z \left(1 - e^{ik_x a_1}\right)$$

$$+ i\lambda_R \left[1 \cdot \left(\vec{S}\times(\vec{d}_3-\vec{d}_1)\right)_z + e^{ik_x a_1}\left(\vec{S}\times(\vec{d}_2-\vec{d}_1)\right)_z\right]$$

$$\mathcal{H}_{AB}^{-1} = 0 \ , \ \mathcal{H}_{BA}^{-1} = t\left(1 + e^{ik_x a}\right)$$

$$\langle ij|\mathcal{H}|ij+1\rangle$$

$$\equiv \mathcal{H}^{+1} \equiv \begin{array}{c|cc} & A & B \\ \hline A & \mathcal{H}_{AA}^{+1} & \mathcal{H}_{AB}^{+1} \\ B & \mathcal{H}_{BA}^{+1} & \mathcal{H}_{BB}^{+1} \end{array}$$

$$\mathcal{H}_{AA}^{+1} = -\lambda_{SO} s_z \left(1 - e^{-ik_x a_1}\right)$$
$$-i\lambda_R \left[1 \cdot \left(\vec{s} \times (\vec{d}_3 - \vec{d}_1)\right)_z + e^{-ik_x a_1} \left(\vec{s} \times (\vec{d}_2 - \vec{d}_1)\right)_z \right]$$

$$\mathcal{H}_{BB}^{+1} = \lambda_{SO} s_z \left(1 - e^{-ik_x a_1}\right)$$
$$-i\lambda_R \left[1 \cdot \left(\vec{s} \times (\vec{d}_3 - \vec{d}_1)\right)_z + e^{-ik_x a_1} \left(\vec{s} \times (\vec{d}_2 - \vec{d}_1)\right)_z \right]$$

$$\mathcal{H}_{AB}^{+1} = t\left(1 + e^{-ik_x a_1}\right), \quad \mathcal{H}_{AB}^{+1} = 0$$

General case:

Hamiltonian of single electrons in crystal

Eigenstates: Bloch state

$$\langle r|k\rangle = \psi_k(\vec{r}) = \sum_n a_n \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \phi_n(\vec{r}-\vec{R}_i)$$

$(n = s, p, d, f, \ldots$ & spin $\uparrow$ or $\downarrow)$

Here, we think the effective Hamiltonian only spanned by p_z orbitals.

$\therefore\ n = p\uparrow$ or $p\downarrow$.

$$\psi_k(\vec{r}) = \sum_\alpha a_\alpha \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \phi_{p_z\alpha}(\vec{r}-\vec{R}_i)$$

$(\alpha = \uparrow$ or $\downarrow)$

This eigenstate can be seen as Fourier transform of localized p_z orbitals.

$$\boxed{\psi(\vec{r}-\vec{R}_i) = \sum_\alpha a_\alpha \phi_{p_z\alpha}(\vec{r}-\vec{R}_i)}$$

$\Longrightarrow$

$$\mathcal{F}[\psi(\vec{r}-\vec{R}_i)](\vec{k})$$

$$= \sum_\alpha a_\alpha \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \phi_{p_z\alpha}(\vec{r}-\vec{R}_i)$$

$\therefore$ First we take the basis as localized p_z orbitals in second quantization, and later take Fourier transform.

$$\boxed{\begin{array}{l} \{|i\alpha\rangle\} : \langle\vec{r}|i\alpha\rangle = \phi_\alpha(\vec{r}-R_i) \quad (p_z \text{ orbital}) \\ \qquad\qquad\qquad\qquad \left(\begin{array}{l}\vec{R}_i : \text{Bravais lattice} \\ \alpha = \uparrow \text{ or } \downarrow\end{array}\right)\end{array}}$$

$$\mathcal{H}_{cryst} = \sum_i V(\vec{r}-\vec{R}_i)$$

crystal Field

$$\mathcal{H}_{kinetic} + \mathcal{H}_{cryst} = \frac{\vec{P}^2}{2m} + \sum_i V(\vec{r}-\vec{R}_i)$$

$$\xrightarrow{\text{quantize}}$$

$$\sum_{ij\alpha\beta} \langle i\alpha| \left(\frac{\vec{P}^2}{2m} + \sum_l V(\vec{r}-\vec{R}_l) \right) |j\beta\rangle \hat{a}^\dagger_{i\alpha} \hat{a}_{j\beta}$$

$$= \sum_{ij\alpha\beta} \int d^3\vec{r}\, \phi_\alpha(\vec{r}-\vec{R}_i) \left(\frac{\vec{P}^2}{2m} + \sum_l V(\vec{r}-\vec{R}_l) \right) \phi_\beta(\vec{r}-\vec{R}_j)$$

$$\times \hat{a}^\dagger_{i\alpha} \hat{a}_{j\beta}$$

$\simeq$ ← tight binding approximation

$$\sum_{i\alpha} \varepsilon_0 \hat{a}^\dagger_{i\alpha} \hat{a}_{i\alpha} + t \sum_{\langle ij \rangle \alpha\beta} \hat{a}^\dagger_{i\alpha} \hat{a}_{j\beta}$$

??

1 orbital × 2 sublattice × 2 spin

↙

Bloch state

$$\psi_{nk} = \sum_{R\tau} \sum_{s} e^{ik\cdot R} \phi_s(\vec{r} - (\vec{R} + \vec{\tau}))$$

$$H_{SO} = \sum_i -\frac{1}{2m^2c^2}\left(\vec{p}\times\vec{\nabla}V(\vec{r}-\vec{R}_i)\right)\cdot\vec{S}$$

Thomas precession

$$= \sum_i -\frac{\hbar}{4m^2c^2}\left(\vec{p}\times\vec{\nabla}V(\vec{r}-\vec{R}_i)\right)\cdot\vec{\sigma}$$

$$\left(\because \vec{S} = \frac{\hbar}{2}\vec{\sigma}\right)$$