Dzyaloshinskii-Moriya interaction

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We use the wannier function as the bases to expand the Hamiltonian.

$$\{\omega_{n\uparrow}(\boldsymbol{r}-\boldsymbol{R}), \omega_{n\downarrow}(\boldsymbol{r}-\boldsymbol{R})\} \tag{1}$$

And the $\widehat{\alpha}_{n\uparrow}(\boldsymbol{R})$ and $\widehat{\alpha}^{\dagger}_{n\downarrow}(\boldsymbol{R})$ are the annihilation and the creation operators of the electrons in the state $\omega_{n\uparrow}(\boldsymbol{r}-\boldsymbol{R})$, etc.

Then the Hamiltionian of a system after considering spin-orbit coupling (SOC) can be writen as,

$$\widehat{H}_1 = \frac{\widehat{\boldsymbol{p}}^2}{2m} + V(\widehat{\boldsymbol{r}}) + \frac{\hbar}{2m^2c^2}\widehat{\boldsymbol{S}} \cdot [\nabla V(\widehat{\boldsymbol{r}}) \times \widehat{\boldsymbol{p}}] \tag{2}$$

The last term is SOC term ($\widehat{H}_{\mathsf{SOC}}$) drive from the Dirac equation[a].

[a] Spin-orbit coupling: Dirac equation

Suppose $V(\boldsymbol{r}) = V(|\boldsymbol{r}|) = V(r)$,

$$\begin{aligned} H_{\mathsf{SOC}} &= \frac{\hbar}{2m^2c^2}\widehat{\boldsymbol{S}} \cdot [\frac{\mathrm{d}V(r)}{\mathrm{d}r}\frac{\widehat{\boldsymbol{r}}}{r} \times \widehat{\boldsymbol{p}}] \\ &= \lambda \widehat{\boldsymbol{L}} \cdot \widehat{\boldsymbol{S}} \\ &= \lambda \left(\widehat{L}_z \widehat{S}_z + \frac{1}{2}(\widehat{L}_+ \widehat{S}_- + \widehat{L}_- \widehat{S}_+) \right) \end{aligned} \tag{3}$$

$$\begin{aligned}
\widehat{H} = \widehat{H}_0^{\text{all}} + \widehat{T}^{\text{all}} = \sum_{\boldsymbol{R}} \sum_{n} \epsilon_n(\boldsymbol{R}) \left[\widehat{\alpha}_{n\uparrow}^{\dagger}(\boldsymbol{R}) \widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) + \widehat{\alpha}_{n\downarrow}^{\dagger}(\boldsymbol{R}) \widehat{\alpha}_{n\downarrow}(\boldsymbol{R}) \right] \\
+ \sum_{\boldsymbol{R} \neq \boldsymbol{R}'} \sum_{n,n'} \Big\{ b_{n'n}(\boldsymbol{R}' - \boldsymbol{R}) \left[\widehat{\alpha}_{n'\uparrow}^{\dagger}(\boldsymbol{R}') \widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) + \widehat{\alpha}_{n'\downarrow}^{\dagger}(\boldsymbol{R}') \widehat{\alpha}_{n\downarrow}(\boldsymbol{R}) \right] \\
+ C_{n'n}^{z}(\boldsymbol{R}' - \boldsymbol{R}) \left[\widehat{\alpha}_{n'\uparrow}^{\dagger}(\boldsymbol{R}') \widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) - \widehat{\alpha}_{n'\downarrow}^{\dagger}(\boldsymbol{R}') \widehat{\alpha}_{n\downarrow}(\boldsymbol{R}) \right] \\
+ C_{n'n}^{-}(\boldsymbol{R}' - \boldsymbol{R}) \widehat{\alpha}_{n'\uparrow}^{\dagger}(\boldsymbol{R}') \widehat{\alpha}_{n\downarrow}(\boldsymbol{R}) \\
+ C_{n'n}^{+}(\boldsymbol{R}' - \boldsymbol{R}) \widehat{\alpha}_{n'\downarrow}^{\dagger}(\boldsymbol{R}') \widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) \Big\}
\end{aligned} \tag{4}$$

$$b_{n'n}(\boldsymbol{R}' - \boldsymbol{R}) + C_{n'n}^{z}(\boldsymbol{R}' - \boldsymbol{R}) = \int \omega_{n'\uparrow}^{*}(\boldsymbol{r} - \boldsymbol{R}') H_1 \omega_{n\uparrow}(\boldsymbol{r} - \boldsymbol{R}) \mathrm{d}\boldsymbol{r} \tag{5a}$$

$$b_{n'n}(\boldsymbol{R}' - \boldsymbol{R}) - C_{n'n}^{z}(\boldsymbol{R}' - \boldsymbol{R}) = \int \omega_{n'\downarrow}^{*}(\boldsymbol{r} - \boldsymbol{R}') H_1 \omega_{n\downarrow}(\boldsymbol{r} - \boldsymbol{R}) \mathrm{d}\boldsymbol{r} \tag{5b}$$

$$C_{n'n}^{x}(\boldsymbol{R}' - \boldsymbol{R}) - iC_{n'n}^{y}(\boldsymbol{R}' - \boldsymbol{R}) = C_{n'n}^{-}(\boldsymbol{R}' - \boldsymbol{R}) = \int \omega_{n'\uparrow}^{*}(\boldsymbol{r} - \boldsymbol{R}') H_1 \omega_{n\downarrow}(\boldsymbol{r} - \boldsymbol{R}) \mathrm{d}\boldsymbol{r} \tag{5c}$$

$$C_{n'n}^{x}(\boldsymbol{R}' - \boldsymbol{R}) + iC_{n'n}^{y}(\boldsymbol{R}' - \boldsymbol{R}) = C_{n'n}^{+}(\boldsymbol{R}' - \boldsymbol{R}) = \int \omega_{n'\downarrow}^{*}(\boldsymbol{r} - \boldsymbol{R}') H_1 \omega_{n\uparrow}(\boldsymbol{r} - \boldsymbol{R}) \mathrm{d}\boldsymbol{r} \tag{5d}$$

Mechanisms of DMI ▷ Perturbation

Basically, there are three techniques to achieve our aims, that perturbed the low energy subspace with the high energy excitation space.

- Downfolding[1]
- Lowdin Perturbation[2]
- Green's Function

All of those three methods gives the same result:

$$\widehat{H}_{\text{eff}} = \widehat{H}_0 - \frac{\widehat{T}^\dagger \widehat{T}}{U} = \widehat{H}_0 + \widehat{H}_{\text{M}} \tag{6}$$

Where U is the Hubbard U refer to the energy cost when move two electrons to the same site. And $\widehat{T}$ only content the hoping terms contribute to this process.

[1] Introduction to the Magnetic Exchange Mechanisms, Yang Li, 2020

[2] https://link.springer.com/content/pdf/bbm%3A978-1-4615-5673-2%2F1.pdf

$$\widehat{H}_{\mathsf{M}} = -\frac{1}{U}\widehat{T}^{\dagger}\widehat{T}$$

$$\begin{aligned}\widehat{T} = {} & b_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\left[\widehat{\alpha}^{\dagger}_{n'\uparrow}(\boldsymbol{R}')\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) + \widehat{\alpha}^{\dagger}_{n'\downarrow}(\boldsymbol{R}')\widehat{\alpha}_{n\downarrow}(\boldsymbol{R})\right] \\ & + C^{z}_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\left[\widehat{\alpha}^{\dagger}_{n'\uparrow}(\boldsymbol{R}')\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) - \widehat{\alpha}^{\dagger}_{n'\downarrow}(\boldsymbol{R}')\widehat{\alpha}_{n\downarrow}(\boldsymbol{R})\right] \\ & + C^{-}_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\widehat{\alpha}^{\dagger}_{n'\uparrow}(\boldsymbol{R}')\widehat{\alpha}_{n\downarrow}(\boldsymbol{R}) \\ & + C^{+}_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\widehat{\alpha}^{\dagger}_{n'\downarrow}(\boldsymbol{R}')\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) + h.c.\end{aligned} \tag{7}$$

The relation between fermi annihilation/creation operators and spin operators is,

$$\widehat{S}_{z,n}(\boldsymbol{R}) = \frac{1}{2}\left[\widehat{\alpha}^{\dagger}_{n\uparrow}(\boldsymbol{R})\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) - \widehat{\alpha}^{\dagger}_{n\downarrow}(\boldsymbol{R})\widehat{\alpha}_{n\downarrow}(\boldsymbol{R})\right] \tag{8a}$$

$$\widehat{S}_{+,n}(\boldsymbol{R}) = \widehat{\alpha}^{\dagger}_{n\uparrow}(\boldsymbol{R})\widehat{\alpha}_{n\downarrow}(\boldsymbol{R}) \tag{8b}$$

$$\widehat{S}_{-,n}(\boldsymbol{R}) = \widehat{\alpha}^{\dagger}_{n\downarrow}(\boldsymbol{R})\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) \tag{8c}$$

$$
\begin{aligned}
\widehat{H}_M = J_{\boldsymbol{R},\boldsymbol{R}'}\ &\widehat{\boldsymbol{S}}(\boldsymbol{R}) \cdot \widehat{\boldsymbol{S}}(\boldsymbol{R}') \\
&+ \boldsymbol{D}_{\boldsymbol{R},\boldsymbol{R}'} \cdot \left[\widehat{\boldsymbol{S}}(\boldsymbol{R}) \times \widehat{\boldsymbol{S}}(\boldsymbol{R}')\right] \\
&+ \widehat{\boldsymbol{S}}(\boldsymbol{R}) \cdot \overleftrightarrow{\Gamma}_{\boldsymbol{R},\boldsymbol{R}'} \cdot \widehat{\boldsymbol{S}}(\boldsymbol{R}')
\end{aligned} \tag{9}
$$

Where,

$$
J_{\boldsymbol{R},\boldsymbol{R}'} = 2|b_{nn'}(\boldsymbol{R}-\boldsymbol{R}')|^2/U \tag{10a}
$$

$$
\boldsymbol{D}_{\boldsymbol{R},\boldsymbol{R}'} = (4i/U)\left[b_{nn'}(\boldsymbol{R}-\boldsymbol{R}')\boldsymbol{C}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) - b_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\boldsymbol{C}_{nn'}(\boldsymbol{R}-\boldsymbol{R}')\right] \tag{10b}
$$

$$
\begin{aligned}
\overleftrightarrow{\Gamma}_{\boldsymbol{R},\boldsymbol{R}'} = 4/U\ &\big[\boldsymbol{C}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \otimes \boldsymbol{C}_{nn'}(\boldsymbol{R}-\boldsymbol{R}') + \boldsymbol{C}_{nn'}(\boldsymbol{R}-\boldsymbol{R}') \otimes \boldsymbol{C}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \\
&- \left(\boldsymbol{C}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \cdot \boldsymbol{C}_{nn'}(\boldsymbol{R}-\boldsymbol{R}')\right) \mathbb{1}\big]
\end{aligned} \tag{10c}
$$

And,

$$
\begin{aligned}
b_{nn'}(\boldsymbol{R}-\boldsymbol{R}') &= b^*_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \\
\boldsymbol{C}_{nn'}(\boldsymbol{R}-\boldsymbol{R}') &= \boldsymbol{C}^*_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \\
\boldsymbol{C} &= (C_x, C_y, C_z)
\end{aligned} \tag{11}
$$

$$\widehat{H}_{\mathsf{DM}} = \boldsymbol{D} \cdot (\widehat{\boldsymbol{S}}_1 \times \widehat{\boldsymbol{S}}_2) \tag{12}$$

Suppose the two ions contribute to the electron transfer is located at point A and B, the point bisecting AB is denoted by C.

- When a center of inversion if located at C, $\boldsymbol{D} = 0$
- When a mirror plane perpendicular to AB passes through C, $\boldsymbol{D} \parallel$ mirror plane
- When a mirror plane including AB, $\boldsymbol{D} \perp$ mirror plane
- When a C_2 axis perpendicular to AB passes C, $\boldsymbol{D} \perp C_2$ axis
- When there is a C_n $(n \geq 2)$ alone AB, $\boldsymbol{D} \parallel AB$