补充材料: Dzyaloshinskii-Moriya (DM) 相互作用推导

Yang Li
lyang.1915@foxmail.com

August 26, 2022

1 Downfolding 二阶微扰

TBA.

2 化简计算二阶微扰项

展开并计算二阶微扰项是一项繁琐但直接的工作. 下面, 我们将具体展示该工作是如何进行的. 同时, 该文档还旨在向您展示如何正确地进行复杂公式推导, 因此行文描述可能略显冗长, 还请耐心评读.

2.1 基本目标

我们具体的目标如下: 计算 *Downfolding* 方法给出的二阶微扰哈密顿量,

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

其中,

$$\begin{aligned}
\widehat{T} = {} & b_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\left[\widehat{\alpha}^{\dagger}_{n'\uparrow}(\boldsymbol{R}')\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) + \widehat{\alpha}^{\dagger}_{n'\downarrow}(\boldsymbol{R}')\widehat{\alpha}_{n\downarrow}(\boldsymbol{R})\right] \\
& + C^{z}_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\left[\widehat{\alpha}^{\dagger}_{n'\uparrow}(\boldsymbol{R}')\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) - \widehat{\alpha}^{\dagger}_{n'\downarrow}(\boldsymbol{R}')\widehat{\alpha}_{n\downarrow}(\boldsymbol{R})\right] \\
& + C^{-}_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\widehat{\alpha}^{\dagger}_{n'\uparrow}(\boldsymbol{R}')\widehat{\alpha}_{n\downarrow}(\boldsymbol{R}) \\
& + C^{+}_{n'n}(\boldsymbol{R}'-\boldsymbol{R})\widehat{\alpha}^{\dagger}_{n'\downarrow}(\boldsymbol{R}')\widehat{\alpha}_{n\uparrow}(\boldsymbol{R}) + h.c.
\end{aligned} \tag{2}$$

2.2 推导前的准备工作

2.2.1 简化记号

将式(2)用简单符号表示,[1]

$$\begin{aligned}\widehat{T} &= b\left(\widehat{\alpha}_{2\uparrow}^{\dagger}\widehat{\alpha}_{1\uparrow}+\widehat{\alpha}_{2\downarrow}^{\dagger}\widehat{\alpha}_{1\downarrow}\right)+C_z\left(\widehat{\alpha}_{2\uparrow}^{\dagger}\widehat{\alpha}_{1\uparrow}-\widehat{\alpha}_{2\downarrow}^{\dagger}\widehat{\alpha}_{1\downarrow}\right)+C_-\widehat{\alpha}_{2\uparrow}^{\dagger}\widehat{\alpha}_{1\downarrow}+C_+\widehat{\alpha}_{2\downarrow}^{\dagger}\widehat{\alpha}_{1\uparrow}+h.c.\\ &= (b+C_z)\widehat{\alpha}_{2\uparrow}^{\dagger}\widehat{\alpha}_{1\uparrow}+(b-C_z)\widehat{\alpha}_{2\downarrow}^{\dagger}\widehat{\alpha}_{1\downarrow}+C_-\widehat{\alpha}_{2\uparrow}^{\dagger}\widehat{\alpha}_{1\downarrow}+C_+\widehat{\alpha}_{2\downarrow}^{\dagger}\widehat{\alpha}_{1\uparrow}+h.c.\end{aligned} \tag{3}$$

其中 $h.c.$ 代指厄米共轭项 (dagger,†), 即将前四项的厄米共轭后完整地加在后面. 进而算符 $\widehat{T}$ 中含有八项跃迁. 不难发现, $\widehat{T}$ 中的前四项代表 1 格点到 2 格点的电子跃迁, 后四项则是格点 2 到格点 1 的电子跃迁. 因此 $\widehat{T}$ 算符本身包含了 1,2 格点间所有的跃迁可能. 即,

$$\widehat{T}=\widehat{t}_{1\to2}+\widehat{t}_{1\to2}^{\dagger}=\widehat{t}_{1\to2}+\widehat{t}_{2\to1} \tag{4}$$

其中 $\widehat{t}_{1\to2}$ 代表 1 格点到 2 格点的四项跃迁, 且我们定义 $\widehat{t}_{2\to1}=\widehat{t}_{1\to2}^{\dagger}$.[2] 将系统全部正反跃迁的可能通路加全, 这保证了哈密顿量的厄米性, 进而保证了粒子数守恒, 使得该系统有稳定的束缚态.

接下来, 我们使用符号 t 来简单表示 $\widehat{t}_{1\to2}$. 式(1)可化简为,

$$\begin{aligned}\widehat{H}_{\mathrm{M}} &= -\frac{1}{U}\widehat{T}^{\dagger}\widehat{T}\\ &= -\frac{1}{U}(t+t^{\dagger})^{\dagger}(t+t^{\dagger})\\ &= -\frac{1}{U}(t^{\dagger}+t)(t+t^{\dagger})\\ &= -\frac{1}{U}(t^{\dagger}t+t^{\dagger}t^{\dagger}+tt+tt^{\dagger})\end{aligned} \tag{5}$$

2.2.2 公式对称性观察

容易验证, $t^{\dagger}t^{\dagger}$ 与 tt 都是 0. 因为我们此处只考虑一个电子的厄米系统, 这两项都是粒子数不守恒的. 或更朴素地, 我们关心的任意电子态作用在这两个算符上的结果都是 0.

[1] 对公式记号的简化是非常有必要的, 这使得我们在纸上书写公式时可以将更多的脑力放在符号间的运算, 而非符号正确性的比对上. **简化符号应该简明扼要地包含该符号所蕴含的所有必要信息**. 而最后在实际成文时, 考虑到科学性和严谨性, 应该再将简化符号扩充为包含足够细节的复杂符号, 这使得我们的文章可以省略大幅描述公式意义的篇幅, 而将重点放在讨论公式背后的物理上来.

[2] 注意, 该处我们还并未对相关的系数做细致考察, 只是声明如果单单从产生湮灭算符角度看, $\widehat{t}_{1\to2}^{\dagger}$ 应该代表的是 2 格点到 1 格点的跃迁

另外, 在式(4)中我们定义了 $\widehat{t}_{2\to1}=\widehat{t}^{\dagger}_{1\to2}$. 而通过仔细比对就不难发现, **算符 $\widehat{t}_{1\to2}$ 与 $\widehat{t}_{2\to1}$ 的区别仅仅是是 1,2 指标互换位置**. 也就是说, 将 t 算符的 1,2 指标互换, 就可以将其变为 $t^{\dagger}$ 算符.[3] 于是,

$$
\begin{aligned}
\widehat{H}_{\mathrm{M}} &= -\frac{1}{U}(t^{\dagger}t+tt^{\dagger}) \\
&= -\frac{1}{U}(\widehat{t}^{\dagger}_{1\to2}\widehat{t}_{1\to2}+\widehat{t}^{\dagger}_{2\to1}\widehat{t}_{2\to1}) \\
&= -\frac{1}{U}\left[t^{\dagger}t+(1\Leftrightarrow 2)\right]
\end{aligned}
\tag{6}
$$

其中 $(1\Leftrightarrow 2)$ 代表前项 1,2 指标互换后的项. 换言之, 如果我们算出了 $t^{\dagger}t$, 只需要将其结果中的 1,2 指标互换位置, 就可以立刻得到 $\widehat{t}^{\dagger}_{2\to1}\widehat{t}_{2\to1}$ 的简式, 而该简式将恰好等于 $tt^{\dagger}$.[4]

应该特别注意的是, 简化表达的系数 $b, C_z, C_\pm$ 是暗含 $(n,\boldsymbol{R})$ 指标的. 当 1,2 指标交换后, 这些系数的变化如下,

$$b_{nn'}(\boldsymbol{R}-\boldsymbol{R}')=b^{*}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \tag{7a}$$
$$C^{z}_{nn'}(\boldsymbol{R}-\boldsymbol{R}')=C^{z*}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \tag{7b}$$
$$C^{\pm}_{nn'}(\boldsymbol{R}-\boldsymbol{R}')=C^{\mp*}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \tag{7c}$$

若设 $C_\pm=C_x\pm iC_y$, 则式(7c)可化为,

$$C^{x}_{nn'}(\boldsymbol{R}-\boldsymbol{R}')=C^{x*}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \tag{8a}$$
$$C^{y}_{nn'}(\boldsymbol{R}-\boldsymbol{R}')=C^{y*}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \tag{8b}$$

令 $\boldsymbol{C}=(C_x,C_y,C_z)$, 则

$$\boldsymbol{C}_{nn'}(\boldsymbol{R}-\boldsymbol{R}')=\boldsymbol{C}^{*}_{n'n}(\boldsymbol{R}'-\boldsymbol{R}) \tag{9}$$

即经历指标互换后, b 会变为 b^*, $\boldsymbol{C}$ 会变为 $\boldsymbol{C}^*$. 上述性质均由系数的定义直接决定. [5]

于是, 我们只需要求出 $t^{\dagger}t$ 的结果, 而后将其结果中的 1,2 指标互换就可以得到 $tt^{\dagger}$. 两项相加, 就可以得到 $\widehat{T}^{\dagger}\widehat{T}$ 的完整表达式. 到此为止, 我们将

[3]这一结论是相当重要的, 在后续的推到中我们会看到, 该结论并没有听起来这么自然和平庸.

[4]请注意, 此处对最终结果进行的 1,2 指标互换的操作, 将不再等价于直接对其做厄米共轭. 因为前者, $t^{\dagger}t$ 内部交换指标后等于 $tt^{\dagger}$; 而后者, $t^{\dagger}t$ 的厄米共轭还是 $t^{\dagger}t$. 而显然 t 和 $t^{\dagger}$ 是不对易的.

[5]如果您没有发现这一点, 那么当实际上手时, 您可能会非常轻易地宣布前文的描述是错的, 因为 "显然"$C_\pm$ 所对应的项在厄米共轭之后不是简单的交换 1,2 指标就能和原先相等的. 事实上他们 "角色互换" 了. 但由于 $\boldsymbol{C}$ 也暗含 1,2 指标, 最终整个哈密顿量仍是形式不变的. 另外, 如果您认为这段不好理解, 不妨实际上手做一做, 这样可以更好地体会本段含义.

一个含 $8\times 8=64$ 项的表达式, 化为了一个 $4\times 4=16$ 项的化简问题. 在此过程中, 我们实际上是使用了 "解的对称性". 接下来我们会看到, 在剩余的 16 项中, 通过合理采纳相关对称性, 也可以极大地简化运算, 减少出错.

2.2.3 算符间的基本关系

注意到, 费米子的产生湮灭算符 $(\widehat{\alpha}_{i\sigma}^{\dagger}, \widehat{\alpha}_{i\sigma})$, 粒子数算符 $(\widehat{n}_{i\sigma})$, 自旋算符 $(\boldsymbol{S}_i)$ 之间有这样几个关系:

$$
\begin{aligned}
\widehat{\alpha}_{i\sigma}\widehat{\alpha}_{j\sigma'} + \widehat{\alpha}_{i\sigma}\widehat{\alpha}_{j\sigma'} &= 0 && \text{(10a)}\\
\widehat{\alpha}_{i\sigma}^{\dagger}\widehat{\alpha}_{j\sigma'}^{\dagger} + \widehat{\alpha}_{i\sigma}^{\dagger}\widehat{\alpha}_{j\sigma'}^{\dagger} &= 0 && \text{(10b)}\\
\widehat{\alpha}_{i\sigma}\widehat{\alpha}_{j\sigma'}^{\dagger} + \widehat{\alpha}_{j\sigma'}^{\dagger}\widehat{\alpha}_{i\sigma} &= \delta_{ij}\delta_{\sigma\sigma'} && \text{(10c)}\\
\widehat{\alpha}_{i\sigma}^{\dagger}\widehat{\alpha}_{i\sigma} &= \widehat{n}_{i\sigma} && \text{(10d)}\\
\widehat{\alpha}_{i\uparrow}^{\dagger}\widehat{\alpha}_{i\uparrow} + \widehat{\alpha}_{i\downarrow}^{\dagger}\widehat{\alpha}_{i\downarrow} &= \widehat{n}_{i} && \text{(10e)}\\
\frac{1}{2}(\widehat{\alpha}_{i\uparrow}^{\dagger}\widehat{\alpha}_{i\uparrow} - \widehat{\alpha}_{i\downarrow}^{\dagger}\widehat{\alpha}_{i\downarrow}) &= \widehat{S}_i^z && \text{(10f)}\\
\widehat{\alpha}_{i\uparrow}^{\dagger}\widehat{\alpha}_{i\downarrow} &= \widehat{S}_i^+ && \text{(10g)}\\
\widehat{\alpha}_{i\downarrow}^{\dagger}\widehat{\alpha}_{i\uparrow} &= \widehat{S}_i^- && \text{(10h)}
\end{aligned}
$$

其中, i, j 表示不同格点 (的不同轨道), σ, σ' 为自旋指标. 自旋升降算符定义为 $\widehat{S}_i^{\pm} = \widehat{S}_i^x \pm i\widehat{S}_i^y$, 总电子数算符 $\widehat{n}_i = \widehat{n}_{i\uparrow} + \widehat{n}_{i\downarrow}$.

同时注意到, 我们考虑的体系是**处在不同格点处的两个轨道之间的单电子跃迁**, 我们已经将双电子态所对应的高能态空间通过 *Downfolding* 技术, "压缩" 到了单电子空间中. 这意味着在我们所关心的态中, 每个轨道上有且仅有一个电子. 也即, 对于我们关心的态, 粒子数算符 $\widehat{n}_i$ 始终为单位算符, $\widehat{n}_i = 1$. 于是, 我们在推导中额外引入了下面一个约束条件,

$$
\widehat{\alpha}_{i\uparrow}^{\dagger}\widehat{\alpha}_{i\uparrow} = 1 - \widehat{\alpha}_{i\downarrow}^{\dagger}\widehat{\alpha}_{i\downarrow} \tag{11}
$$

结合式(10)和式(11)可以立刻推出,

$$
\begin{aligned}
\widehat{\alpha}_{i\downarrow}\widehat{\alpha}_{i\downarrow}^{\dagger} = \widehat{\alpha}_{i\uparrow}^{\dagger}\widehat{\alpha}_{i\uparrow} = \widehat{n}_{i\uparrow} &= \frac{1}{2} + \widehat{S}_i^z && \text{(12a)}\\
\widehat{\alpha}_{i\uparrow}\widehat{\alpha}_{i\uparrow}^{\dagger} = \widehat{\alpha}_{i\downarrow}^{\dagger}\widehat{\alpha}_{i\downarrow} = \widehat{n}_{i\downarrow} &= \frac{1}{2} - \widehat{S}_i^z && \text{(12b)}
\end{aligned}
$$

2.3 公式推导

2.3.1 原项展开

为了方便, 我们首先将 $t^\dagger$ 和 t 清晰地写出来, 所有 α 上的 “hat” 都被省略, 以此缩减手写成本.

$$t^\dagger = (b^* + C_z^*)\alpha_{1\uparrow}^\dagger\alpha_{2\uparrow} + (b^* - C_z^*)\alpha_{1\downarrow}^\dagger\alpha_{2\downarrow} + C_-^*\alpha_{1\downarrow}^\dagger\alpha_{2\uparrow} + C_+^*\alpha_{1\uparrow}^\dagger\alpha_{2\downarrow} \tag{13a}$$

$$t = (b + C_z)\alpha_{2\uparrow}^\dagger\alpha_{1\uparrow} + (b - C_z)\alpha_{2\downarrow}^\dagger\alpha_{1\downarrow} + C_-\alpha_{2\uparrow}^\dagger\alpha_{1\downarrow} + C_+\alpha_{2\downarrow}^\dagger\alpha_{1\uparrow} \tag{13b}$$

接下来, 我们需要写出对应的 16 项分式. 注意 $t^\dagger$ 在前, t 在后. α 是算符, 不能轻易调动顺序; $b, \boldsymbol{C}$ 是复数, 可以自由换位.[6] 令 $\widehat{h}_{\mathrm{M}} = t^\dagger t$,

$$\begin{aligned}
\widehat{h}_{\mathrm{M}} = &(b^* + C_z^*) & \alpha_{1\uparrow}^\dagger\alpha_{2\uparrow} & \quad (b + C_z) & \alpha_{2\uparrow}^\dagger\alpha_{1\uparrow} \\
+ &(b^* + C_z^*) & \alpha_{1\uparrow}^\dagger\alpha_{2\uparrow} & \quad (b - C_z) & \alpha_{2\downarrow}^\dagger\alpha_{1\downarrow} \\
+ &(b^* + C_z^*) & \alpha_{1\uparrow}^\dagger\alpha_{2\uparrow} & \quad C_- & \alpha_{2\uparrow}^\dagger\alpha_{1\downarrow} \\
+ &(b^* + C_z^*) & \alpha_{1\uparrow}^\dagger\alpha_{2\uparrow} & \quad C_+ & \alpha_{2\downarrow}^\dagger\alpha_{1\uparrow} \\
+ &(b^* - C_z^*) & \alpha_{1\downarrow}^\dagger\alpha_{2\downarrow} & \quad (b + C_z) & \alpha_{2\uparrow}^\dagger\alpha_{1\uparrow} \\
+ &(b^* - C_z^*) & \alpha_{1\downarrow}^\dagger\alpha_{2\downarrow} & \quad (b - C_z) & \alpha_{2\downarrow}^\dagger\alpha_{1\downarrow} \\
+ &(b^* - C_z^*) & \alpha_{1\downarrow}^\dagger\alpha_{2\downarrow} & \quad C_- & \alpha_{2\uparrow}^\dagger\alpha_{1\downarrow} \\
+ &(b^* - C_z^*) & \alpha_{1\downarrow}^\dagger\alpha_{2\downarrow} & \quad C_+ & \alpha_{2\downarrow}^\dagger\alpha_{1\uparrow} \\
+ &C_-^* & \alpha_{1\downarrow}^\dagger\alpha_{2\uparrow} & \quad (b + C_z) & \alpha_{2\uparrow}^\dagger\alpha_{1\uparrow} \\
+ &C_-^* & \alpha_{1\downarrow}^\dagger\alpha_{2\uparrow} & \quad (b - C_z) & \alpha_{2\downarrow}^\dagger\alpha_{1\downarrow} \\
+ &C_-^* & \alpha_{1\downarrow}^\dagger\alpha_{2\uparrow} & \quad C_- & \alpha_{2\uparrow}^\dagger\alpha_{1\downarrow} \\
+ &C_-^* & \alpha_{1\downarrow}^\dagger\alpha_{2\uparrow} & \quad C_+ & \alpha_{2\downarrow}^\dagger\alpha_{1\uparrow} \\
+ &C_+^* & \alpha_{1\uparrow}^\dagger\alpha_{2\downarrow} & \quad (b + C_z) & \alpha_{2\uparrow}^\dagger\alpha_{1\uparrow} \\
+ &C_+^* & \alpha_{1\uparrow}^\dagger\alpha_{2\downarrow} & \quad (b - C_z) & \alpha_{2\downarrow}^\dagger\alpha_{1\downarrow} \\
+ &C_+^* & \alpha_{1\uparrow}^\dagger\alpha_{2\downarrow} & \quad C_- & \alpha_{2\uparrow}^\dagger\alpha_{1\downarrow} \\
+ &C_+^* & \alpha_{1\uparrow}^\dagger\alpha_{2\downarrow} & \quad C_+ & \alpha_{2\downarrow}^\dagger\alpha_{1\uparrow}
\end{aligned} \tag{14}$$

[6] 书写该处时应该特别小心, 因为接下来的复杂运算都是基于该处的, 稳扎稳打, 步步为营. 推公式切忌心浮气躁, 想得到结果又不舍得花费精力和时间.

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}} = (b+C_z)(b^*+C_z^*) \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\uparrow} \alpha_{2\uparrow}^\dagger \alpha_{1\uparrow} \\
+ (b-C_z)(b^*+C_z^*) \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\uparrow} \alpha_{2\downarrow}^\dagger \alpha_{1\downarrow} \\
+ C_-(b^*+C_z^*) \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\uparrow} \alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} \\
+ C_+(b^*+C_z^*) \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\uparrow} \alpha_{2\downarrow}^\dagger \alpha_{1\uparrow} \\
+ (b+C_z)(b^*-C_z^*) \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\downarrow} \alpha_{2\uparrow}^\dagger \alpha_{1\uparrow} \\
+ (b-C_z)(b^*-C_z^*) \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\downarrow} \alpha_{2\downarrow}^\dagger \alpha_{1\downarrow} \\
+ C_-(b^*-C_z^*) \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\downarrow} \alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} \\
+ C_+(b^*-C_z^*) \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\downarrow} \alpha_{2\downarrow}^\dagger \alpha_{1\uparrow} \\
+ (b+C_z)C_-^* \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\uparrow} \alpha_{2\uparrow}^\dagger \alpha_{1\uparrow} \\
+ (b-C_z)C_-^* \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\uparrow} \alpha_{2\downarrow}^\dagger \alpha_{1\downarrow} \\
+ C_-C_-^* \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\uparrow} \alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} \\
+ C_+C_-^* \quad & \alpha_{1\downarrow}^\dagger \alpha_{2\uparrow} \alpha_{2\downarrow}^\dagger \alpha_{1\uparrow} \\
+ (b+C_z)C_+^* \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\downarrow} \alpha_{2\uparrow}^\dagger \alpha_{1\uparrow} \\
+ (b-C_z)C_+^* \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\downarrow} \alpha_{2\downarrow}^\dagger \alpha_{1\downarrow} \\
+ C_-C_+^* \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\downarrow} \alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} \\
+ C_+C_+^* \quad & \alpha_{1\uparrow}^\dagger \alpha_{2\downarrow} \alpha_{2\downarrow}^\dagger \alpha_{1\uparrow}
\end{aligned}
\tag{15}
$$

结合式(10)和式(12), 我们可以继续对式(15)做如下化简[7],

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}} = &(|b|^2+|C_z|^2+bC_z^*+b^*C_z) &\cdot \quad &(\quad n_{1\uparrow}n_{2\downarrow}) \\
&+(|b|^2-|C_z|^2+bC_z^*-b^*C_z) &\cdot \quad &(- \quad S_1^+S_2^-) \\
&+(b^*C_-+C_z^*C_-) &\cdot \quad &(\quad S_1^+n_{2\downarrow}) \\
&+(b^*C_++C_z^*C_+) &\cdot \quad &(- \quad n_{1\uparrow}S_2^-) \\
&+(|b|^2-|C_z|^2-bC_z^*+b^*C_z) &\cdot \quad &(- \quad S_1^-S_2^+) \\
&+(|b|^2+|C_z|^2-bC_z^*-b^*C_z) &\cdot \quad &(\quad n_{1\downarrow}n_{2\uparrow}) \\
&+(b^*C_--C_z^*C_-) &\cdot \quad &(- \quad n_{1\downarrow}S_2^+) \\
&+(b^*C_+-C_z^*C_+) &\cdot \quad &(\quad S_1^-n_{2\uparrow}) \\
&+(bC_-^*+C_zC_-^*) &\cdot \quad &(\quad S_1^-n_{2\downarrow}) \\
&+(bC_-^*-C_zC_-^*) &\cdot \quad &(- \quad n_{1\downarrow}S_2^-) \\
&+C_-C_-^* &\cdot \quad &(\quad n_{1\downarrow}n_{2\downarrow}) \\
&+C_+C_-^* &\cdot \quad &(- \quad S_1^-S_2^-) \\
&+(bC_+^*+C_zC_+^*) &\cdot \quad &(- \quad n_{1\uparrow}S_2^+) \\
&+(bC_+^*-C_zC_+^*) &\cdot \quad &(\quad S_1^+n_{2\uparrow}) \\
&+C_-C_+^* &\cdot \quad &(- \quad S_1^+S_2^+) \\
&+C_+C_+^* &\cdot \quad &(\quad n_{1\uparrow}n_{2\uparrow})
\end{aligned}
\tag{16}
$$

2.3.2 展开结果分类

通过一些其他的途径, 我们已经知晓, 各向同性的交换是 $|b|^2$ 的效果, DM 相互作用是 $|b||\boldsymbol{C}|$ 的效果, 对称的各向异性交换相互作用是 $|\boldsymbol{C}|^2$ 的效果. 于是, 我们可以对式(16)中的各项按所含 $b, \boldsymbol{C}$ 参数做如下分类. 令 $\widehat{h}_{\mathrm{M}} = \widehat{h}_{\mathrm{M}}^{(b2)} + \widehat{h}_{\mathrm{M}}^{(bC)} + \widehat{h}_{\mathrm{M}}^{(C2)}$, 其中,

$$
\widehat{h}_{\mathrm{M}}^{(b2)} = |b|^2(n_{1\uparrow}n_{2\downarrow}+n_{1\downarrow}n_{2\uparrow}-S_1^+S_2^--S_1^-S_2^+) \tag{17}
$$

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}}^{(bC)} = &\, bC_z^*(n_{1\uparrow}n_{2\downarrow}-n_{1\downarrow}n_{2\uparrow}+S_1^-S_2^+-S_1^+S_2^-) \\
&+b^*C_z(n_{1\uparrow}n_{2\downarrow}-n_{1\downarrow}n_{2\uparrow}+S_1^+S_2^--S_1^-S_2^+) \\
&+bC_-^*(S_1^-n_{2\downarrow}-n_{1\downarrow}S_2^-) \\
&+b^*C_-(S_1^+n_{2\downarrow}-n_{1\downarrow}S_2^+) \\
&+bC_+^*(S_1^+n_{2\uparrow}-n_{1\uparrow}S_2^+) \\
&+b^*C_+(S_1^-n_{2\uparrow}-n_{1\uparrow}S_2^-)
\end{aligned}
\tag{18}
$$

[7]为了用笔书写时的简单, 我们依然略去 hat 记号.

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}}^{(C2)} &= |C_z|^2(n_{1\uparrow}n_{2\downarrow} + n_{1\downarrow}n_{2\uparrow} + S_1^+S_2^- + S_1^-S_2^+) \\
&+ |C_-|^2 n_{1\downarrow}n_{2\downarrow} + |C_+|^2 n_{1\uparrow}n_{2\uparrow} \\
&+ C_z C_-^*(S_1^- n_{2\downarrow} + n_{1\downarrow}S_2^-) \\
&+ C_z^* C_-(S_1^+ n_{2\downarrow} + n_{1\downarrow}S_2^+) \\
&+ C_z C_+^*(-S_1^+ n_{2\uparrow} - n_{1\uparrow}S_2^+) \\
&+ C_z^* C_+(-S_1^- n_{2\uparrow} - n_{1\uparrow}S_2^-) \\
&+ C_- C_+^*(-S_1^+S_2^+) + C_-^* C_+(-S_1^-S_2^-)
\end{aligned} \tag{19}
$$

2.3.3 各向同性交换相互作用: $|b|^2$ 项

将式(10)和式(12)中的条件带入式(17)可得,

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}}^{(b2)} &= |b|^2[(\frac{1}{2} + S_1^z)(\frac{1}{2} - S_2^z) + (\frac{1}{2} - S_1^z)(\frac{1}{2} + S_2^z) - 2S_1^xS_2^x - 2S_1^zS_2^z] \\
&= |b|^2(\frac{1}{2} - 2S_1^zS_2^z - 2S_1^xS_2^x - 2S_1^zS_2^z) \\
&\overset{\text{eff.}}{=} -2|b|^2 \boldsymbol{S}_1 \cdot \boldsymbol{S}_2
\end{aligned} \tag{20}
$$

2.3.4 DM 交换相互作用: $|b||\mathbf{C}|$ 项

其次来看 $|b||\boldsymbol{C}|$ 项,

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}}^{(bC)} &= bC_z^*(n_{1\uparrow}n_{2\downarrow} - n_{1\downarrow}n_{2\uparrow} + S_1^-S_2^+ - S_1^+S_2^-) + h.c. \\
&+ bC_-^*(S_1^- n_{2\downarrow} - n_{1\downarrow}S_2^-) + h.c. \\
&+ bC_+^*(S_1^+ n_{2\uparrow} - n_{1\uparrow}S_2^+) + h.c.
\end{aligned} \tag{21}
$$

其中, 式(21)的第一二项,

$$
\begin{aligned}
& bC_z^*(n_{1\uparrow}n_{2\downarrow} - n_{1\downarrow}n_{2\uparrow} + S_1^-S_2^+ - S_1^+S_2^-) + h.c. \\
&= bC_z^*[(\frac{1}{2} + S_1^z)(\frac{1}{2} - S_2^z) - (\frac{1}{2} - S_1^z)(\frac{1}{2} + S_2^z) \\
&\qquad + (S_1^x - iS_1^y)(S_2^x + iS_2^y) - (S_1^x + iS_1^y)(S_2^x - iS_2^y)] + h.c. \\
&= bC_z^*[(S_1^z - S_2^z) + 2i(S_1^xS_2^y - S_1^yS_2^x)] + h.c. \\
&= (bC_z^* + b^*C_z)(S_1^z - S_2^z) + 2i(bC_z^* - b^*C_z)(S_1^xS_2^y - S_1^yS_2^x)
\end{aligned} \tag{22}
$$

式(21)的第三到六项,

$$
\begin{aligned}
&bC_-^*(S_1^- n_{2\downarrow} - n_{1\downarrow}S_2^-) + bC_+^*(S_1^+ n_{2\uparrow} - n_{1\uparrow}S_2^+) + h.c.\\
&= b(C_x^* + iC_y^*)[(S_1^x - iS_1^y)(\frac{1}{2} - S_2^z) - (\frac{1}{2} - S_1^z)(S_2^x - iS_2^y)] + h.c.\\
&+ b(C_x^* - iC_y^*)[(S_1^x + iS_1^y)(\frac{1}{2} + S_2^z) - (\frac{1}{2} + S_1^z)(S_2^x + iS_2^y)] + h.c.\\
&= b(C_x^* + iC_y^*)(\frac{1}{2}S_1^x - \frac{i}{2}S_1^y - S_2^zS_1^x + iS_2^zS_1^y - \frac{1}{2}S_2^x + \frac{i}{2}S_2^y + S_1^zS_2^x - iS_1^zS_2^y) + h.c.\\
&+ b(C_x^* - iC_y^*)(\frac{1}{2}S_1^x + \frac{i}{2}S_1^y + S_2^zS_1^x + iS_2^zS_1^y - \frac{1}{2}S_2^x - \frac{i}{2}S_2^y - S_1^zS_2^x - iS_1^zS_2^y) + h.c.\\
&= bC_x^*[(S_1^x - S_2^x) + 2i(S_2^zS_1^y - S_1^zS_2^y)] + ibC_y^*[-i(S_1^y - S_2^y) - 2S_2^zS_1^x + 2S_1^zS_2^x] + h.c.\\
&= bC_x^*[(S_1^x - S_2^x) + 2i(S_1^yS_2^z - S_1^zS_2^y)] + bC_y^*[(S_1^y - S_2^y) + 2i(S_1^zS_2^x - S_2^zS_1^x)] + h.c.\\
&= (bC_x^* + b^*C_x)(S_1^x - S_2^x) + 2i(bC_x^* - b^*C_x)(S_1^yS_2^z - S_1^zS_2^y)\\
&+ (bC_y^* + b^*C_y)(S_1^y - S_2^y) + 2i(bC_y^* - b^*C_y)(S_1^zS_2^x - S_2^zS_1^x)
\end{aligned}
\tag{23}
$$

于是, $|b||\boldsymbol{C}|$ 项最终可化简为,

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}}^{(bC)} &= (bC_z^* + b^*C_z)(S_1^z - S_2^z) + 2i(bC_z^* - b^*C_z)(S_1^xS_2^y - S_1^yS_2^x)\\
&+ (bC_x^* + b^*C_x)(S_1^x - S_2^x) + 2i(bC_x^* - b^*C_x)(S_1^yS_2^z - S_1^zS_2^y)\\
&+ (bC_y^* + b^*C_y)(S_1^y - S_2^y) + 2i(bC_y^* - b^*C_y)(S_1^zS_2^x - S_2^zS_1^x)\\
&= (b\boldsymbol{C}^* + b^*\boldsymbol{C})(\boldsymbol{S}_1 - \boldsymbol{S}_2) + 2i(b\boldsymbol{C}^* - b^*\boldsymbol{C})\cdot(\boldsymbol{S}_1 \times \boldsymbol{S}_2)
\end{aligned}
\tag{24}
$$

2.3.5 对称各向异性交换相互作用: $|\mathbf{C}|^2$ 项

最后看 $|\boldsymbol{C}|^2$ 项,

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}}^{(C2)} &= |C_z|^2(n_{1\uparrow}n_{2\downarrow} + n_{1\downarrow}n_{2\uparrow} + S_1^+S_2^- + S_1^-S_2^+)\\
&+ C_-C_-^*n_{1\downarrow}n_{2\downarrow} + C_+C_+^*n_{1\uparrow}n_{2\uparrow}\\
&+ C_zC_-^*(+S_1^-n_{2\downarrow} + n_{1\downarrow}S_2^-) + h.c.\\
&+ C_zC_+^*(-S_1^+n_{2\uparrow} - n_{1\uparrow}S_2^+) + h.c.\\
&+ C_-C_+^*(-S_1^+S_2^+) + h.c.
\end{aligned}
\tag{25}
$$

式(25)的第一项,

$$
\begin{aligned}
&|C_z|^2(n_{1\uparrow}n_{2\downarrow} + n_{1\downarrow}n_{2\uparrow} + S_1^+S_2^- + S_1^-S_2^+)\\
&= |C_z|^2(\frac{1}{2} - 2S_1^zS_2^z + 2S_1^xS_2^x + 2S_1^yS_2^y)\\
&\overset{\text{eff.}}{=} 2|C_z|^2S_1^xS_2^x + 2|C_z|^2S_1^yS_2^y - 2|C_z|^2S_1^zS_2^z
\end{aligned}
\tag{26}
$$

式(25)的第二三项,

$$
\begin{aligned}
&C_-C_-^*n_{1\downarrow}n_{2\downarrow}+C_+C_+^*n_{1\uparrow}n_{2\uparrow}\\
&=(C_x-iC_y)(C_x^*+iC_y^*)(\frac{1}{2}-S_1^z)(\frac{1}{2}-S_2^z)\\
&+(C_x+iC_y)(C_x^*-iC_y^*)(\frac{1}{2}+S_1^z)(\frac{1}{2}+S_2^z)\\
&=[(C_xC_x^*+C_yC_y^*)+i(C_xiC_y^*-C_yC_x^*)](\frac{1}{4}-\frac{1}{2}S_1^z-\frac{1}{2}S_2^z+S_1^zS_2^z)\\
&+[(C_xC_x^*+C_yC_y^*)-i(C_xiC_y^*-C_yC_x^*)](\frac{1}{4}+\frac{1}{2}S_1^z+\frac{1}{2}S_2^z+S_1^zS_2^z)\\
&=(C_xC_x^*+C_yC_y^*)(\frac{1}{2}+2S_1^zS_2^z)+i(C_xC_y^*-C_yC_x^*)(-S_1^z-S_2^z)\\
&\overset{\text{eff.}}{=}2(|C_x|^2+|C_y|^2)S_1^zS_2^z-i(C_xC_y^*-C_yC_x^*)(S_1^z+S_2^z)
\end{aligned}
\tag{27}
$$

式(25)的第四到七项,

$$
\begin{aligned}
&C_zC_-^*(S_1^-n_{2\downarrow}+n_{1\downarrow}S_2^-)+C_zC_+^*(-S_1^+n_{2\uparrow}-n_{1\uparrow}S_2^+)+h.c.\\
&=C_z(C_x^*+iC_y^*)[+(S_1^x-iS_1^y)(\frac{1}{2}-S_2^z)+(\frac{1}{2}-S_1^z)(S_2^x-iS_2^y)]+h.c.\\
&+C_z(C_x^*-iC_y^*)[-(S_1^x+iS_1^y)(\frac{1}{2}+S_2^z)-(\frac{1}{2}+S_1^z)(S_2^x+iS_2^y)]+h.c.\\
&=C_z(C_x^*+iC_y^*)(+\frac{1}{2}S_1^x-\frac{i}{2}S_1^y-S_1^xS_2^z+iS_1^yS_2^z+\frac{1}{2}S_2^x-\frac{i}{2}S_2^y-S_1^zS_2^x+iS_1^zS_2^y)+h.c.\\
&+C_z(C_x^*-iC_y^*)(-\frac{1}{2}S_1^x-\frac{i}{2}S_1^y-S_1^xS_2^z-iS_1^yS_2^z-\frac{1}{2}S_2^x-\frac{i}{2}S_2^y-S_1^zS_2^x-iS_1^zS_2^y)+h.c.\\
&=C_zC_x^*[-iS_1^y-2S_1^xS_2^z-iS_2^y-2S_1^zS_2^x]+iC_zC_y^*[S_1^x+2iS_1^yS_2^z+S_2^x+2iS_1^zS_2^y]+h.c.\\
&=C_zC_x^*[-i(S_1^y+S_2^y)-2(S_1^xS_2^z+2S_1^zS_2^x)]+C_zC_y^*[i(S_1^x+S_2^x)-2(S_1^yS_2^z+S_1^zS_2^y)]+h.c.\\
&=-i(C_zC_x^*-C_z^*C_x)(S_1^y+S_2^y)-2(C_zC_x^*+C_z^*C_x)(S_1^xS_2^z+S_1^zS_2^x)\\
&++i(C_zC_y^*-C_z^*C_y)(S_1^x+S_2^x)-2(C_zC_y^*+C_z^*C_y)(S_1^yS_2^z+S_1^zS_2^y)\\
&=-i(C_zC_x^*-C_z^*C_x)(S_1^y+S_2^y)-2(C_zC_x^*+C_z^*C_x)(S_1^xS_2^z+S_1^zS_2^x)\\
&+-i(C_yC_z^*-C_zC_y^*)(S_1^x+S_2^x)-2(C_yC_z^*+C_zC_y^*)(S_1^yS_2^z+S_1^zS_2^y)
\end{aligned}
\tag{28}
$$

式(25)的第八九项,

$$
\begin{aligned}
&C_-C_+^*(-S_1^+S_2^+)+h.c.\\
&=-(C_x-iC_y)(C_x^*-iC_y^*)(S_1^x+iS_1^y)(S_2^x+iS_2^y)+h.c.\\
&=-[(C_xC_x^*-C_yC_y^*)-i(C_yC_x^*+C_xC_y^*)][(S_1^xS_2^x-S_1^yS_2^y)+i(S_1^xS_2^y+S_1^yS_2^x)]+h.c.\\
&=-2(C_xC_x^*-C_yC_y^*)(S_1^xS_2^x-S_1^yS_2^y)-2(C_yC_x^*+C_xC_y^*)(S_1^xS_2^y+S_1^yS_2^x)\\
&=-2(|C_x|^2-|C_y|^2)S_1^xS_2^x-2(-|C_x|^2+|C_y|^2)S_1^yS_2^y-2(C_yC_x^*+C_xC_y^*)(S_1^xS_2^y+S_1^yS_2^x)
\end{aligned}
\tag{29}
$$

因此，$|\boldsymbol{C}|^2$ 项化简结果为，

$$
\begin{aligned}
\widehat{h}_{\mathrm{M}}^{(C2)} &= 2|C_z|^2 S_1^x S_2^x + 2|C_z|^2 S_1^y S_2^y - 2|C_z|^2 S_1^z S_2^z \\
&+ 2(|C_x|^2 + |C_y|^2) S_1^z S_2^z - i(C_x C_y^* - C_y C_x^*)(S_1^z + S_2^z) \\
&+ -i(C_z C_x^* - C_z^* C_x)(S_1^y + S_2^y) - 2(C_z C_x^* + C_z^* C_x)(S_1^x S_2^z + S_1^z S_2^x) \\
&+ -i(C_y C_z^* - C_z C_y^*)(S_1^x + S_2^x) - 2(C_y C_z^* + C_z C_y^*)(S_1^y S_2^z + S_1^z S_2^y) \\
&+ -2(|C_x|^2 - |C_y|^2) S_1^x S_2^x - 2(-|C_x|^2 + |C_y|^2) S_1^y S_2^y - 2(C_y C_x^* + C_x C_y^*)(S_1^x S_2^y + S_1^y S_2^x) \\
&= -2(+|C_x|^2 - |C_y|^2 - C_z|^2) S_1^x S_2^x \\
&+ -2(-|C_x|^2 + |C_y|^2 - |C_z|^2) S_1^y S_2^y \\
&+ -2(-|C_x|^2 - |C_y|^2 + |C_z|^2) S_1^z S_2^z \\
&+ -2(C_z C_x^* + C_z^* C_x)(S_1^z S_2^x + S_1^x S_2^z) \\
&+ -2(C_y C_z^* + C_z C_y^*)(S_1^y S_2^z + S_1^z S_2^y) \\
&+ -2(C_y C_x^* + C_x C_y^*)(S_1^x S_2^y + S_1^y S_2^x) \\
&+ -i(C_x C_y^* - C_y C_x^*)(S_1^z + S_2^z) \\
&+ -i(C_z C_x^* - C_z^* C_x)(S_1^y + S_2^y) \\
&+ -i(C_y C_z^* - C_z C_y^*)(S_1^x + S_2^x) \\
&= \begin{pmatrix} S_1^x \\ S_1^y \\ S_1^z \end{pmatrix} \gamma (S_2^x, S_2^y, S_2^z) - i(\boldsymbol{C} \times \boldsymbol{C}^*) \cdot (\boldsymbol{S}_1 + \boldsymbol{S}_2) \\
&= \boldsymbol{S}_1 \cdot \gamma \cdot \boldsymbol{S}_2 - i(\boldsymbol{C} \times \boldsymbol{C}^*) \cdot (\boldsymbol{S}_1 + \boldsymbol{S}_2)
\end{aligned} \tag{30}
$$

其中，

$$\gamma = -2(\boldsymbol{C} \otimes \boldsymbol{C}^* + \boldsymbol{C}^* \otimes \boldsymbol{C} - \mathbb{I}\boldsymbol{C} \cdot \boldsymbol{C}^*) \tag{31}$$

注意到，

$$\gamma^\dagger = \gamma^* = \gamma \tag{32}$$

2.3.6 结果合并

因此，

$$
\begin{aligned}
t^\dagger t = \widehat{h}_{\mathrm{M}} &= \widehat{h}_{\mathrm{M}}^{(b2)} + \widehat{h}_{\mathrm{M}}^{(bC)} + \widehat{h}_{\mathrm{M}}^{(C2)} \\
&= -2|b|^2 \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \\
&+ (b\boldsymbol{C}^* + b^*\boldsymbol{C})(\boldsymbol{S}_1 - \boldsymbol{S}_2) + 2i(b\boldsymbol{C}^* + b^*\boldsymbol{C}) \cdot (\boldsymbol{S}_1 \times \boldsymbol{S}_2) \\
&+ \boldsymbol{S}_1 \cdot \gamma \cdot \boldsymbol{S}_2 - i(\boldsymbol{C} \times \boldsymbol{C}^*) \cdot (\boldsymbol{S}_1 + \boldsymbol{S}_2)
\end{aligned} \tag{33}
$$

于是, [8]

$$
\begin{aligned}
\widehat{H}_{\mathrm{M}} &= -\frac{1}{U}\widehat{T}^\dagger\widehat{T} \\
&= -\frac{1}{U}(t^\dagger t + tt^\dagger) \\
&= -\frac{1}{U}[t^\dagger t + (1 \Leftrightarrow 2)] \\
&= -\frac{1}{U}[-2|b|^2\boldsymbol{S}_1\cdot\boldsymbol{S}_2 - 2|b|^2\boldsymbol{S}_2\cdot\boldsymbol{S}_1 \\
&\qquad + (b\boldsymbol{C}^* + b^*\boldsymbol{C})(\boldsymbol{S}_1 - \boldsymbol{S}_2) + 2i(b\boldsymbol{C}^* - b^*\boldsymbol{C})\cdot(\boldsymbol{S}_1\times\boldsymbol{S}_2) \\
&\qquad + (b^*\boldsymbol{C} + b\boldsymbol{C}^*)(\boldsymbol{S}_2 - \boldsymbol{S}_1) + 2i(b^*\boldsymbol{C} - b\boldsymbol{C}^*)\cdot(\boldsymbol{S}_2\times\boldsymbol{S}_1) \\
&\qquad + \boldsymbol{S}_1\cdot\gamma\cdot\boldsymbol{S}_2 - i(\boldsymbol{C}\times\boldsymbol{C}^*)\cdot(\boldsymbol{S}_1 + \boldsymbol{S}_2) \\
&\qquad + \boldsymbol{S}_2\cdot\gamma^*\cdot\boldsymbol{S}_1 - i(\boldsymbol{C}^*\times\boldsymbol{C})\cdot(\boldsymbol{S}_2 + \boldsymbol{S}_1)] \\
&= \frac{4|b|^2}{U}\boldsymbol{S}_1\cdot\boldsymbol{S}_2 + \frac{4i}{U}(b^*\boldsymbol{C} - b\boldsymbol{C}^*)\cdot(\boldsymbol{S}_1\times\boldsymbol{S}_2) + \boldsymbol{S}_1\cdot\frac{-2\gamma}{U}\cdot\boldsymbol{S}_2
\end{aligned}
\tag{34}
$$

2.4 推导结果

于是, 我们最终得到

$$\widehat{H}_{\mathrm{M}} = J\boldsymbol{S}_1\cdot\boldsymbol{S}_2 + \boldsymbol{D}\cdot(\boldsymbol{S}_1\times\boldsymbol{S}_2) + \boldsymbol{S}_1\cdot\Gamma\cdot\boldsymbol{S}_2 \tag{35a}$$

$$J = \frac{4|b|^2}{U} \tag{35b}$$

$$\boldsymbol{D} = \frac{4i}{U}(b^*\boldsymbol{C} - b\boldsymbol{C}^*) \tag{35c}$$

$$\Gamma = \frac{4}{U}(\boldsymbol{C}\otimes\boldsymbol{C}^* + \boldsymbol{C}^*\otimes\boldsymbol{C} - \mathbb{I}\boldsymbol{C}\cdot\boldsymbol{C}^*) \tag{35d}$$

其中, b 为 $b_{n'n}(\boldsymbol{R}'-\boldsymbol{R})$ 的简化标记, $\boldsymbol{C}$ 为 $\boldsymbol{C}_{n'n}(\boldsymbol{R}'-\boldsymbol{R})$ 的简化标记, $\boldsymbol{S}_1$ 为 $\boldsymbol{S}_n(\boldsymbol{R})$ 的简化标记, $\boldsymbol{S}_2$ 为 $\boldsymbol{S}_{n'}(\boldsymbol{R}')$ 的简化标记. $\mathbb{I}$ 为单位矩阵.

该结果与文献仅在各向同性交换相互作用 J 上差 2 倍,[9] 初步估计该处应是原文有 typo.

[8] $\boldsymbol{S}_2\cdot\gamma^*\cdot\boldsymbol{S}_1 = \boldsymbol{S}_1\cdot\gamma^\dagger\cdot\boldsymbol{S}_2 = \boldsymbol{S}_1\cdot\gamma\cdot\boldsymbol{S}_2$

[9] Moriya, T., Anisotropic superexchange interaction and weak ferromagnetism. Phys. Rev. **120**, 91.(1960)