$$T = \cancel{\alpha\alpha\alpha} \; (b+C_z)[\alpha_{2\uparrow}^\dagger \alpha_{1\uparrow}] + (b-C_z)\,\alpha_{2\downarrow}^\dagger \alpha_{1\downarrow} + C^-\alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} + C^+\alpha_{2\downarrow}^\dagger \alpha_{1\uparrow}$$

$$T^\dagger = (b^*+C_z^*)\,\alpha_{1\uparrow}^\dagger \alpha_{2\uparrow} + (b^*-C_z^*)\,\alpha_{1\downarrow}^\dagger \alpha_{2\downarrow} + C^{-*}\,\alpha_{1\downarrow}^\dagger \alpha_{2\uparrow} + C^{+*}\,\alpha_{1\uparrow}^\dagger \alpha_{2\downarrow}$$

$$T^\dagger T = (b^*+C_z^*)(b+C_z)\,\alpha_{1\uparrow}^\dagger \alpha_{2\uparrow}\,\alpha_{2\uparrow}^\dagger \alpha_{1\uparrow} + (b^*+C_z^*)\,\alpha_{1\uparrow}^\dagger \alpha_{2\uparrow}\,(b-C_z)\,\alpha_{2\downarrow}^\dagger \alpha_{1\downarrow}$$

$$(b^*+C_z^*)\,C_-\,\cancel{\alpha_{2\uparrow}^\dagger\alpha_{2\uparrow}}\,\alpha_{1\uparrow}^\dagger \alpha_{2\uparrow}\,\alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} + (b^*+C_z^*)\,C_+\,\alpha_{1\uparrow}^\dagger \alpha_{2\uparrow}\,\alpha_{2\downarrow}^\dagger \alpha_{1\uparrow}$$

$$(b^*-C_z^*)(b+C_z)\,\alpha_{1\downarrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\uparrow}^\dagger \alpha_{1\uparrow} + (b^*-C_z^*)(b-C_z)\,\alpha_{1\downarrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\downarrow}^\dagger \alpha_{1\downarrow}$$

$$(b^*-C_z^*)\,C^-\,\alpha_{1\downarrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} + (b^*-C_z^*)\,C_+\,\alpha_{1\downarrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\downarrow}^\dagger \alpha_{1\uparrow}$$

$$C_-^*\,\alpha_{1\downarrow}^\dagger \alpha_{2\uparrow}\,(b+C_z)\,(\alpha_{2\uparrow}^\dagger \alpha_{1\uparrow}) + C_-^*\,(b-C_z)\,\alpha_{1\downarrow}^\dagger \alpha_{2\uparrow}\,\alpha_{2\downarrow}^\dagger \alpha_{1\downarrow}$$

$$C_-^*\,\alpha_{1\downarrow}^\dagger \alpha_{2\uparrow}\,C_-\,\alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} + C_-^*\,C_+\,\alpha_{1\downarrow}^\dagger \alpha_{2\uparrow}\,\alpha_{2\downarrow}^\dagger \alpha_{1\uparrow}$$

$$C_+^*\,(b+C_z)\,\alpha_{1\uparrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\uparrow}^\dagger \alpha_{1\uparrow} + C_+^*\,(b-C_z)\,\alpha_{1\uparrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\downarrow}^\dagger \alpha_{1\downarrow}$$

$$C_+^*\,C_-^*\,\alpha_{1\uparrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\uparrow}^\dagger \alpha_{1\downarrow} + C_+^*\,C_+\,\alpha_{1\uparrow}^\dagger \alpha_{2\downarrow}\,\alpha_{2\downarrow}^\dagger \alpha_{1\uparrow}$$

$$\cancel{b}\,(|b|^2+|C_z|^2+C_z^* b + b^* C_z)\,\cancel{n_{1\uparrow}\,n_{2\downarrow}}$$

$$(|b|^2-|C_z|^2-b^* C_z + C_z^* b^*)\,\cancel{S_1^+(1-S_2^-)}$$

$$(b^*+C_z^*)\,C_-$$

$$\cancel{S_1^+ n_{2\downarrow}}$$

$$(b^*+C_z^*)\,C_+$$

$+ |C_z|^2 + C_z^* b + b^* C_z)$ $\cdot$ $n_{1\uparrow} n_{2\downarrow}$

$\pm |C_z|^2 - b^* C_z + C_z^* b)$ $\cdot$ $- S_1^+ \; \cancel{\;\;} \; S_2^-)$

$C_- + C_z^* C_-$ $S_1^+ n_{2\downarrow}$

$C_+ + C_z^* C_+$ $- n_{1\uparrow} S_2^-$

$|^2 - |C_z|^2 - C_z^* b + b^* C_z)$ $\cdot$ $- S_1^- S_2^+$

$^* C_+ - C_z^* C_+$ $\cdot$ $S_1^- n_{2\uparrow}$

$_-^* b + C_-^* C_z$ $S_1^- n_{2\downarrow}$

$^* b - C_-^* C_z$ $\cdot$ $- n_{1\downarrow} S_2^-$

$|C_-|^2$ $\cdot$ $n_{1\downarrow} n_{2\downarrow}$

$C_-^* C_+$ $\cdot$ $- S_1^- S_2^-$

$C_+^* b + C_+^* C_z$ $\cdot$ $- n_{1\uparrow} S_2^+$

$C_+^* b - C_+^* C_z$ $\cdot$ $S_1^+ n_{2\uparrow}$

$C_+^* C_-$ $\cdot$ $- S_1^+ S_2^+$

$|C_+|^2$ $\cdot$ $n_{1\uparrow} n_{2\uparrow}$

$b|^2 + |C_z|^2 - b^* C_z - b C_z^*$ $\cdot$ $n_{1\downarrow} n_{2\uparrow}$

$b^* C_- - C_z^* C_-$ $\cdot$ $- n_{1\downarrow} S_2^+$

$$S_1^+ = S_x + i S_y$$
$$S_1^- = S_1^x - i S_1^y$$

~~$$~~

$$2 S_z = \tfrac{1}{2}(n_\uparrow - n_\downarrow) \cdot$$
$$1 = n_\uparrow + n_\downarrow \cdot$$
$$n_\uparrow = S_z + \tfrac{1}{2}$$
$$n_\downarrow = \tfrac{1}{2} - S_z$$

$(1) b^2$

$$n_{1\uparrow} n_{2\downarrow} + n_{1\downarrow} n_{2\uparrow} - S_1^+ S_2^- - S_1^- S_2^+$$

$$= n_{1\uparrow} n_{2\downarrow} + n_{1\downarrow} n_{2\uparrow} + 2 S_1^z S_2^z - 2\left(S_1^z S_2^z + S_1^x S_2^x + S_1^y S_2^y \right)$$

$$= n_{1\uparrow} n_{2\downarrow} + n_{1\downarrow} n_{2\uparrow} + 2 \cdot \tfrac{1}{2}(n_{1\uparrow} - n_{1\downarrow}) \tfrac{1}{2}(n_{2\uparrow} - n_{2\downarrow}) - 2 \vec{S}_1 \cdot \vec{S}_2$$

$$= \tfrac{1}{2}(n_{1\uparrow} + n_{1\downarrow})(n_{2\uparrow} + n_{2\downarrow}) - 2 \vec{S}_1 \cdot \vec{S}_2$$

$$= \tfrac{1}{2} - 2 \vec{S}_1 \cdot \vec{S}_2$$

$$-2 \vec{S}_1 \cdot \vec{S}_2 \qquad \otimes \; H_m^{(1)} = - \frac{2|b|^2}{V} \vec{S}_1 \cdot \vec{S}_2 \quad \checkmark \qquad\qquad S_1^x S_2^x$$
$$S_1^x$$

$C_z^* b + C_z \quad (2) \; bC$

$$\left(b C_z^* + b^* C_z \right) \cdot \left(n_{1\uparrow} n_{2\downarrow} - n_{1\downarrow} n_{2\uparrow} \right) + \left(b^* C_z - b C_z^* \right) \left(S_1^+ S_2^- - S_1^- S_2^+ \right)$$

$$\left(b C_z^* + b^* C_z \right) \left(n_{1\uparrow} - n_{2\uparrow} \right) + \left(b^* C_z - b C_z^* \right) \left[(S_{1x} + i S_{1y})(S_{2x} - i S_{2y}) - (S_{1x} - i S_{1y})(S_{2x} + i S_{2y}) \right]$$

$$= \left(b C_z^* + b^* C_z \right) \left(n_{1\uparrow} - n_{2\uparrow} \right) + \underline{\left(b^* C_z - b C_z^* \right) (-2i)(S_{1x} S_{2y} - S_{1y} S_{2x})}$$

$$S_{1z} - S_{2z}$$

$$b^* C_- S_1^+ n_{2\downarrow} - b^* C_+ n_{1\uparrow} S_2^- \pm b^* C_+ S_1^- S_{2\uparrow} + b C_-^* S_1^- n_{2\downarrow}$$

$$+ b C_-^*$$

$$b^* C_- C \; (S_1^+ n_{2\downarrow} - n_{1\downarrow} S_2^+) \qquad = \; \left(S_1^+ (2 - S_2) - (2 - S_1^z) S_2^+ \right)$$

$$b^* C_+ C \; (-n_{1\uparrow} S_2^- + S_1^- n_{2\uparrow})$$

$$b C_-^* \; (S_1^- n_{2\downarrow} - n_{1\uparrow} S_2^-) \qquad\qquad b \cdot \vec{C} \cdot \cdot (\vec{S}_1 - \vec{S}_2) + h.c$$

$$b C_+^* \; (-n_{1\uparrow} S_2^+ + S_1^+ n_{2\uparrow})$$

$$\begin{vmatrix} S_1^x S_2^y & S_1^z \\ S_1^x & S_1^y & S_2^z \end{vmatrix}$$

$$b C_z^* [n_{1\uparrow} n_{2\downarrow} - S_1^+ S_2^- + S_1^- S_2^+ - n_{1\downarrow} n_{2\uparrow}]$$ ①

$$b^* C_z [n_{1\uparrow} n_{2\downarrow} + S_1^+ S_2^- - S_1^- S_2^+ - n_{1\downarrow} n_{2\uparrow}]$$

$$b C_-^* [S_1^- n_{2\downarrow} - n_{1\uparrow} S_2^-]$$ ②

$$b^* C_- [S_1^+ n_{2\downarrow} - n_{1\downarrow} S_2^+]$$

$$b C_+^* [-n_{1\uparrow} S_2^+ + S_1^+ n_{2\uparrow}]$$ ③

$$b^* C_+ [-n_{1\uparrow} S_2^- + S_1^- n_{2\uparrow}]$$

$$① = (b C_z^* + b^* C_z) \overbrace{(n_{1\uparrow} n_{2\downarrow} - n_{1\downarrow} n_{2\uparrow})}^{} + (b C_z^* - b^* C_z)(S_1^- S_2^+ - S_1^+ S_2^-)$$

$$= (b C_z^* + b^* C_z)(S_1^z - S_2^z) + (b C_z^* - b^* C_z)[(S_1^x - i S_1^y)(S_2^x + i S_2^y) - (S_1^x + i S_1^y)(S_2^x - i S_2^y)]$$

$$= \cdots + (b C_z^* - b^* C_z)[(S_1^x S_2^x - i S_1^y S_2^x + i S_1^x S_2^y + S_1^y S_2^y) - (S_1^x S_2^x - i S_1^x S_2^y + i S_1^y S_2^x + S_1^y S_2^y)]$$

$$= \cdots + (b C_z^* - b^* C_z) \, 2i (S_1^x S_2^y - S_1^y S_2^x)$$

$$= (b C_z^* + b^* C_z)(S_1^z - S_2^z) + (b C_z^* - b^* C_z) 2i (S_1^x S_2^y - S_1^y S_2^x)$$

$$② \quad b(C_x^* + i C_y^*)[(S_1^x - i S_1^y)(\tfrac{1}{2} - S_2^z) - (\tfrac{1}{2} \mp S_1^z)(S_2^x - i S_2^y)] +$$

$$b^*(C_x - i C_y)[(S_1^x + i S_1^y)(\tfrac{1}{2} - S_2^z) - (\tfrac{1}{2} - S_1^z)(S_2^x + i S_2^y)]$$

$$= b(C_x^* + i C_y^*)[\tfrac{1}{2} S_1^x - \tfrac{i}{2} S_1^y - S_1^x S_2^z + i S_1^y S_2^z - (\tfrac{1}{2} S_2^x - \tfrac{i}{2} S_2^y - S_1^z S_2^x + i S_1^z S_2^y \cdots$$

$$b^*(C_x - i C_y)[\tfrac{1}{2} S_1^x + \tfrac{i}{2} S_1^y - S_1^x S_2^z -$$

$$\textcircled{2} = b(C_x^* + iC_y^*)\left[(S_1^x - iS_1^y)(\tfrac{1}{2} - S_2^z) - (\tfrac{1}{2} - S_1^z)(S_2^x - iS_2^y)\right] + h.c.$$

$$+ b(C_x^* - iC_y^*)\left[(S_1^x + iS_1^y)(\tfrac{1}{2} + S_2^z) - (\tfrac{1}{2} + S_1^z)(S_2^x + iS_2^y)\right] + h.c.$$

$$= b(C_x^* + iC_y^*)\left[\tfrac{1}{2}S_1^x - \tfrac{i}{2}S_1^y - S_1^x S_2^z + iS_1^y S_2^z - (\tfrac{1}{2}S_2^x - \tfrac{i}{2}S_2^y - S_1^z S_2^x + iS_1^z S_2^y)\right]$$

$$= b(C_x^* + iC_y^*)\left(\tfrac{1}{2}(S_1^x - S_2^x) - \tfrac{i}{2}(S_1^y - S_2^y) + (S_1^z S_2^x - S_1^x S_2^z) + i(S_1^y S_2^z - S_1^z S_2^y)\right)$$

$$+ b(C_x^* - iC_y^*)\left(\tfrac{1}{2}(S_1^x - S_2^x) + \tfrac{i}{2}(S_1^y - S_2^y) + (S_1^x S_2^z - S_1^z S_2^x) + i(S_1^y S_2^z - S_1^z S_2^y)\right)$$

$$= bC_x^*\left((S_1^x - S_2^x) + 2i(S_1^y S_2^z - S_1^z S_2^y)\right) + iC_y^* b\left(-i(S_1^y - S_2^y) + 2(S_1^z S_2^x - S_1^x S_2^z)\right)$$
$$+ h.c.$$

$$= \cancel{bC_x^* \Xi}$$

$$= (bC_x^* + b^* C_x)(S_1^x - S_2^x) + (bC_x^* - b^* C_x)2i(S_1^y S_2^z - S_1^z S_2^y) +$$

$$(bC_y^* + b^* C_y)(S_1^y - S_2^y) + (bC_x^* - b^* C_x)2i(S_1^z S_2^x - S_1^x S_2^z)$$

$$\textcircled{1} + \textcircled{2} + \textcircled{3} = (b\vec{C}^* + b^*\vec{C})(\vec{S}_1 - \vec{S}_2) + 2i(b\vec{C}^* - b^*\vec{C})\,\vec{S}_1 \times \vec{S}_2$$

$$\textcircled{1} + \textcircled{2} + \textcircled{3} + (1 \leftrightarrow 2) = 0 + 4i(b\vec{C}^* - b^*\vec{C})\cdot(\vec{S}_1 \times \vec{S}_2)$$

$$C^2$$

$$|C_z|^2 \left(n_{1\uparrow} n_{2\downarrow} + S_1^+ S_2^- + S_1^- S_2^+ + n_{1\downarrow} n_{2\uparrow} \right) + \quad ①$$

$$\left. \begin{array}{l} C_z^* C_- \left[S_1^+ n_{2\downarrow} + n_{1\downarrow} S_2^+ \right] \\ C_z C_-^* \left[S_1^- n_{2\downarrow} + n_{1\uparrow} S_2^- \right] \end{array} \right] ⊕$$

$$\left. \begin{array}{l} C_z^* C_+ \left[-n_{1\uparrow} S_2^- - S_1^- n_{2\uparrow} \right] \\ C_z C_+^* \left[-n_{1\uparrow} S_2^+ - S_1^+ n_{2\uparrow} \right] \end{array} \right] \triangle$$

$$|C_-|^2 \, n_{1\downarrow} n_{2\downarrow} \quad ②$$

$$\left. \begin{array}{l} C_-^* C_+ \left[-S_1^- S_2^- \right] \\ C_- C_+^* \left[-S_1^+ S_2^+ \right] \end{array} \right] ⊠$$

$$|C_+|^2 \, n_{1\uparrow} n_{2\uparrow} \quad ③$$

$$① = |C_z|^2 \left(n_{1\downarrow} n_{2\uparrow} + n_{1\uparrow} n_{2\downarrow} + S_1^+ S_2^- + S_1^- S_2^+ \right)$$

$$= |C_z|^2 \left(\frac{1}{2} - 2 S_1^z S_2^z + 2 S_1^x S_2^x + 2 S_1^y S_2^y \right)$$

$$= + 2 C_z C_z^* S_1^x S_2^x + 2 C_z C_z^* S_1^y S_2^y - 2 C_z C_z^* S_1^z S_2^z$$

$$②+③ = C_- C_-^* \, n_{1\downarrow} n_{2\downarrow} + C_+ C_+^* \, n_{1\uparrow} n_{2\uparrow}$$

$$= (C_x - iC_y)(C_x^* + iC_y^*) \left(\frac{1}{2} - S_1^z \right) \left(\frac{1}{2} - S_2^z \right) +$$
$$(C_x + iC_y)(C_x^* - iC_y^*) \left(\frac{1}{2} + S_1^z \right) \left(\frac{1}{2} + S_2^z \right)$$

$$= \left(C_x C_x^* + i C_x C_y^* - i C_x^* C_y + C_y C_y^* \right) \left(\frac{1}{4} - \frac{1}{2} S_1^z - \frac{1}{2} S_2^z + S_1^z S_2^z \right)$$
$$\left(C_x C_x^* - i C_x C_y^* + i C_x^* C_y + C_y C_y^* \right) \left(\frac{1}{4} + \frac{1}{2} S_1^z + \frac{1}{2} S_2^z + S_1^z S_2^z \right)$$

$$= (C_x C_x^* + C_y C_y^*) \left[\frac{1}{2} + 2 S_1^z S_2^z \right] +$$
$$i (C_x C_y^* - C_x^* C_y) \left[- S_1^z - S_2^z \right]$$

$$= (C_x C_x^* + C_y C_y^*) \frac{1}{2} 2 S_1^z S_2^z \mp i (C_x C_y^* - C_y C_x^*)(S_1^z + S_2^z)$$

$$+① +③ = 2 C_z C_z^* S_1^x S_2^x + 2 C_z C_z^* S_1^y S_2^y - 2 C_z C_z^* S_1^z S_2^z + 2(C_x C_x^* + C_y C_y^*) 2 S_1^z S_2^z$$
$$- i (C_x C_y^* - C_y C_x^*)(S_1^z + S_2^z)$$

$$= 2 |C_z|^2 \underset{xy}{S_1^x S_2^x} + 2 |C_z|^2 \underset{xy}{S_1^y S_2^y} + 2 [2(|C_x|^2 + |C_y|^2 - |C_z|^2] \underset{zz}{S_1^z S_2^z} \cdot$$
$$- i (C_x C_y^* - C_y C_x^*)(S_1^z + S_2^z)$$

$$④ + △ = C_z^* (C_x - i C_y)[(S_1^x + i S_1^y)(\tfrac{1}{2} - S_2^z) + (\tfrac{1}{2} - S_1^z)(S_2^x + i S_2^y)] + h.C. +$$
$$C_z^* (C_x + i C_y)[-(S_1^x - i S_1^y)(\tfrac{1}{2} + S_2^z) - (\tfrac{1}{2} + S_1^z)(S_2^x - i S_2^y)] + h.C.$$

$$\tfrac{1}{2} S_1^x + \tfrac{i}{2} S_1^y - S_1^x S_2^z - i S_1^y S_2^z + \tfrac{1}{2} S_2^x + \tfrac{i}{2} S_2^y - S_1^z S_2^x - i S_1^z S_2^y$$
$$-\tfrac{1}{2} S_1^x + \tfrac{i}{2} S_1^y - S_1^x S_2^z + i S_1^y S_2^z - \tfrac{1}{2} S_2^x + \tfrac{i}{2} S_2^y - S_1^z S_2^x + i S_1^z S_2^y$$

$$= C_z^* C_x [i (S_1^y + S_2^y) - 2(S_1^x S_2^z + S_1^z S_2^x)] +$$
$$C_z^* i C_y [-(S_1^x + S_2^x) + 2i(S_1^y S_2^z + S_1^z S_2^y)] + h.C$$

$$-i C_z^* C_x = i (C_z^* C_x - C_x^* C_z)(S_1^y + S_2^y) - 2(C_z^* C_x + C_x^* C_z)(S_1^x S_2^z + S_1^z S_2^x)$$
$$-i (C_y C_z^* - C_z C_y^*)(S_1^x + S_2^x) - 2(\underset{yz}{C_y C_z^*} + \underset{zy}{C_z C_y^*})(S_1^y S_2^z + S_1^z S_2^y)$$

$$\boxed{×} = C_-^* C_+ (-S_1^- S_2^-) + C_+ C_-^* h.C.$$

$$= -(C_x^* + i C_y^*)(C_x + i C_y)(S_1^x - i S_1^y)(S_2^x - i S_2^y)$$

$$= -[(C_x^* C_x - C_y^* C_y) + i(C_x^* C_y + C_x C_y^*)][(S_1^x S_2^x - S_1^y S_2^y) - i(S_1^y S_2^x + S_1^x S_2^y)]$$

$$= -[2(C_x^* C_x - C_y^* C_y)(\underset{xx}{S_1^x S_2^x} - \underset{yy}{S_1^y S_2^y}) + 2(C_x^* C_y + C_x C_y^*)(\underset{xy}{S_1^y S_2^x} + \underset{xy}{S_1^x S_2^y})] \quad +h.C.$$

$$= 2(C_x^* C_x - C_y^* C_y)$$

$$All = 2\{ (-|C_x|^2 + |C_y|^2 + |C_z|^2) S_1^x S_2^x + (|C_x|^2 - |C_y|^2 + |C_z|^2) S_1^y S_2^y + (|C_x|^2 + |C_y|^2 - |C_z|^2) $$
$$S_1^z S_2^z$$

$$- \sum_{i \neq j = x,y,z} (C_i^* C_j + C_j^* C_i)(S_1^i S_2^j + S_1^j S_2^i) \} - i (\vec{C} \times \vec{C}^*) \cdot (\vec{S}_1 + \vec{S}_2)$$

$$All + (1 \leftrightarrow 2) = -4(C \otimes C^* + C^* \otimes C - (C \cdot C^*) \vec{1}) \frac{\vec{S}_1}{|c|}$$

$$\therefore \hat{H}_M = +\frac{4|b|^2}{U}\vec{S}_1\cdot\vec{S}_2 + \frac{4i}{U}(b\vec{c}^*-b^*\vec{c})(\vec{S}_1\times\vec{S}_2) + \frac{4}{U}[\vec{c}\otimes\vec{c}^*+\vec{c}^*\otimes\vec{c} - (\vec{c}\cdot\vec{c})\cdot\vec{\vec{I}}]\begin{vmatrix}\vec{S}_2\\\vec{S}_1\end{vmatrix}$$

与原文整体差少个负号,

该结果应该是正确的,

因为 $+\frac{4t^2}{U}$ 可从 ~~Heis~~ Hubbard 模型推出.

原文中 $+\frac{2|b|^2}{U}$ 显然不对.