2016/11/10 (목)

mean-field decoupling of Hubbard interaction.

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow} \rightarrow -U \sum_i \left(2 \langle \vec{S}_i \rangle \cdot \vec{S}_i - \langle \vec{S}_i \rangle^2 \right)$$

where $\vec{S}_i = \sum_{\sigma,\sigma'} \frac{C^\dagger_{i\sigma} \vec{\sigma}_{\sigma\sigma'} C_{i\sigma'}}{2}$

$$= -U \sum_i \Big(2 \langle S_i^x \rangle S_i^x + 2 \langle S_i^y \rangle S_i^y + 2 \langle S_i^z \rangle S_i^z$$

$$- \langle S_i^x \rangle \langle S_i^x \rangle - \langle S_i^y \rangle \langle S_i^y \rangle - \langle S_i^z \rangle \langle S_i^z \rangle \Big)$$

$$= -U \sum_i \Big(\langle S_i^x \rangle \sum_{\sigma\sigma'} C^\dagger_{i\sigma} \sigma^x_{\sigma\sigma'} C_{i\sigma'} + \langle S_i^y \rangle \sum_{\sigma\sigma'} C^\dagger_{i\sigma} \sigma^y_{\sigma\sigma'} C_{i\sigma'}$$

$$+ \langle S_i^z \rangle \sum_{\sigma\sigma'} C^\dagger_{i\sigma} \sigma^z_{\sigma\sigma'} C_{i\sigma'} - \langle S_i^x \rangle \langle S_i^x \rangle - \langle S_i^y \rangle \langle S_i^y \rangle - \langle S_i^z \rangle \langle S_i^z \rangle \Big)$$

$$= -U \sum_i$$

$$\begin{pmatrix} C^\dagger_{i\uparrow} & C^\dagger_{i\downarrow} \end{pmatrix} \begin{pmatrix} \langle S_i^z \rangle - \langle S_i^x \rangle^2 - \langle S_i^y \rangle^2 - \langle S_i^z \rangle^2 & \langle S_i^x \rangle - i \langle S_i^y \rangle \\ \langle S_i^x \rangle + i \langle S_i^y \rangle & -\langle S_i^z \rangle - \langle S_i^x \rangle^2 - \langle S_i^y \rangle^2 - \langle S_i^z \rangle^2 \end{pmatrix}.$$

$$\times \begin{pmatrix} C_{i\uparrow} \\ C_{i\downarrow} \end{pmatrix}$$