Hartree-Fock approximation: triangular Hubbard model at half filling ($n = 1$)

1 Mean-field Hamiltonian

$$
\begin{aligned}
H &= -t \sum_{\langle ij\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} && (1)\\
&\downarrow \\
H_{\mathrm{MF}} &= \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} \\
&\quad + U \sum_i \left[\langle n_{i,\uparrow}\rangle n_{i,\downarrow} + \langle n_{i,\downarrow}\rangle n_{i,\uparrow} \right] \\
&\quad - U \sum_i \left[\left\langle c^\dagger_{i,\uparrow} c_{i,\downarrow} \right\rangle c^\dagger_{i,\downarrow} c_{i,\uparrow} + \left\langle c^\dagger_{i,\downarrow} c_{i,\uparrow} \right\rangle c^\dagger_{i,\uparrow} c_{i,\downarrow} \right] \\
&\quad + \mathrm{const.} && (2)\\
\mathrm{const.} &= -U \sum_i \langle n_{i,\uparrow}\rangle \langle n_{i,\downarrow}\rangle \\
&\quad + U \sum_i \left\langle c^\dagger_{i,\uparrow} c_{i,\downarrow} \right\rangle \left\langle c^\dagger_{i,\downarrow} c_{i,\uparrow} \right\rangle && (3)\\
\epsilon_k &= -2t \left[\cos k_x + \cos k_y + \cos(k_x + k_y) \right] && (4)
\end{aligned}
$$

2 Order parameter

Assuming the 120° Neel state

$$
\begin{aligned}
\langle S^x_i \rangle &= m \,\mathrm{Re}\, e^{iQR_i} && (5)\\
\langle S^y_i \rangle &= m \,\mathrm{Im}\, e^{iQR_i} && (6)\\
\langle S^z_i \rangle &= 0 && (7)\\
Q &= (2\pi/3, 2\pi/3), && (8)
\end{aligned}
$$

we obtain

$$
\begin{aligned}
\langle n_{i,\uparrow} \rangle &= \langle n_{i,\downarrow} \rangle = n && (9)\\
\left\langle c^\dagger_{i,\uparrow} c_{i,\downarrow} \right\rangle &= \left\langle S^+_i \right\rangle = \langle S^x_i \rangle + i \langle S^y_i \rangle = m\, e^{iQR_i} && (10)\\
\left\langle c^\dagger_{i,\downarrow} c_{i,\uparrow} \right\rangle &= \left\langle S^-_i \right\rangle = \left\langle S^+_i \right\rangle^* && (11)
\end{aligned}
$$

3 Hamiltonian to be diagonalized

$$
\begin{aligned}
H_{\mathrm{MF}} &= \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} \\
&\quad + Un \sum_i \left(n_{i,\downarrow} + n_{i,\uparrow}\right) \\
&\quad - Um \sum_i \left(e^{iQR_i} c^\dagger_{i,\downarrow} c_{i,\uparrow} + e^{-iQR_i} c^\dagger_{i,\uparrow} c_{i,\downarrow} \right) \\
&\quad + \text{const.} \\
&= \sum_{k,\sigma} \left(\epsilon_k + Un\right) c^\dagger_{k,\sigma} c_{k,\sigma} \\
&\quad - Um \sum_k \left(c^\dagger_{k,\downarrow} c_{k-Q,\uparrow} + c^\dagger_{k,\uparrow} c_{k+Q,\downarrow} \right) \\
&\quad + \text{const.} \\
&= \sum_{k,\sigma}^{\mathrm{RBZ}} \begin{pmatrix} c^\dagger_{k,\uparrow} & c^\dagger_{k+Q,\uparrow} & c^\dagger_{k+2Q,\uparrow} & c^\dagger_{k,\downarrow} & c^\dagger_{k+Q,\downarrow} & c^\dagger_{k+2Q,\downarrow} \end{pmatrix} \\
&\quad \left(\begin{array}{ccc|ccc}
\tilde{\epsilon}_k & & & & \Delta & \\
& \tilde{\epsilon}_{k+Q} & & & & \Delta \\
& & \tilde{\epsilon}_{k+2Q} & \Delta & & \\
\hline
& & \Delta & \tilde{\epsilon}_k & & \\
\Delta & & & & \tilde{\epsilon}_{k+Q} & \\
& \Delta & & & & \tilde{\epsilon}_{k+2Q}
\end{array}\right)
\begin{pmatrix} c_{k,\uparrow} \\ c_{k+Q,\uparrow} \\ c_{k+2Q,\uparrow} \\ c_{k,\downarrow} \\ c_{k+Q,\downarrow} \\ c_{k+2Q,\downarrow} \end{pmatrix} \\
&\quad + \text{const.}
\end{aligned} \tag{12}
$$

Here,

$$\tilde{\epsilon}_k = \epsilon_k + Un \tag{13}$$

$$\Delta = -Um \tag{14}$$

$$\text{const.} = -Un^2 N_s + Um^2 N_s \tag{15}$$

The RBZ is given as

$$k_x + k_y < \frac{2\pi}{3},\ k_x + k_y > -\frac{2\pi}{3}, \tag{16}$$

$$k_x - 2k_y < \frac{5\pi}{3},\ k_x - 2k_y > -\frac{5\pi}{3}, \tag{17}$$

$$2k_x - k_y < \frac{5\pi}{3},\ \text{ and }\ 2k_x - k_y > -\frac{5\pi}{3} \tag{18}$$

so that the number of k points is $N_s/3$.

4 Self-consistent equation

$$
\begin{aligned}
n &= \frac{1}{2N_s}\sum_{i,\sigma}\langle n_{i,\sigma}\rangle \\
&= \frac{1}{2N_s}\sum_{k,\sigma}\left\langle c^\dagger_{k,\sigma}c_{k,\sigma}\right\rangle \\
&= \frac{1}{2N_s}\sum_{k,\sigma}^{\mathrm{RBZ}}\left[\left\langle c^\dagger_{k,\sigma}c_{k,\sigma}\right\rangle + \left\langle c^\dagger_{k+Q,\sigma}c_{k+Q,\sigma}\right\rangle + \left\langle c^\dagger_{k+2Q,\sigma}c_{k+2Q,\sigma}\right\rangle\right] \qquad (19)
\end{aligned}
$$

$$
\begin{aligned}
m &= \frac{1}{2N_s}\sum_{i}\left[\langle S^+_i\rangle e^{-iQR_i} + \langle S^-_i\rangle e^{iQR_i}\right] \\
&= \frac{1}{2N_s}\sum_{k}\left[\left\langle c^\dagger_{k,\uparrow}c_{k+Q,\downarrow}\right\rangle + \left\langle c^\dagger_{k,\downarrow}c_{k-Q,\uparrow}\right\rangle\right] \\
&= \frac{1}{2N_s}\sum_{k}^{\mathrm{RBZ}}\left[\left\langle c^\dagger_{k,\uparrow}c_{k+Q,\downarrow}\right\rangle + \left\langle c^\dagger_{k+Q,\uparrow}c_{k+2Q,\downarrow}\right\rangle + \left\langle c^\dagger_{k+2Q,\uparrow}c_{k,\downarrow}\right\rangle\right. \\
&\quad \left. + \left\langle c^\dagger_{k,\downarrow}c_{k+2Q,\uparrow}\right\rangle + \left\langle c^\dagger_{k+Q,\downarrow}c_{k,\uparrow}\right\rangle + \left\langle c^\dagger_{k+2Q,\downarrow}c_{k+Q,\uparrow}\right\rangle\right] \qquad (20)
\end{aligned}
$$

5 Comparison with the previous result

For $N_s = 6\times 6$ under periodic-periodic boundary condition, we obtain

total energy	-0.4229593004
Coulomb energy	0.3744104588
charge n	0.5
magnetization m	0.4610411632

The energy $E_{\mathrm{tot}}N_s = -15.22653481$ is consistent with the previous mean-field result $E_{\mathrm{tot}}N_s = -15.226$ by Maruyama et al. [J. Phys.: Conf. Ser. **320**, 012061].