

HS

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Equations

The self-consistent gap equation to be solved is given by:

$$\Delta_{s,d} = \frac{1}{N} \sum_k (v_{k1} u_{k3} + v_{k2} u_{k4}) (\cos(k_x) \pm \cos(k_y))$$

Here, u_{k1} and v_{k2} are given by:

$$u_{k1}^2 = v_{k2}^2 = \frac{1}{2} \left[1 + \frac{\omega_\uparrow + \omega_\downarrow}{\sqrt{(\omega_\uparrow + \omega_\downarrow)^2 + 4\nu^2}} \right]$$

And u_{k2} and v_{k1} are given by:

$$u_{k2}^2 = v_{k1}^2 = \frac{1}{2} \left[1 - \frac{\omega_\uparrow + \omega_\downarrow}{\sqrt{(\omega_\uparrow + \omega_\downarrow)^2 + 4\nu^2}} \right]$$

The coefficients u_{k3} , u_{k4} , v_{k3} , and v_{k4} are given by:

$$u_{k3}^2 = v_{k4}^2 = \frac{1}{2} \left[1 + \frac{\omega_\uparrow + \omega_\downarrow}{\sqrt{(\omega_\uparrow + \omega_\downarrow)^2 + 4\nu^2}} \right]$$

$$u_{k4}^2 = v_{k3}^2 = \frac{1}{2} \left[1 - \frac{\omega_\uparrow + \omega_\downarrow}{\sqrt{(\omega_\uparrow + \omega_\downarrow)^2 + 4\nu^2}} \right]$$

where:

$$\omega_\sigma = h_{1\sigma}(k)(\alpha_{k\sigma}^2 - \beta_{k\sigma}^2) - 2h_{2\sigma}(k)\alpha_{k\sigma}\beta_{k\sigma}$$

$$\nu = -h_3(k)(\alpha_{k\uparrow}\beta_{k\downarrow} + \alpha_{k\downarrow}\beta_{k\uparrow})$$

where,

$$\begin{aligned} h_{1\sigma}(k) &= \frac{U - \Delta}{2} \left(\frac{1 + \delta - \sigma m_s}{2} \right) - \frac{t^2}{\Delta} \left[4(1 - 2\delta) + g_{1\sigma}(2\chi_{BB\bar{\sigma}} + 4\chi_{B\bar{x}y\bar{\sigma}}) + g_{1\sigma} \frac{1 - \delta + \sigma m_s}{2} \gamma_k \right] \\ &\quad - \frac{2t^2}{U + \Delta} g_s \sigma m_s + \frac{2t^2}{U + \Delta} (1 - \delta) \end{aligned}$$

$$h_{2\sigma}(k) = \left[-tg_{1\sigma} - \frac{t^2}{\Delta} (-2\chi_{AB\sigma} + 6g_2\chi_{AB\bar{\sigma}}) - \frac{t^2}{U + \Delta} \left[g_s \left(\frac{1}{2} \chi_{AB\sigma} + \chi_{AB\bar{\sigma}} \right) + \frac{1}{2} \chi_{AB\sigma} \right] \right] \gamma_k$$

$$h_3(k) = \left[\frac{4t^2}{\Delta} (1 - g_2) + \frac{4t^2}{U + \Delta} \left(\frac{3g_s}{4} - \frac{1}{4} \right) - \frac{2t^2}{\Delta} (g_{t\downarrow} + g_{t\uparrow}) \right] \frac{\Delta_{AB}}{2} [\cos(k_x) - \cos(k_y)]$$

Here,

$$\gamma_k = 2[\cos(k_x) + \cos(k_y)]$$

$$\gamma'_k = 2[\cos(2k_x) + \cos(2k_y)] + 4[\cos(k_x + k_y) + \cos(k_x - k_y)]$$

This results in,

$$2\alpha_{k\sigma}^2 = [1 - h_{1\sigma}(k)/E_\sigma(k)]$$

$$2\beta_{k\sigma}^2 = [1 + h_{1\sigma}(k)/E_\sigma(k)]$$

with,

$$E_\sigma(k) = \sqrt{h_{1\sigma}(k)^2 + h_{2\sigma}(k)^2}$$

At half-filling, the magnetizations on the A and B sub-lattices are equal and opposite to each other owing to the particle-hole symmetry. Hence, $m_s = (m_A - m_B)/2 = m_A$. Self-consistent equations for the various mean-field order parameters are

$$\begin{aligned} m_s &= \frac{1}{N} \sum_k (\alpha_{k\uparrow}^2 - \alpha_{k\downarrow}^2), \\ \delta &= \frac{1}{2N} \sum_{k\sigma} (\alpha_{k\sigma}^2 - \beta_{k\sigma}^2), \\ \chi_{AB\sigma} &= -\frac{1}{4N} \sum_k \gamma_k \alpha_{k\sigma} \beta_{k\sigma}, \\ \chi_{BB\sigma} &= \frac{1}{N} \sum_k [\cos(2k_x) + \cos(2k_y)] \beta_{k\sigma}^2, \\ \chi_{BBxy\sigma} &= \frac{1}{N} \sum_k 2\beta_{k\sigma}^2 \cos(k_x) \cos(k_y). \end{aligned}$$

Also,

$$\begin{aligned} g_{t\sigma} &= \frac{2\delta}{1 + \delta + \sigma m_s} \\ g_s &= \frac{4}{(1 + \delta)^2 - m_s^2} \\ g_1 &= 1 \\ g_2 &= \frac{4\delta}{(1 + \delta)^2 - m_s^2} \end{aligned}$$

Here σ can be either \uparrow or \downarrow ; depending on the spin up or down respectively