

# Perturbative calculations

Hao Chen

November 27, 2023

The full Hamiltonian is

$$H = H_0 + H_I = \underbrace{\sum_{\mathbf{k}s} \epsilon_{\mathbf{k}} c_{\mathbf{k},s}^\dagger c_{\mathbf{k},s}^{\phantom\dagger} - g \sum_j n_{j\uparrow} n_{j\downarrow}}_{H_0} + \underbrace{\sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)}_{H_I}, \quad (1)$$

where the kinetic energy  $\epsilon_{\mathbf{k}} = -2t[\cos(k_x a) + \cos(k_y a)] - \mu$ , the spin-spin coupling  $D_{ij} = D(\mathbf{z} \times (\mathbf{r}_i - \mathbf{r}_j))$ , and  $\langle ij \rangle$  denotes the nearest-neighbors. We study Eq. (1) on a square lattice and treat  $H_I$  as a perturbation.

Let's first summarize the mean-field results for the unperturbed Hamiltonian  $H_0$ . By condensing the pairing operator  $c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$  and  $c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$ , and diagonalizing the resulting mean-field Hamiltonian, we arrive at

$$H_0 = \sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1}^{\phantom\dagger} + E_{\mathbf{k}} \gamma_{\mathbf{k}2}^\dagger \gamma_{\mathbf{k}2}^{\phantom\dagger} \right\}, \quad (2)$$

where additional constants are ignored, the excitation energy  $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$ , and the Bogoliubov particle ( $\gamma_{\mathbf{k}}, \gamma_{\mathbf{k}}^\dagger$ ) is defined as

$$\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \gamma_{\mathbf{k}1} \\ \gamma_{\mathbf{k}2}^\dagger \end{pmatrix} \quad (3)$$

with coefficients

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right) \quad \text{and} \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right). \quad (4)$$

The gap  $\Delta$  satisfies the following self-consistent equation at  $T = 0$ :

$$\Delta = \frac{g}{2\Omega} \sum_{\mathbf{k}} \frac{\Delta}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}. \quad (5)$$

The ground state  $|g_0\rangle$  of Eq. (2) is the state that gets annihilated by all  $\gamma$  operators:  $\gamma_{\mathbf{k},\sigma} |g_0\rangle = 0, \forall \mathbf{k}, \sigma$ .

The inversion-symmetry-breaking term written in terms of the bare electron creation/annihilation operators is

$$H_I = \frac{iD}{\Omega} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} \sum_{s_1 s_2 s_3 s_4} \left\{ -\sin[q_y a] \left( \frac{\sigma_{s_1 s_2}^y}{2} \frac{\sigma_{s_3, s_4}^z}{2} - \frac{\sigma_{s_1 s_2}^z}{2} \frac{\sigma_{s_3, s_4}^y}{2} \right) \right. \\ \left. + \sin[q_x a] \left( \frac{\sigma_{s_1 s_2}^z}{2} \frac{\sigma_{s_3, s_4}^x}{2} - \frac{\sigma_{s_1 s_2}^x}{2} \frac{\sigma_{s_3, s_4}^z}{2} \right) \right\} c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2}. \quad (6)$$

Analogous to the mean-field treatment, we approximate the quartic term by a sum of quadratic terms:

$$\begin{aligned} c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2} &= \langle c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger \rangle_0 c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2} + c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 s_3}^\dagger \langle c_{\mathbf{k}_2 - \mathbf{q} s_4} c_{\mathbf{k}_1 + \mathbf{q} s_2} \rangle_0 \\ &\quad - \langle c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} \rangle_0 c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} - c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} \langle c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} \rangle_0 \quad (7) \\ &\quad + \langle c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} \rangle_0 c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} + c_{\mathbf{k}_1 s_1}^\dagger c_{\mathbf{k}_1 + \mathbf{q} s_2} \langle c_{\mathbf{k}_2 s_3}^\dagger c_{\mathbf{k}_2 - \mathbf{q} s_4} \rangle_0. \end{aligned}$$

To treat  $H_I$  perturbatively, we evaluate the expectation values using the unperturbed ground state  $|g_0\rangle$ , i.e.,  $\langle \cdot \rangle_0 = \langle g_0 | \cdot | g_0 \rangle$ , instead of determining the expectation values through self-consistent equations. After some algebra work, we obtain the resulting Bogoliubov-de-Gennes (BdG) Hamiltonian

$$H_{\text{BdG}} = \sum_{\mathbf{k}} \frac{1}{2} \begin{pmatrix} \gamma_{\mathbf{k}1}^\dagger & \gamma_{\mathbf{k}2}^\dagger & \gamma_{-\mathbf{k}1} & \gamma_{-\mathbf{k}2} \end{pmatrix} \begin{pmatrix} E_{\mathbf{k}} & A_{\mathbf{k}} & B_{\mathbf{k}} & 0 \\ A_{\mathbf{k}}^* & E_{\mathbf{k}} & 0 & -B_{\mathbf{k}}^* \\ B_{\mathbf{k}}^* & 0 & -E_{\mathbf{k}} & -A_{\mathbf{k}}^* \\ 0 & -B_{\mathbf{k}} & -A_{\mathbf{k}} & -E_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \gamma_{\mathbf{k}1} \\ \gamma_{\mathbf{k}2} \\ \gamma_{-\mathbf{k}1}^\dagger \\ \gamma_{-\mathbf{k}2}^\dagger \end{pmatrix}, \quad (8)$$

where

$$A_{\mathbf{k}} = \frac{D}{\Omega} \sum_{\mathbf{k}'} \left( \sin[(k'_y - k_y)a] + i \sin[(k'_x - k_x)a] \right) u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}, \quad (9)$$

$$B_{\mathbf{k}} = -\frac{D}{\Omega} \sum_{\mathbf{k}'} \left( \sin[(k'_y - k_y)a] + i \sin[(k'_x - k_x)a] \right) v_{\mathbf{k}}^2 u_{\mathbf{k}'} v_{\mathbf{k}'}. \quad (10)$$

The BdG Hamiltonian (8) is diagonalized by introducing the new particle  $(\alpha_{\mathbf{k}\lambda}, \alpha_{\mathbf{k}\lambda}^\dagger)$ :

$$\begin{pmatrix} \gamma_{\mathbf{k}1} \\ \gamma_{\mathbf{k}2} \\ \gamma_{-\mathbf{k}1}^\dagger \\ \gamma_{-\mathbf{k}2}^\dagger \end{pmatrix} = S_{\mathbf{k}} \begin{pmatrix} \alpha_{\mathbf{k}1} \\ \alpha_{\mathbf{k}2} \\ \alpha_{-\mathbf{k}1}^\dagger \\ \alpha_{-\mathbf{k}2}^\dagger \end{pmatrix} \quad (11)$$

with  $S_{\mathbf{k}}$  a unitary  $4 \times 4$  matrix. The diagonalized Hamiltonian is

$$H_{\text{BdG}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}1} \alpha_{\mathbf{k}1}^\dagger \alpha_{\mathbf{k}1} + \omega_{\mathbf{k}2} \alpha_{\mathbf{k}2}^\dagger \alpha_{\mathbf{k}2}, \quad (12)$$

where

$$\omega_{\mathbf{k},1} = \sqrt{|A_{\mathbf{k}}|^2 + |B_{\mathbf{k}}|^2 + E_{\mathbf{k}}^2 - \sqrt{(A_{\mathbf{k}}^* B_{\mathbf{k}} + A_{\mathbf{k}} B_{\mathbf{k}}^*)^2 + 4|A_{\mathbf{k}}|^2 E_{\mathbf{k}}^2}}, \quad (13)$$

$$\omega_{\mathbf{k},2} = \sqrt{|A_{\mathbf{k}}|^2 + |B_{\mathbf{k}}|^2 + E_{\mathbf{k}}^2 + \sqrt{(A_{\mathbf{k}}^* B_{\mathbf{k}} + A_{\mathbf{k}} B_{\mathbf{k}}^*)^2 + 4|A_{\mathbf{k}}|^2 E_{\mathbf{k}}^2}}. \quad (14)$$

The new ground state  $|g\rangle$  is defined as the state that gets annihilated by all  $\alpha_{\mathbf{k}\lambda}$ .

In order to study the pairing structure of the ground state  $|g\rangle$ , we define the order parameter

$$\Phi_{s_1 s_2} = \langle g | c_{-\mathbf{k}s_1} c_{\mathbf{k}s_2} | g \rangle. \quad (15)$$

Note that we use the bare electron operators in the bracket. Figures. 1, 2, 3 show the order parameter  $\Phi_{s_1 s_2}$  for three different choices of the chemical potential  $\mu$  while fixing

$t = 1, g = 2, D = 0.5$ . From Fig. 1(a-d) and Fig. 2(a-d), we observe that odd-parity pairing emerges on top the original even-parity pairing. Furthermore, we can get the perturbation effect on the original s-wave singlet pairing by subtracting  $\langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$  from  $\Phi_{\downarrow\uparrow}$ , and we denote the new quantity as  $\Phi'_{\downarrow\uparrow}$ , as shown in Fig. 1(g-h) and Fig. 2(g-h). The pattern of  $\Phi'_{\downarrow\uparrow}$  implies the additional extended s-wave pairing.

However, surprisingly the non-centrosymmetric perturbation does not alter the pairing structure at half-filling ( $\mu = 0$ ) in our calculations, as shown in Fig. 3. Specifically, at  $\mu = 0$ ,

$$\begin{aligned} A_{\mathbf{k}} &= -\frac{u_{\mathbf{k}} v_{\mathbf{k}} D}{2} \int \frac{d^2 k'}{(2\pi)^2} \frac{\Delta [\cos(k'_y) \sin(k_y) + i \cos(k'_x) \sin(k_x)]}{\sqrt{4t^2(\cos(k'_x) + \cos(k'_y))^2 + \Delta^2}} = 0, \\ B_{\mathbf{k}} &= \frac{v_{\mathbf{k}}^2 D}{2} \int \frac{d^2 k'}{(2\pi)^2} \frac{\Delta [\cos(k'_y) \sin(k_y) + i \cos(k'_x) \sin(k_x)]}{\sqrt{4t^2(\cos(k'_x) + \cos(k'_y))^2 + \Delta^2}} = 0. \end{aligned} \quad (16)$$

Therefore, in our perturbation scheme,  $H_I$  doesn't couple to  $H_0$  at half-filling.

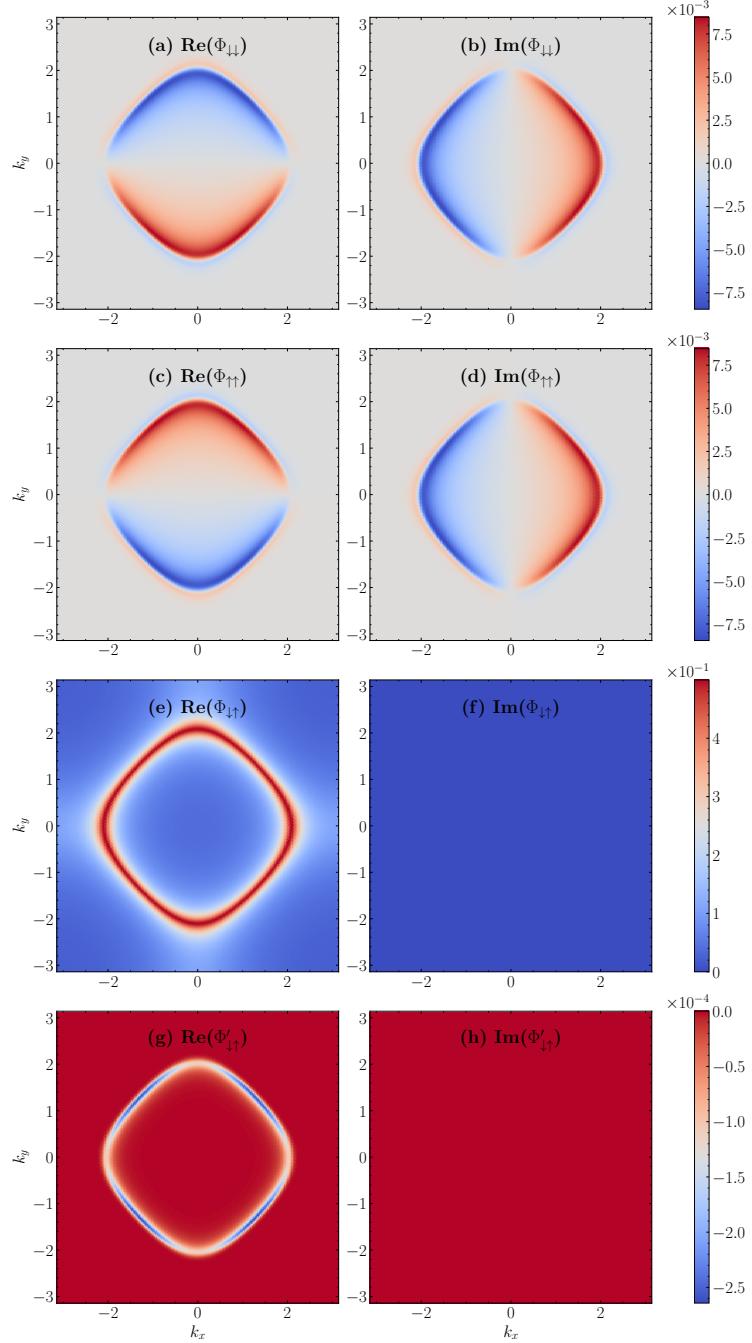


Figure 1: Order parameters  $\Phi_{s_1 s_2}$  at chemical potential  $\mu = -1$ . Other parameters are fixed as  $(t, g, D) = (1, 2, 0.5)$ . The quantity  $\Phi'_{\downarrow\uparrow} = \Phi_{\downarrow\uparrow} - \langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$  characterizes the new singlet pairing structure due to the perturbation.

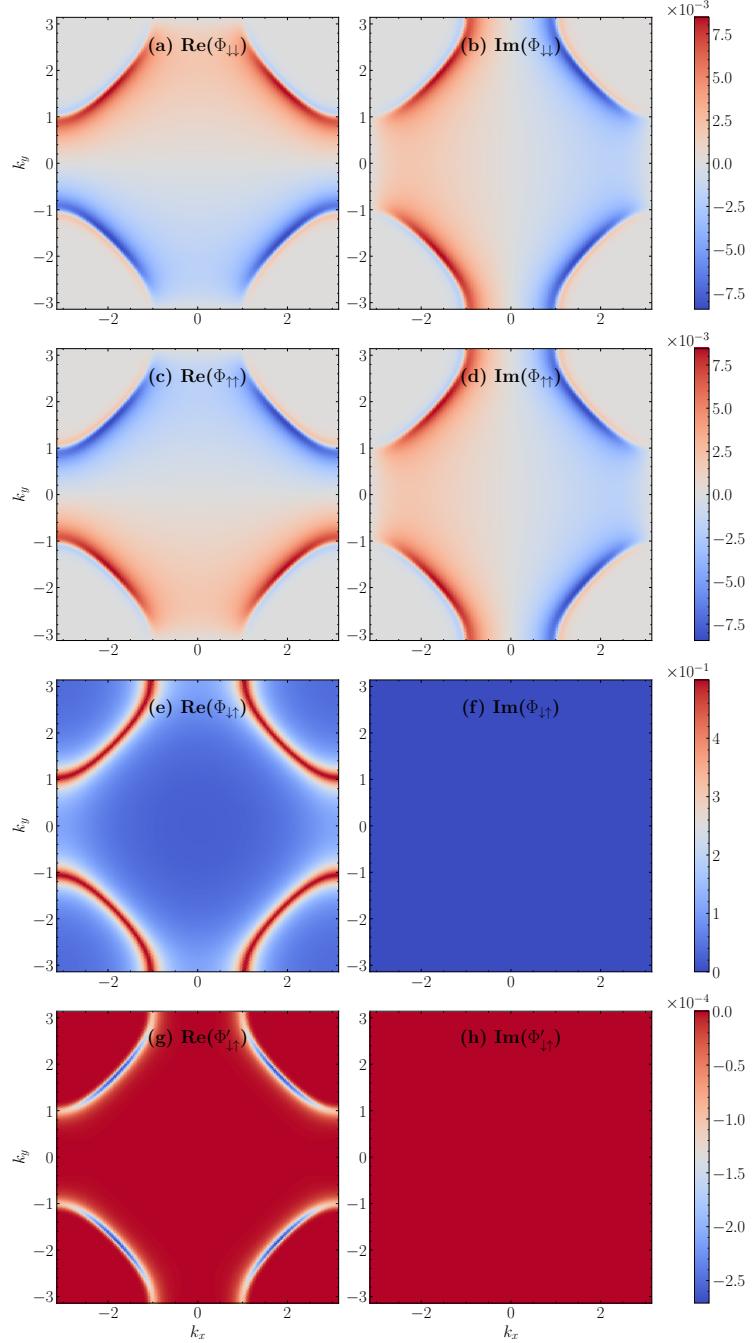


Figure 2: Order parameters  $\Phi_{s_1s_2}$  at chemical potential  $\mu = 1$ . Other parameters are fixed as  $(t, g, D) = (1, 2, 0.5)$ . The quantity  $\Phi'_{\downarrow\uparrow} = \Phi_{\downarrow\uparrow} - \langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$  characterizes the new singlet pairing structure due to the perturbation.

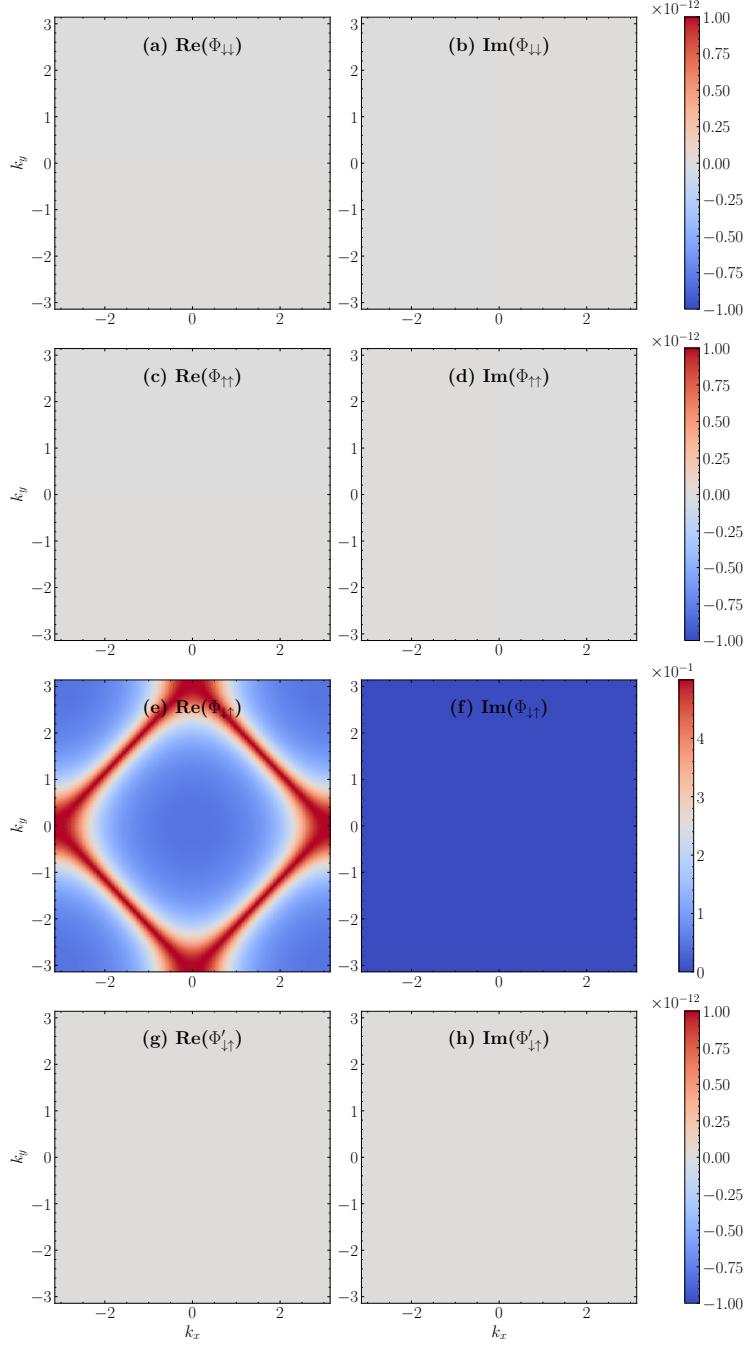


Figure 3: Order parameters  $\Phi_{s_1 s_2}$  at chemical potential  $\mu = 0$ . Other parameters are fixed as  $(t, g, D) = (1, 2, 0.5)$ . The quantity  $\Phi'_{\downarrow\uparrow} = \Phi_{\downarrow\uparrow} - \langle g_0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | g_0 \rangle$  characterizes the new singlet pairing structure due to the perturbation.