Bogoliubov-Valatin Canonical Transformation and the Model Hamiltonian

To describe the superconducting state at $T > 0$, the variational approach that we have followed so far is not very useful. An approach developed independently by Bogoliubov and Valatin and now known as Bogoliubov-Valatin canonical transformation, which we describe next, is more appropriate.

Our pair Hamiltonian, including the $-\mu\hat{N}$ term is given by

$$H - \mu\hat{N} = \sum_{\vec{k}\sigma} \xi_{\vec{k}} C^{+}_{\vec{k}\sigma} C^{+}_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}} C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} C_{-\vec{l}\downarrow} C_{\vec{l}\downarrow} \tag{1}$$

Since we are dealing with a large number of particles, the fluctuation about the average of $C_{-\vec{k}\downarrow} C_{\vec{k}\uparrow}$ would be small. With that in mind we define a c-number $b_{\vec{k}}$ as

$$C_{-\vec{k}\downarrow} C_{\vec{k}\uparrow} = b_{\vec{k}} + (C_{-\vec{k}\downarrow} C_{\vec{k}\uparrow} - b_{\vec{k}}) \tag{2}$$

Now the interaction term can be rewritten as

$$\sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}} C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} C_{-\vec{k}\downarrow} C_{\vec{k}\uparrow} = \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}} \, (b^{*}_{\vec{k}} + (C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} - b^{*}_{\vec{k}}))(b_{\vec{l}} + (C_{-\vec{l}\downarrow} C_{\vec{l}\uparrow} - b_{\vec{l}})) \tag{3}$$

$$= \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}} [b_{\vec{l}} C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} - b^{*}_{\vec{k}} b_{\vec{l}} + b^{*}_{\vec{k}} C_{-\vec{l}\downarrow} C_{\vec{l}\uparrow} + (C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} - b^{*}_{\vec{k}})(C_{-\vec{l}\downarrow} C_{\vec{l}\uparrow} - b_{\vec{l}}) \tag{4}$$

we assume that the last term on the right hand side of the above equation is small due to large number of particles and therefore we ignore it,

$$= \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}} (b^{*}_{\vec{k}} C_{-\vec{l}\downarrow} C_{\vec{l}\uparrow} + b_{\vec{l}} C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} - b^{*}_{\vec{k}} b_{\vec{l}}) \tag{5}$$

The model Hamiltonian now becomes

$$H - \mu N \simeq H_m = \sum_{\vec{k}\sigma} \xi_{\vec{k}} C^{+}_{\vec{k}\sigma} C^{+}_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}} \left[b^{*}_{\vec{k}} C_{-\vec{l}\downarrow} C_{\vec{l}\uparrow} + b_{\vec{l}} C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} - b^{*}_{\vec{k}} b_{\vec{l}} \right] \tag{6}$$

subject to the constraint

$$b_{\vec{k}} = \langle C_{-\vec{k}|} C_{\vec{k}|} \rangle_{av} \tag{7}$$

Now we define

$$\Delta_{\vec{k}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} b_{\vec{l}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} \langle C_{-\vec{l}\downarrow} C_{\vec{l}\uparrow} \rangle \tag{8}$$

leading to

$$H_m = \sum_{\vec{k}\sigma} \xi_{\vec{k}} C^{+}_{\vec{k}\sigma} C_{\vec{k}\sigma} - \sum_{\vec{l}} \Delta^{*}_{\vec{l}} C_{-\vec{l}\downarrow} C_{\vec{l}\uparrow} - \sum_{\vec{k}} \Delta_{\vec{k}} C^{+}_{\vec{k}\uparrow} C^{+}_{-\vec{k}\downarrow} - \sum_{\vec{k}} \Delta_{\vec{k}} b^{*}_{\vec{k}} \tag{9}$$

Relabeling the summation index, we get

$$H_m = \sum_{\vec{k}\sigma} \xi_{\vec{k}} C^+_{\vec{k}\sigma} C_{\vec{k}\sigma} - \sum_{\vec{k}} \left(\Delta_{\vec{k}} C^+_{\vec{k}\uparrow} C^+_{-\vec{k}\downarrow} + \Delta^*_{\vec{k}} C_{-\vec{k}\downarrow} C_{\vec{k}\uparrow} - \Delta_{\vec{k}} b^*_{\vec{k}} \right) \tag{10}$$

Noting that the operators in the model Hamiltonian appear in a bilinear form, it can be written in a diagonal form by appropriate transformations using C operators, as shown by Bogoliubov and Valatin. We define

$$C_{\vec{k}|} = u^*_{\vec{k}} \gamma_{\vec{k}0} + v_{\vec{k}} \gamma^+_{\vec{k}1} \tag{11}$$

$$C^+_{-\vec{k}|} = -v^*_{\vec{k}} \gamma_{\vec{k}0} + u_{\vec{k}} \gamma^+_{\vec{k}1} \tag{12}$$

where $\gamma' s$ satisfy the following anticommutation rules,

$$\left[\gamma^+_{\vec{k}0}, \gamma \right]_+ = \delta_{\vec{k}\vec{k}'} \tag{13}$$

$$\left[\gamma^+_{\vec{k}1}, \gamma_{\vec{k}'1} \right]_+ = \delta_{\vec{k}\vec{k}'} \tag{14}$$

We also note that $u_{\vec{k}}$ and $v_{\vec{k}}$ satisfy $[u_{\vec{k}}]^2 + [v_{\vec{k}}]^2 = 1$. Now substituting for $C's$ in terms of $\gamma's$ in the Hamiltonian we will have terms that we consider separately,

$$C^+_{\vec{k}|} C_{\vec{k}|} = \left(u_{\vec{k}} \gamma^+_{\vec{k}0} + u^*_{\vec{k}} \gamma_{\vec{k}1} \right) \left(u^*_{\vec{k}} \gamma_{\vec{k}0} + u_{\vec{k}} \gamma^+_{\vec{k}1} \right) \tag{15}$$

$$= \left| u_{\vec{k}} \right|^2 \gamma^+_{\vec{k}0} \gamma_{\vec{k}0} + u^*_{\vec{k}} v^*_{\vec{k}} \gamma_{\vec{k}1} \gamma_{\vec{k}0} + u_{\vec{k}} v_{\vec{k}} \gamma^+_{\vec{k}0} \gamma^+_{\vec{k}1} + \left| v_{\vec{k}} \right|^2 \gamma_{\vec{k}1} \gamma^+_{\vec{k}1} \tag{16}$$

$$C^+_{\vec{k}|} C_{\vec{k}|} = \left(-v^*_{\vec{k}} \gamma_{\vec{k}0} + u_{\vec{k}} \gamma^+_{\vec{k}1} \right) \left(-v_{\vec{k}} \gamma^+_{\vec{k}0} + u^*_{\vec{k}} \gamma_{\vec{k}1} \right) \tag{17}$$

$$= \left| v_{\vec{k}} \right|^2 \gamma_{\vec{k}0} \gamma^+_{\vec{k}0} - u_{\vec{k}} v_{\vec{k}} \gamma^+_{\vec{k}1} \gamma^+_{\vec{k}0} - u^*_{\vec{k}} v^*_{\vec{k}} \gamma_{\vec{k}0} \gamma_{\vec{k}1} + \left| v^*_{\vec{k}} \right|^2 \gamma^+_{\vec{k}1} \gamma_{\vec{k}1} \tag{18}$$

Similarly,

$$C^+_{\vec{k}|} C^+_{-\vec{k}|} = \left(u_{\vec{k}} \gamma^+_{\vec{k}0} + u^*_{\vec{k}} \gamma_{\vec{k}1} \right) \left(-v^*_{\vec{k}} \gamma_{\vec{k}0} + u_{\vec{k}} \gamma^+_{\vec{k}1} \right) \tag{19}$$

$$= -u_{\vec{k}} v^*_{\vec{k}} \gamma^+_{\vec{k}0} \gamma_{\vec{k}0} - \left| v_{\vec{k}} \right|^2 \gamma_{\vec{k}1} \gamma_{\vec{k}0} + u^2_{\vec{k}} \gamma^+_{\vec{k}0} \gamma^+_{\vec{k}1} + u^*_{\vec{k}} v^*_{\vec{k}} \gamma_{\vec{k}1} \gamma^+_{\vec{k}1} \tag{20}$$

and

$$C_{-\vec{k}|} C_{\vec{k}|} = \left(-v_{\vec{k}} \gamma^+_{\vec{k}0} + u^*_{\vec{k}} \gamma^+_{\vec{k}1} \right) \left(u^*_{\vec{k}} \gamma_{\vec{k}0} + v_{\vec{k}} \gamma^+_{\vec{k}1} \right) \tag{21}$$

$$= -v_{\vec{k}} u^*_{\vec{k}} \gamma^+_{\vec{k}0} \gamma_{\vec{k}0} + \left| u_{\vec{k}} \right|^2 \gamma_{\vec{k}1} \gamma_{\vec{k}0} - \left| v_{\vec{k}} \right|^2 \gamma^+_{\vec{k}0} \gamma^+_{\vec{k}1} + u^*_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}1} \gamma^+_{\vec{k}1} \tag{22}$$

We now substitute these values in the Hamiltonian. Considering the first term we have,

$$= \sum_{\vec{k}} \xi_{\vec{k}} \left\{ \left| u_{\vec{k}} \right|^2 \gamma^+_{\vec{k}0} \gamma_{\vec{k}0} + u^*_{\vec{k}} v^*_{\vec{k}} \gamma_{\vec{k}1} \gamma_{\vec{k}0} + u_{\vec{k}} v_{\vec{k}} \gamma^+_{\vec{k}0} \gamma^+_{\vec{k}1} + \left| v_{\vec{k}} \right|^2 \underbrace{\gamma_{\vec{k}1} \gamma^+_{\vec{k}1}} \right\}$$

$$+ \xi_{\vec{k}} \left\{ \left| v_{\vec{k}} \right|^2 \underbrace{\gamma_{\vec{k}0} \gamma^+_{\vec{k}0}} - u_{\vec{k}} v_{\vec{k}} \gamma^+_{\vec{k}1} \gamma^+_{\vec{k}0} - u^*_{\vec{k}} v^*_{\vec{k}} \gamma_{\vec{k}0} \gamma_{\vec{k}1} + \left| u_{\vec{k}} \right|^2 \gamma^+_{\vec{k}1} \gamma_{\vec{k}1} \right\}$$

$$=\sum_{\vec{k}} \xi_{\vec{k}}\Big[|u_{\vec{k}}|^2\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0} + u^{*}_{\vec{k}}v^{*}_{\vec{k}}\gamma_{\vec{k}1}\gamma_{\vec{k}0} + u_{\vec{k}}v_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1}$$

$$+ |v_{\vec{k}}|^2\left(1-\gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}\right) + |v_{\vec{k}}|^2\left(1-\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0}\right) + u_{\vec{k}}v_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1} + u^{*}_{\vec{k}}v^{*}_{\vec{k}}\gamma_{\vec{k}1}\gamma_{\vec{k}0} + |u_{\vec{k}}|^2\gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}\Big]$$

$$=\sum_{\vec{k}}\xi_{\vec{k}}\Big[\left(|u_{\vec{k}}|^2-|v_{\vec{k}}|^2\right)\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0} + 2u^{*}_{\vec{k}}v^{*}_{\vec{k}}\gamma_{\vec{k}1}\gamma_{\vec{k}0} + 2u_{\vec{k}}v_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1} + 2|v_{\vec{k}}|^2 + \left(|u_{\vec{k}}|^2-|v_{\vec{k}}|^2\right)\gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}\Big]$$

$$=\sum_{\vec{k}} \xi_{\vec{k}}\Big[\left(|u_{\vec{k}}|^2-|v_{\vec{k}}|^2\right)\left(\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0}+\gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}\right) + 2u^{*}_{\vec{k}}v^{*}_{\vec{k}}\gamma_{\vec{k}1}\gamma_{\vec{k}0} + 2u_{\vec{k}}v_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1} + 2|v_{\vec{k}}|^2\Big] \tag{23}$$

The second term can be simplified as,

$$\sum_{\vec{k}} \Delta_{\vec{k}}\Big[\left(-u_{\vec{k}}v^{*}_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0} - |v_{\vec{k}}|^2\gamma_{\vec{k}1}\gamma_{\vec{k}0} + u^{2}_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1} + u_{\vec{k}}v^{*}_{\vec{k}}\gamma_{\vec{k}1}\gamma^{+}_{\vec{k}1}\right)$$

$$+\left(-u^{*}_{\vec{k}}v_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0} + |u_{\vec{k}}|^2\gamma_{\vec{k}1}\gamma_{\vec{k}0} - |v_{\vec{k}}|^2\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1} + u^{*}_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}1}\gamma^{+}_{\vec{k}1}\right) - b^{*}_{\vec{k}}\Big]$$

$$=\sum_{\vec{k}} \Delta_{\vec{k}}\Big[\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0}\left(-u_{\vec{k}}v^{*}_{\vec{k}} - u^{*}_{\vec{k}}v_{\vec{k}}\right) + \gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}\left(-u_{\vec{k}}v^{*}_{\vec{k}} - u^{*}_{\vec{k}}v_{\vec{k}}\right)$$

$$+\gamma_{\vec{k}1}\gamma_{\vec{k}0}\left(|u_{\vec{k}}|^2-|v_{\vec{k}}|^2\right) + \left(|u_{\vec{k}}|^2-|v_{\vec{k}}|^2\right)\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1} + u_{\vec{k}}v^{*}_{\vec{k}} + u^{*}_{\vec{k}}v_{\vec{k}} - b^{*}_{\vec{k}}\Big]$$

$$=\sum_{\vec{k}}\Delta_{\vec{k}}\Big[\left(-u_{\vec{k}}v^{*}_{\vec{k}} - u^{*}_{\vec{k}}v_{\vec{k}}\right)\left(\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0}+\gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}-1\right) + \left(|u_{\vec{k}}|^2-|v_{\vec{k}}|^2\right)\left(\gamma_{\vec{k}1}\gamma_{\vec{k}0}+\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1}\right) - b^{*}_{\vec{k}}\Big] \tag{24}$$

Putting all the terms together, our model Hamiltonian becomes

$$H_m=\sum_{\vec{k}}\xi_{\vec{k}}\Big\{\left(|u_{\vec{k}}|^2-|v_{\vec{k}}|^2\right)\left(\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0}+\gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}\right) + 2u^{*}_{\vec{k}}v^{*}_{\vec{k}}\gamma_{\vec{k}1}\gamma_{\vec{k}0} + 2u_{\vec{k}}v_{\vec{k}}\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1} + 2|v_{\vec{k}}|^2\Big\}$$

$$+\sum_{\vec{k}}\Big\{\left(u_{\vec{k}}v^{*}_{\vec{k}} - u^{*}_{\vec{k}}v_{\vec{k}}\right)\left(\gamma^{+}_{\vec{k}0}\gamma_{\vec{k}0}+\gamma^{+}_{\vec{k}1}\gamma_{\vec{k}1}\right) + \left(v^{2}_{\vec{k}} - u^{2}_{\vec{k}}\right)\left(\gamma_{\vec{k}1}\gamma_{\vec{k}0}+\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1}\right) + b_{\vec{k}}\Big\} \tag{25}$$

If the coefficients of $\gamma_{\vec{k}1}\gamma_{\vec{k}0}$ and $\gamma^{+}_{\vec{k}0}\gamma^{+}_{\vec{k}1}$ vanish then the model Hamiltonian is diagonalized. That we do next.