

A similar result holds in the tight binding model, where we have (assuming only on-site interactions)

$$\langle \tilde{t}|V_c|\tilde{t} \rangle = \langle t|V_c|t \rangle = 0 \quad (25a)$$

$$\langle \tilde{s}|V_c|\tilde{s} \rangle = \frac{2U}{N^2} \sum_i \cos^2 2\mathbf{k} \cdot \mathbf{R}_i \quad (25b)$$

$$\langle s|V_c|s \rangle = \frac{2U}{N} \quad (25c)$$

Again the average of Eq. (25a) and Eqs. (25b) or (25c) yields Eq. (19) or (18) for $\mathbf{k}' = -\mathbf{k}$.

IV. RELEVANCE TO SUPERCONDUCTIVITY

Our findings in the previous sections suggest that the new basis is relevant to superconductivity. The fact that the BCS wavefunction Eq. (4) singles out pairs $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ could naturally be explained by the fact that the direct Coulomb repulsion between an \uparrow -spin electron in state $\tilde{\varphi}_{\mathbf{k}}$ and a \downarrow -spin electron in $\tilde{\varphi}_{-\mathbf{k}}$ is particularly small.

Consider then as an alternative to the BCS wavefunction a wavefunction of the form Eq. (4) but with the new states instead of the Bloch states:

$$|\Psi\rangle_{new} = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \tilde{c}_{\mathbf{k}\uparrow}^\dagger \tilde{c}_{-\mathbf{k}\downarrow}^\dagger) |0\rangle \quad (26)$$

Deep in the Fermi sea, $u_{\mathbf{k}} = u_{-\mathbf{k}} = 0$ and $v_{\mathbf{k}} = v_{-\mathbf{k}} = 1$. Since

$$(\tilde{c}_{\mathbf{k}\uparrow}^\dagger \tilde{c}_{-\mathbf{k}\downarrow}^\dagger)(\tilde{c}_{-\mathbf{k}\uparrow}^\dagger \tilde{c}_{\mathbf{k}\downarrow}^\dagger) = (c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)(c_{-\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger) \quad (27)$$

deep in the Fermi sea the new wavefunction is the same as the BCS wavefunction. This also means that in the normal state ($u_{\mathbf{k}} v_{\mathbf{k}} = 0$ for all \mathbf{k}) the wavefunctions Eq. (4) and Eq. (26) are identical. However, in the region where $u_{\mathbf{k}} v_{\mathbf{k}} \neq 0$ there is a difference. We have for $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ and $(-\mathbf{k} \uparrow, \mathbf{k} \downarrow)$ pairs in the BCS wavefunction

$$\begin{aligned} |\Psi\rangle_{BCS}^{k,-k} &= (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)(u_{-\mathbf{k}} + v_{-\mathbf{k}} c_{-\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger) \\ &= u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 (\tilde{c}_{\mathbf{k}\uparrow}^\dagger \tilde{c}_{-\mathbf{k}\downarrow}^\dagger)(\tilde{c}_{-\mathbf{k}\uparrow}^\dagger \tilde{c}_{\mathbf{k}\downarrow}^\dagger) \\ &\quad - i u_{\mathbf{k}} v_{\mathbf{k}} ((\tilde{c}_{\mathbf{k}\uparrow}^\dagger \tilde{c}_{\mathbf{k}\downarrow}^\dagger) + (\tilde{c}_{-\mathbf{k}\uparrow}^\dagger \tilde{c}_{-\mathbf{k}\downarrow}^\dagger)) \end{aligned} \quad (28)$$

(assuming as usual $u_{\mathbf{k}} = u_{-\mathbf{k}}$, $v_{\mathbf{k}} = v_{-\mathbf{k}}$). Instead, in the new wavefunction Eq. (26)

$$\begin{aligned} |\Psi\rangle_{new}^{k,-k} &= (u_{\mathbf{k}} + v_{\mathbf{k}} \tilde{c}_{\mathbf{k}\uparrow}^\dagger \tilde{c}_{-\mathbf{k}\downarrow}^\dagger)(u_{-\mathbf{k}} + v_{-\mathbf{k}} \tilde{c}_{-\mathbf{k}\uparrow}^\dagger \tilde{c}_{\mathbf{k}\downarrow}^\dagger) \\ &= u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 (\tilde{c}_{\mathbf{k}\uparrow}^\dagger \tilde{c}_{-\mathbf{k}\downarrow}^\dagger)(\tilde{c}_{-\mathbf{k}\uparrow}^\dagger \tilde{c}_{\mathbf{k}\downarrow}^\dagger) \\ &\quad + u_{\mathbf{k}} v_{\mathbf{k}} ((\tilde{c}_{\mathbf{k}\uparrow}^\dagger \tilde{c}_{\mathbf{k}\downarrow}^\dagger) + (\tilde{c}_{-\mathbf{k}\uparrow}^\dagger \tilde{c}_{-\mathbf{k}\downarrow}^\dagger)) \end{aligned} \quad (29)$$

Eqs. (28) and (29) differ in the last line. The BCS wavefunction has an amplitude for having double occupancy

of the state $\tilde{\varphi}_{\mathbf{k}}$ with the state $\tilde{\varphi}_{-\mathbf{k}}$ being empty, and vice versa, and no amplitude for the states $\tilde{\varphi}_{\mathbf{k}}$ and $\tilde{\varphi}_{-\mathbf{k}}$ being both singly occupied. Instead, the new state has amplitude for the states $\tilde{\varphi}_{\mathbf{k}}$ and $\tilde{\varphi}_{-\mathbf{k}}$ being both singly-occupied and no amplitude for the state $\tilde{\varphi}_{\mathbf{k}}$ being doubly-occupied with the state $\tilde{\varphi}_{-\mathbf{k}}$ empty, nor vice versa. Single occupancy of both $\tilde{\varphi}_{\mathbf{k}}$ and $\tilde{\varphi}_{-\mathbf{k}}$ minimizes the direct Coulomb repulsion between the electrons while double occupancy of either state maximizes the direct Coulomb repulsion. Consequently, we conclude that the new wavefunction Eq. (26) will be strongly favored energetically over the BCS wavefunction Eq. (4) as far as the Coulomb interaction between electrons is concerned.

In summary, in the normal state where states \mathbf{k} and $-\mathbf{k}$ are both either occupied or empty, the new basis is completely equivalent to the conventional one. However in a state of the BCS form that allows for partial occupation of pair states the new basis appears to be favorable.

Furthermore, Eqs. (29), (16b) and (14b) indicate that the advantage of the new basis over the conventional one will be greatest if $u_{\mathbf{k}} v_{\mathbf{k}} \neq 0$ in a region where k is small. Instead, for \mathbf{k} near the edge of the Brillouin zone there is no advantage to the new basis according to Eq. (19). This suggests that in a superconducting state described by the wavefunction Eq. (26) the region where $u_{\mathbf{k}} v_{\mathbf{k}} \neq 0$ should occur near $k = 0$, and the states with \mathbf{k} near the Brillouin zone edge should be full ($v_{\mathbf{k}} = 1, u_{\mathbf{k}} = 0$) (to conserve the number of particles). This is precisely the scenario predicted in Ref.[6].

V. 4-ELECTRON STATE

We consider in the following the plane wave case only. Let us consider further the two candidate wavefunctions Eqs. (4) and (26) for the case of only two pairs, in states $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ and $(-\mathbf{k} \uparrow, \mathbf{k} \downarrow)$. The Coulomb energy in the BCS case is

$$\langle V_c \rangle_{BCS} = \frac{4V(0)}{\Omega} |v_{\mathbf{k}}|^4 + \frac{2(V(0) + V(2k))}{\Omega} |u_{\mathbf{k}}|^2 |v_{\mathbf{k}}|^2 \quad (30a)$$

and with the new wavefunction Eq. (26) it is

$$\langle V_c \rangle_{new} = \frac{4V(0)}{\Omega} |v_{\mathbf{k}}|^4 + \frac{2V(0)}{\Omega} |u_{\mathbf{k}}|^2 |v_{\mathbf{k}}|^2 \quad (30b)$$

Since the Coulomb repulsion $V(2k)$ is positive for all k , the new state has clearly lower Coulomb energy than the BCS state.

However in adding the second electron pair we have lost the lowering of energy proportional to $V(2k)$ that occurred for the single pair (Eq. (16b)) due to interference effects. How can it be restored? In deriving Eq. (30), we assumed $u_{\mathbf{k}} = u_{-\mathbf{k}}$, $v_{\mathbf{k}} = v_{-\mathbf{k}}$. Not making that