More pairs

- we build up the grnd. state from pairs.

$i = (\vec{r}_i, s_i)$, N: even.

$$\Psi(1,2,\dots N) = \underset{\substack{\uparrow \\ \text{anti-sym} \\ \text{operator}}}{\hat{A}} \{\varphi(1,2)\varphi(3,4)\dots\varphi(N-1,N)\}$$

$\varphi(i,j) = \varphi(\vec{r}_i - \vec{r}_j)\alpha(s_i)\beta(s_j)$ since it is under the $\hat{A}$ operator

$$\hat{A}\varphi(i,j) = \varphi(\vec{r}_i - \vec{r}_j)\underbrace{\left[\alpha(s_i)\beta(s_j) - \alpha(s_j)\beta(s_i)\right]}_{\sqrt{2}\,\hat{}\,\chi(s_i,s_j)}$$

$$\varphi(\vec{r}_i - \vec{r}_j) = \sum_{k_i} c(\vec{k}_i)\, e^{i\vec{k}_i(\vec{r}_i - \vec{r}_j)} \qquad c(k) = c(-k)$$

$$\Psi(1,2,\dots,N) = \sum_{k_1}\sum_{k_3}\dots\sum_{k_{N-1}} c(k_1)c(k_2)\dots c(k_{N-1})\cdot SD$$

$$\underset{\substack{\uparrow \\ \text{Slater-determinant}}}{SD} = \hat{A}\left\{e^{i\vec{k}_1\vec{r}_1}\alpha(s_1)\,e^{-i\vec{k}_1\vec{r}_2}\beta(s_2)\dots e^{i\vec{k}_{N-1}\vec{r}_{N-1}}\alpha(s_{N-1})\,e^{-i\vec{k}_{N-1}\vec{r}_N}\beta(s_N)\right\}$$

- we can convert this to 2nd quant. form.

$$|\hat{\Psi}_N\rangle = \sum_{k_1}\sum_{k_3}\dots\sum_{k_{N-1}} c_{k_1}c_{k_2}\dots c_{k_{N-1}}\,\hat{a}^+_{k_1\uparrow}\hat{a}^+_{-k_1\downarrow}\dots\hat{a}^+_{k_{N-1}\uparrow}\hat{a}^+_{-k_{N-1}\downarrow}|\emptyset\rangle$$

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Bardeen - Cooper - Schrieffer grnd. state

$$|BCS\rangle = \prod_{\vec{k}}\left(u_{\vec{k}} + v_{\vec{k}}\, a^+_{\vec{k}\uparrow}a^+_{-\vec{k}\downarrow}\right)|\emptyset\rangle \leftarrow \text{BCS-ansatz}$$

• this is for <u>all</u> $\vec{k}$, not just for the Fermi-sphere.

$u_{\vec k_1} u_{\vec k_2} \dots u_{\vec k} |\emptyset\rangle \rightsquigarrow$ belongs to 0 particles

$\sum_{k} \beta_k a^+_{\vec k\uparrow} a^+_{-\vec k\downarrow} |\emptyset\rangle \rightsquigarrow$ all are 2 particle states (creates pairs...)

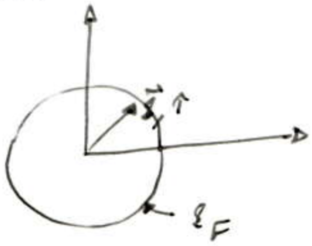
• a grund. stat like $|BCS\rangle$ does not belong to a given particle-number states, but a linear comb. of many even particle-number states.

$$|BCS\rangle = \sum_{N,\vec k} \varphi_{N,\vec k} \, |\varphi_{N,\vec k}\rangle \qquad N: \text{even}$$

$\langle BCS|BCS\rangle = 1$ if $u_k^2 + v_k^2 = 1$, no vector-pot ($\vec B$ field)

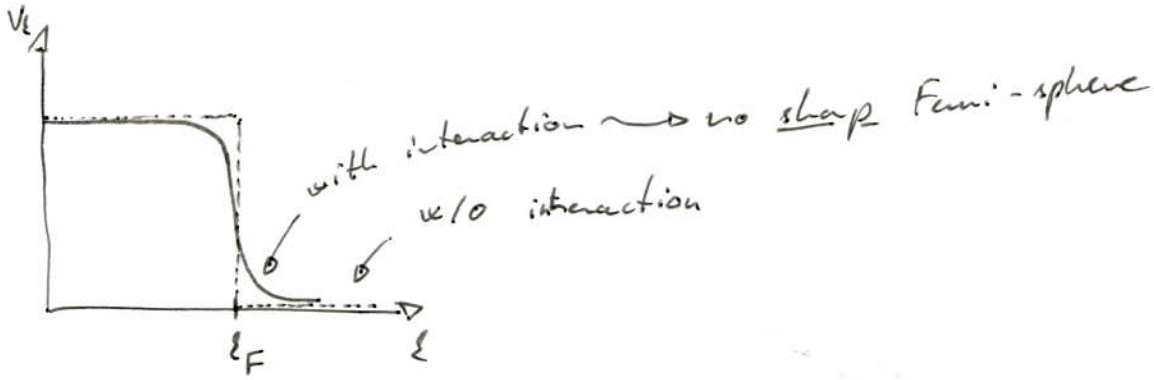
u_k, v_k can be choosen to be real.

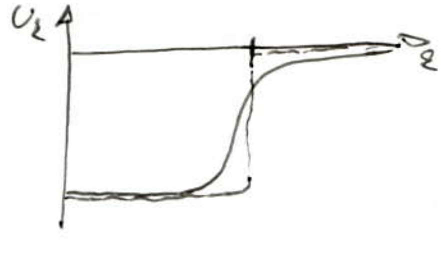
• BCS ansatz can describe the <u>Normal-state</u> /at T=0.../



$$\left.\begin{aligned} v_k &= 1 \\ u_k &= 0 \end{aligned}\right\} \text{ if } k < k_F$$

$$\left.\begin{aligned} v_k &= 0 \\ u_k &= 1 \end{aligned}\right\} \text{ if } k > k_F$$





- the order can be changed in $|BCS\rangle$, since there is always 2 fermionic creation ops. $\rightsquigarrow$ anticommute ...
  $\hookrightarrow (-1)^2 = 1 \ldots$

$$\langle BCS | BCS \rangle = \langle \emptyset | \prod_{\substack{k' \\ k' \neq k}} (u_{k'} + v_{k'} a_{-k'\downarrow} a_{k'\uparrow}) \underbrace{(u_k + v_k a_{-k\downarrow} a_{k\uparrow})(u_k + v_k a^+_{k\uparrow} a^+_{-k\downarrow})}_{} \cdot$$

$$\cdot \prod_{k''} (u_{k''} + v_{k''} a^+_{k''\uparrow} a^+_{-k''\downarrow}) |\emptyset\rangle$$

$$(u_k^2 + u_k v_k (a_{-k\downarrow} a_{k\uparrow} + a^+_{k\uparrow} a^+_{-k\downarrow}) + + v_k^2 a_{-k\downarrow} a_{k\uparrow} a^+_{k\uparrow} a^+_{-k\downarrow})$$

$$(u_k^2 + v_k^2 a_{-k\downarrow} a^+_{-k\downarrow} a_{k\uparrow} a^+_{k\uparrow}) =$$

$$= (u_k^2 + v_k^2 (1 - a^+_{-k\downarrow} a_{-k\downarrow})(1 - a^+_{k\uparrow} a_{k\uparrow})) =$$

$$= (u_k^2 + v_k^2 + (\text{operators}))$$

$\downarrow$ moving them all to gives 0.

$$a_{k\uparrow} |\emptyset\rangle = 0 \qquad a_{k\downarrow} |\emptyset\rangle = 0 \qquad \langle \emptyset | a^+_{k\uparrow} = 0 \qquad \langle \emptyset | a^+_{k\downarrow} = 0$$

$\rightsquigarrow$ process can be repeated for $\forall \vec{k}$ $\rightsquigarrow$ $\langle BCS | BCS \rangle = 0$ (if $u_k^2 + v_k^2 = 1$ for $\forall \vec{k}$)

- now we build a new creation and annihilation ops. that keep the canonical properties.

<u>Bogoliubov - Valatin Canonical transformation</u>

- making new quasi-particle ops.
  $a^+_{k\uparrow}$ and $a_{-k\downarrow}$ are related. $\rightsquigarrow$ both increase momentum with k, spin with $1/2$

$$\alpha^+_{k\uparrow} = u_k a^+_{k\uparrow} - v_k a_{-k\downarrow} \qquad \alpha_{k\uparrow} = u_k a_{k\uparrow} - v_k a^+_{-k\downarrow}$$

$$\alpha^+_{k\downarrow} = u_k a^+_{k\downarrow} + v_k a_{-k\uparrow} \qquad \alpha_{k\downarrow} = u_k a_{k\downarrow} + v_k a^+_{-k\uparrow}$$

• New α-s have the same commutation relations

$\{A,B\}$	$\alpha_{k\uparrow}$	$\alpha_{k'\downarrow}$	$\alpha^+_{k'\uparrow}$	$\alpha^+_{k'\downarrow}$
$\alpha_{k\uparrow}$	0	0	$\delta_{kk'}$	0
$\alpha_{k\downarrow}$	0	0	0	$\delta_{kk'}$
$\alpha^+_{k\uparrow}$	$\delta_{kk'}$	0	0	0
$\alpha^+_{k\downarrow}$	0	$\delta_{kk'}$	0	0

$$\{\alpha^+_{k\uparrow}, \alpha^+_{k'\downarrow}\} = \{u_k a^+_{k\uparrow} - v_k a_{-k\downarrow}, u_{k'} a^+_{k'\downarrow} + v_k a_{-k'\uparrow}\}$$

$$= -v_k u_{k'} \delta_{-k,k'} + u_k v_{k'} \delta_{k,-k'} =$$

$$= -v_k u_{-k} + u_{-k'} v_{k'} = 0 \quad \square$$

$$\{\alpha_{k\uparrow}, \alpha^+_{k'\uparrow}\} = \{u_k a_{k\uparrow} - v_k a^+_{-k\downarrow}, u_{k'} a^+_{k'\uparrow} - v_{k'} a_{-k'\downarrow}\} =$$

$$= u_k u_{k'} \delta_{kk'} - v_k v_{k'} \delta_{kk'} = \underbrace{(u_k^2 + v_k^2)}_{1} \delta_{kk'} = \delta_{kk'} \quad \square$$

⇝ can be done for the rest of the table...

• Important property:

$$\boxed{\begin{aligned} \alpha_{k\uparrow}|BCS\rangle &= 0 \\ \alpha_{k\downarrow}|BCS\rangle &= 0 \end{aligned}}$$

if u_k, v_k are the same in α, BCS.

$$\hat{H} = \sum_k \varepsilon_k (\alpha^+_{k\uparrow}\alpha_{k\uparrow} + \alpha^+_{k\downarrow}\alpha_{k\downarrow})$$ ⇝ diagonalized Hamiltonian

⇝ we know how many pairs with energy ε_k...

$$\alpha_{k\uparrow}|BCS\rangle = \alpha_{k\uparrow} \prod_{k'\neq k} (u_{k'} + v_{k'} a^+_{k'\uparrow} a^+_{-k'\downarrow})(u_k + v_k a^+_{k\uparrow} a^+_{-k\downarrow})|\emptyset\rangle =$$

$$= \prod_{k'\neq k} (u_{k'} + v_{k'} a^+_{k'\uparrow} a_{-k'\downarrow}) \cdot \alpha_{k\uparrow}(u_k + v_k a^+_{k\uparrow} a^+_{-k\downarrow})|\emptyset\rangle =$$

$$= \prod_{k'\neq k} (\dots)(u_k a_{k\uparrow} - v_k a^+_{-k\downarrow})(u_k + v_k a^+_{k\uparrow} a^+_{-k\downarrow})|\emptyset\rangle =$$

$$= \prod_{k'\neq k}(\dots)\left(-v_k u_k a^+_{-k\downarrow} + u_k v_k a_{k\uparrow} a^+_{k\uparrow} a^+_{-k\downarrow} \underbrace{- v_k^2 a^+_{-k\downarrow} a^+_{k\uparrow} a^+_{-k\downarrow}}_{+ v_k^2 a^+_{k\uparrow} (a^+_{-k\downarrow})^2}\right)|\emptyset\rangle =$$

⇝ 0! due to the Fermi-statistics.

$$= \prod_{\ell' \neq \ell} (\ldots)\left(-v_\ell u_\ell a^+_{-\ell\downarrow} + u_\ell v_\ell (1 - a^+_{\ell\uparrow} a_{\ell\uparrow}) a^+_{-\ell\downarrow}\right)|\emptyset\rangle =$$

$$= (\ldots)\Big(\underbrace{-v_\ell u_\ell a^+_{-\ell\downarrow} + u_\ell v_\ell a^+_{-\ell\downarrow}}_{\emptyset} - u_\ell v_\ell a^+_{\ell\uparrow} a^+_{-\ell\downarrow} \underset{\emptyset}{a_{\ell\uparrow}}\Big)|\emptyset\rangle = \underline{\underline{0}} \quad \square$$

- one can build up a quasi-particle Fock space.

$\alpha^+_{\ell\uparrow} \ldots |BCS\rangle$ ⇝ excited states built upon the BCS ground. state.

$\Updownarrow$

$|BCS\rangle$ is the vacuum for the α-s

- Inverse transformation:

$$\alpha^+_{\ell\uparrow} = u_\ell a^+_{\ell\uparrow} - v_\ell a_{-\ell\downarrow} \quad / \cdot u_\ell$$

$$\alpha_{-\ell\downarrow} = u_{-\ell} a_{-\ell\downarrow} + v_\ell a^+_{\ell\uparrow} \quad / \cdot v_\ell \qquad / u_{-\ell} = u_\ell = u_{|\ell|} = u_\ell \ldots /$$

$$u_\ell \alpha^+_{\ell\uparrow} + v_\ell \alpha_{-\ell\downarrow} = a^+_{\ell\uparrow}$$

⇝ others can be derived similarly.

$$a^+_{\ell\downarrow} = u_\ell \alpha^+_{\ell\downarrow} - v_\ell \alpha_{-\ell\uparrow}$$

$$a_{\ell\uparrow} = u_\ell \alpha_{\ell\uparrow} + v_\ell \alpha^+_{-\ell\downarrow}$$

$$a_{\ell\downarrow} = u_\ell \alpha_{\ell\downarrow} - v_\ell \alpha^+_{-\ell\uparrow}$$

$$\langle\emptyset| a^+_{\ell\uparrow} a^+_{-\ell\downarrow} |\emptyset\rangle = 0$$

$\langle BCS| a^+_{k\uparrow} a^+_{-k\downarrow} |BCS\rangle \neq 0$ $\rightsquigarrow$ pair-state

$$a^+_{k\uparrow} a^+_{-k\downarrow} = (u_k \alpha^+_{k\uparrow} + v_k \alpha_{-k\downarrow})(u_k \alpha^+_{-k\downarrow} - v_k \alpha_{k\uparrow})$$

$$u_k v_k \langle BCS| (1 - \alpha^+_{-k\downarrow} \alpha_{-k\downarrow}) |BCS\rangle = u_k v_k$$

$$\langle BCS| \overbrace{a^+_{k\uparrow} a_{k\uparrow}}^{n_{k\uparrow}} |BCS\rangle = \langle BCS| (\cancel{u_k \alpha^+_{k\uparrow}} + v_k \alpha_{-k\downarrow})(\cancel{u_k \alpha_{k\uparrow}} + v_k \alpha^+_{-k\downarrow}) |BCS\rangle =$$

$$= \langle BCS| v_k^2 (1 - \alpha^+_{-k\downarrow} \alpha_{-k\downarrow}) |BCS\rangle = v_k^2$$

$$\langle BCS| n_{k\downarrow} |BCS\rangle = v_k^2$$

$$\langle BCS| \hat{N} |BCS\rangle = \sum_k \langle BCS| a^+_{k\uparrow} a_{k\uparrow} + a^+_{k\downarrow} a_{k\downarrow} |BCS\rangle = 2 \sum_k v_k^2$$

this is the definite avg. value.

What is the fluctuation?

$$\hat{N}^2 = 4 \sum_k \hat{n}_{k\uparrow} \sum_{k'} \hat{n}_{k'\uparrow} \quad \text{if } k \neq k'$$

$$\langle BCS| \hat{n}_{k\uparrow} \hat{n}_{k'\uparrow} |BCS\rangle = v_k^2 v_{k'}^2 \quad \text{if } k \neq k'$$

$$\langle BCS| \hat{n}_{k\uparrow} \hat{n}_{k\uparrow} |BCS\rangle = (u_k^2 + v_k^2) v_k^2$$