Mean-field approximation for the repulsive one band Hubbard model

The Hamiltonian is

$$H = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Let us propose a spin-density-wave solution.

We replace $n_{i\sigma}$ by a mean value. First we write:

$$n_{i\sigma} = \langle n_{i\sigma} \rangle + (n_{i\sigma} - \langle n_{i\sigma} \rangle)$$

and then we say that $n_{i\sigma} - \langle n_{i\sigma} \rangle$ is "small". This quantity tell us how much the system deviates from the mean value, which has to be found self-consistently. The interaction becomes

$$n_{i\uparrow} n_{i\downarrow} = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + (n_{i\uparrow} - \langle n_{i\uparrow} \rangle) \langle n_{i\downarrow} \rangle$$

$$+ (n_{i\downarrow} - \langle n_{i\downarrow} \rangle) \langle n_{i\uparrow} \rangle$$

This is the Hartree-Fock approximation.

$$+ \underbrace{(n_{i\uparrow} - \langle n_{i\uparrow} \rangle)(n_{i\downarrow} - \langle n_{i\downarrow} \rangle)}$$

This term is of "second order" in the small deviation from the MF Ansatz. Thus, we neglect it. Then:

$$\boxed{n_{i\uparrow} n_{i\downarrow} \approx - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + n_{i\uparrow} \langle n_{i\downarrow} \rangle + n_{i\downarrow} \langle n_{i\uparrow} \rangle}$$

As Ansatz we propose

$$\langle n_{i\uparrow} \rangle = \frac{1}{2}\left(1 + S\, e^{i\vec{Q}.\vec{r}}\right)$$

$$\langle n_{i\downarrow} \rangle = \frac{1}{2}\left(1 - S\, e^{i\vec{Q}.\vec{r}}\right)$$

where $\vec{Q} = (\pi, \pi)$ in 2D. S is the parameter that we have to find by energy minimization.

$e^{i\vec{Q}.\vec{r}} = (-1)^{i_x + i_y}$ where i_x, i_y are the components of the site vector $\vec{r}$. This factor is 1 for "even" sites, and (-1) for "odd" sites i.e. it divides the square lattice into two sublattices:

-1	1	-1
1	-1	1
-1	1	-1

If $S = 0$, then $\langle n_{i\uparrow} \rangle = \langle n_{i\downarrow} \rangle = 1/2$ and this is the correct result at $U = 0$ and half-filling. In this case translational invariance is unbroken.

If $S = 1$,

$$\langle n_{i\uparrow} \rangle = \begin{cases} 1 \text{ for even sites} \\ 0 \text{ for odd sites} \end{cases}$$

$$\langle n_{i\downarrow} \rangle = \begin{cases} 0 \text{ for even sites} \\ 1 \text{ for odd sites} \end{cases}$$

This is correct. It is the result we expect at U large where we have one particle per site at half-filling, and the effective Hamiltonian is the Heisenberg model with antiferromagnetic coupling.

Note that the interaction in the Hubbard model is usually written in a "particle-hole symmetric way" as

$$U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$$

which, after the MF Ansatz, becomes:

$$U \sum_i \left(n_{i\uparrow} n_{i\downarrow} - \tfrac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) + 1/4 \right) \approx$$

$$\approx U \sum_i \Big[- \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + n_{i\uparrow} \tfrac{1}{2}(1 - S e^{i\vec{Q}\cdot\vec{r}}) + n_{i\downarrow} \tfrac{1}{2}(1 + S e^{i\vec{Q}\cdot\vec{r}}) - \tfrac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) + 1/4 \Big] =$$

$$= U \sum_i \left[-\frac{1}{4} \underbrace{(1 + S e^{i\vec{Q}\cdot\vec{r}})(1 - S e^{i\vec{Q}\cdot\vec{r}})}_{1 - S^2} + \frac{S}{2} e^{i\vec{Q}\cdot\vec{r}} (n_{i\downarrow} - n_{i\uparrow}) + 1/4 \right]$$

$$= U \sum_i \left[\frac{S^2}{4} + \frac{S}{2} e^{i\vec{Q}\cdot\vec{r}} (n_{i\downarrow} - n_{i\uparrow}) \right]$$

Then, the MF Hubbard model is

$$H_{MF} = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c.}) + UN\frac{S^2}{4}$$

$$- \frac{US}{2} \sum_i e^{i\vec{Q}\cdot\vec{i}} (n_{i\uparrow} - n_{i\downarrow})$$

where N is the total # of sites.
Note that the last term resembles the interaction of a particle in a "staggered" magnetic field $\vec{h}_i$ which is of the form:

$$\sum_i \vec{h}_i \cdot \vec{S}_i = \sum_i \underbrace{h e^{i\vec{Q}\cdot\vec{i}}}_{\text{staggered field}} \underbrace{\left(\frac{n_{i\uparrow} - n_{i\downarrow}}{2}\right)}_{S_i^z}$$

↑ Assume $\vec{h}$ points along z

The MF Hamiltonian can be handled better in momentum space where the kinetic energy is explicitly diagonal. Note that H_{MF}, being quadratic in $c^{\dagger}, c$, must be exactly solvable unlike the full Hamiltonian that contains a "$c^{\dagger}c^{\dagger}cc$" complicated interaction.

The kinetic energy becomes:

$$H_{K.E.} = -t \sum_{l\sigma} \left(c^{+}_{l\sigma} c_{l+\mu\sigma} + c^{+}_{l+\mu\sigma} c_{l\sigma} \right)$$

$(\mu = \hat{x}, \hat{y})$

This is another way to represent nearest-neighbors. $\hat{x}, \hat{y}$ are unit vectors along the axis.

Let us introduce a standard Fourier transformation as:

$$c_{l\sigma} = \frac{1}{\sqrt{N}} \sum_{p} e^{i\vec{p}.\vec{l}} c_{p\sigma}$$

Then,

$$H_{K.E.} = -t \sum_{l,\mu,\sigma} \frac{1}{N} \sum_{pp'} \left[e^{-i\vec{p}.\vec{l}} e^{i\vec{p}'.(\vec{l}+\vec{\mu})} c^{+}_{p\sigma} c_{p'\sigma} + e^{-i(\vec{l}+\vec{\mu}).\vec{p}} e^{i\vec{p}'.\vec{l}} c^{+}_{p\sigma} c_{p'\sigma} \right]$$

But we know that

$$\frac{1}{N} \sum_{l} e^{-i\vec{p}.\vec{l}} e^{i\vec{p}'.\vec{l}} = \delta_{\vec{p}\vec{p}'}.$$

Then:

$$H_{K.E.} = -t \sum_{\mu,\sigma} \sum_{p} c^{+}_{p\sigma} c_{p\sigma} \left(e^{i\vec{p}.\vec{\mu}} + e^{-i\vec{p}.\vec{\mu}} \right)$$

$$H_{K.E.} = -t \sum_{p\sigma} c^{+}_{p\sigma} c_{p\sigma} \sum_{\mu} 2\cos(\vec{p}\cdot\vec{\mu})$$

$$= \sum_{p\sigma} c^{+}_{p\sigma} c_{p\sigma}\, \varepsilon_p$$

where $\varepsilon_p = -2t(\cos p_x + \cos p_y)$ in 2D since $\vec{\mu}$ is either $(1,0)$ or $(0,1)$.

The kinetic energy is indeed diagonal in p-space.

Now, let us Fourier transform the other term that appears in H_{MF}:

$$-\frac{US}{2} \sum_{\ell} e^{i\vec{Q}\cdot\vec{\ell}} (n_{\ell\uparrow} - n_{\ell\downarrow}) =$$

$$= -\frac{US}{2} \sum_{\ell} e^{i\vec{Q}\cdot\vec{\ell}} \left(c^{+}_{\ell\uparrow} c_{\ell\uparrow} - c^{+}_{\ell\downarrow} c_{\ell\downarrow}\right) =$$

$$= -\frac{US}{2} \sum_{\ell} \frac{1}{N} \sum_{pp'} e^{i\vec{Q}\cdot\vec{\ell}}\, e^{-i\vec{p}\cdot\vec{\ell}}\, e^{i\vec{p}'\cdot\vec{\ell}} \left(c^{+}_{p\uparrow} c_{p'\uparrow} - c^{+}_{p\downarrow} c_{p'\downarrow}\right)$$

Now we have to use the identity:

$$\frac{1}{N}\sum_{\ell} e^{-i(\vec{p}-\vec{p}'-\vec{Q})\cdot\vec{\ell}} = \delta_{\vec{p},\vec{p}'+\vec{Q}}$$

and we get

$$-\frac{US}{2}\sum_{p'}\left(c^{+}_{p'+Q\uparrow}c_{p'\uparrow} - c^{+}_{p'+Q\downarrow}c_{p'\downarrow}\right).$$

(Note that Q or $-Q$ are equivalent)

The full MF Hamiltonian is

$$H_{MF} = \frac{UNS^2}{4} + \sum_{p\sigma} c^{+}_{p\sigma}c_{p\sigma}\varepsilon_p - \frac{US}{2}\sum_{p}\left(c^{+}_{p+Q\uparrow}c_{p\uparrow} - c^{+}_{p+Q\downarrow}c_{p\downarrow}\right).$$

Note that the last term contains terms that change momentum from p to $p+Q$. This is an apparent violation of p-conservation. The effect is caused by the MF approximation. The spins are like in a staggered field that allows for p-non conservation in Q.

Note also that H_{MF} is "almost" diagonal but not quite yet. Momentum p interacts with itself in the K.E. and with $p+Q$ in the other term. But $p+Q$ interacts with itself and with $p+2Q$ which is p. Then, p and $p+Q$ interact with each other and no other momentum. The Hamiltonian is thus in a simple block form, where each block is

$$\begin{array}{c} \\ C^{\dagger}_{p\sigma} \\ C^{\dagger}_{p+Q\sigma} \end{array} \begin{array}{c} \begin{array}{cc} C_{p\sigma} & C_{p+Q\sigma} \end{array} \\ \begin{pmatrix} \varepsilon_p & -\frac{US}{2}\sigma \\ -\frac{US\sigma}{2} & \varepsilon_{p+Q} \end{pmatrix} \end{array}$$

where $\sigma = +1$ if spin up,
$= -1$ if spin down.

Note that $\varepsilon_{p+Q} = -2t \sum_{\mu} \cos(\vec{p}+\vec{Q}\cdot\vec{\mu})$

$= -2t\left[\cos(p_x+\pi) + \cos(p_y+\pi)\right] = +2t\,(\cos p_x + \cos p_y)$

$= -\varepsilon_p$

and the matrix becomes:

$$\begin{pmatrix} \varepsilon_p & -\frac{US}{2}\sigma \\ -\frac{US}{2}\sigma & -\varepsilon_p \end{pmatrix}$$

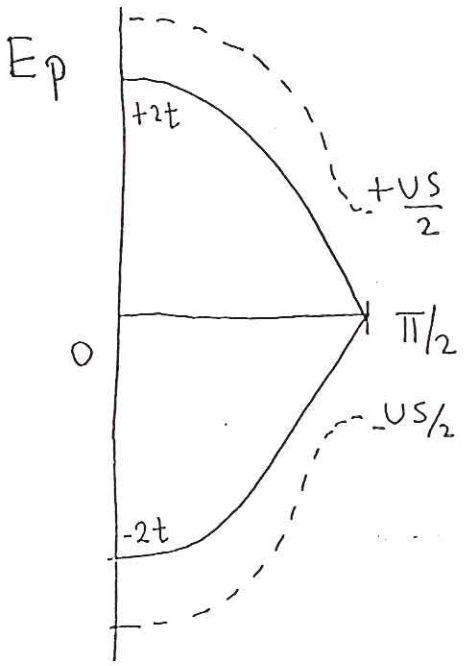
The eigenvalues, E_p, are obtain from:

$$\underbrace{(\varepsilon_p - E_p)(-\varepsilon_p - E_p)}_{-\varepsilon_p^2 + E_p^2} - \frac{U^2 S^2}{4}\underbrace{\sigma^2}_{1} = 0$$

$$\boxed{E_p = \pm\sqrt{\varepsilon_p^2 + \frac{U^2 S^2}{4}}}$$

Note that p is now restricted to <u>half</u> the Brillouin zone. The reason is that the eigenvalues E_p are obtained after putting in one block p and $p+Q$. At $S=0$ which is the noninteracting limit I had $2N$ eigenvalues (2 for spin, N for # of momenta). Now I have $2 \times 2 \times \frac{N}{2} = 2N$ also where 2 is for spin, the second 2 is for the $\pm$ values in the equation for E_p and $\frac{N}{2}$ are the possible values p takes.

To plot this we use half the Brillouin zone.
Consider the 1D case:



At $U=0$ we have the solid line
The dashed line represents the MF solution. This solution at $p=0$ is

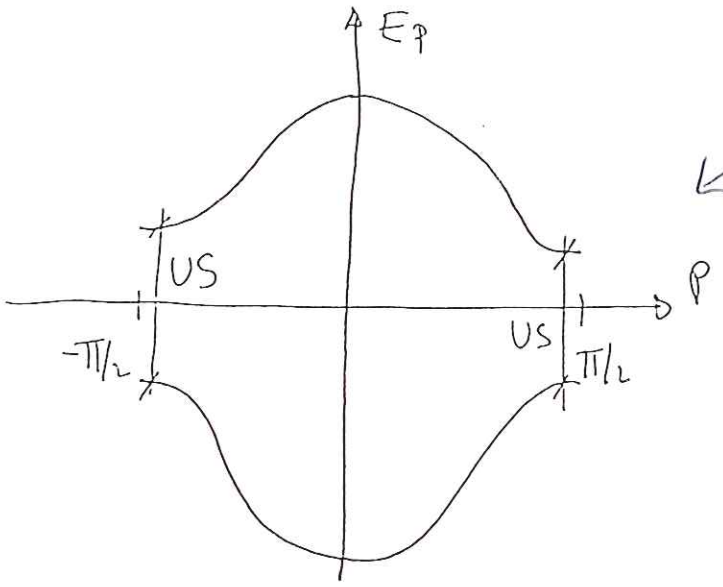
$$E_0 = \pm\sqrt{\varepsilon_0^2 + \frac{U^2 S^2}{4}}$$

$$= \pm\sqrt{(2t)^2 + \frac{U^2 S^2}{4}}$$

and at $p=\pi/2$ we know $\varepsilon_p = 0$
and

$$E_{\pi/2} = \pm \frac{US}{2}$$

Then, now we have a gap in the spectrum which is the smallest at $\pi/2$. Including negative values for the momenta we have



why a gap opens!

In a state ↑ ↓ ↑ ↓, adding a charge costs energy U

↑ ↓ ↑ (↓↑) ↑ ↓ ...

As simple as that!

The total gap is $U \cdot S = 2\Delta$ and the dispersion is

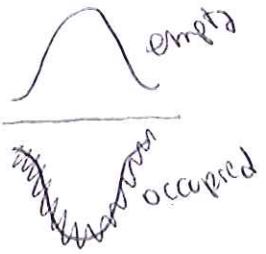
$$E_p = \pm \sqrt{\varepsilon_p^2 + \Delta^2}$$

as in the BCS superconductors.

So far we haven't said anything about S. We have to find its self-consistent equation. What is the energy of the problem in the MF Ansatz? Well, we have to fill all levels of negative energy which is fine since we are at half-filling and we have enough particles. The energy is:

$$E_{MF} = 2 \sum_{\substack{\text{(such that} \\ E_p < 0)}} E_p + \frac{UNS^2}{4}$$

(2 ↑ spin)



$$\frac{\partial E_{MF}}{\partial S} = 0 = \frac{\partial}{\partial S}\left(2 \sum_{E_p<0} (-)\sqrt{\varepsilon_p^2 + \frac{U^2 S^2}{4}} + \frac{UNS^2}{4}\right)$$

$$= -2 \sum_{E_p<0} \frac{U^2/4 \, 2S}{2\sqrt{\varepsilon_p^2 + \frac{U^2S^2}{4}}} + \frac{UN}{4} 2S$$

$$= -\frac{U^2 S}{2} \sum_{p} \frac{1}{\sqrt{\varepsilon_p^2 + \frac{U^2S^2}{4}}} + \frac{UNS}{2}$$

(For each p in the "reduced" Brillouin zone there is a negative E_p

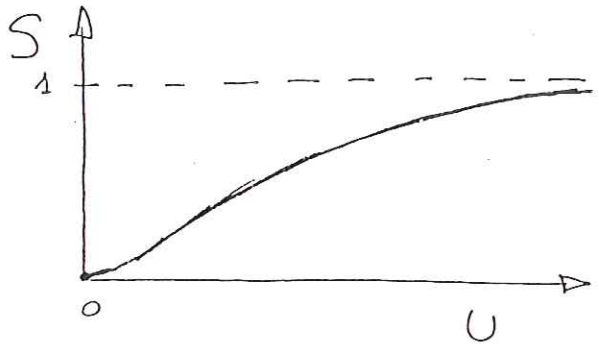
Let us forget about the trivial $S=0$ solution.

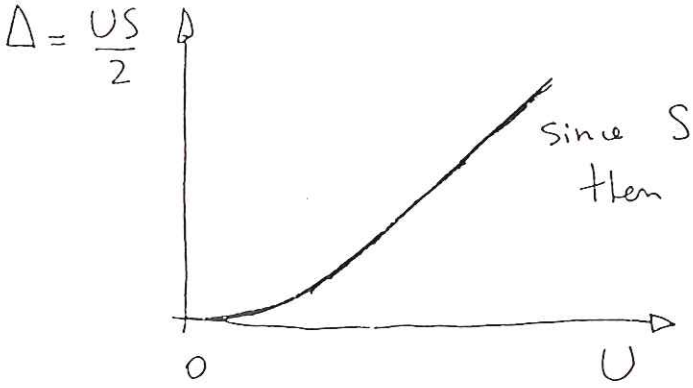
Then we get:

$$\frac{1}{N} \sum_{p \in \text{reduced BZ}} \frac{U}{\sqrt{\varepsilon_p^2 + \frac{U^2 S^2}{4}}} = 1$$

This is the "gap" equation. Again, very similar to BCS.

This is the "gap equation" in the context of antiferromagnetism.





Since $S \to 1$ as $U \to \infty$, then $\Delta \approx U/2$ at large U.

Now, let us calculate the eigenvectors. For $\sigma = +1$, i.e. spin up, the matrix is

$$\begin{pmatrix} \varepsilon_p & -\Delta \\ -\Delta & -\varepsilon_p \end{pmatrix}$$

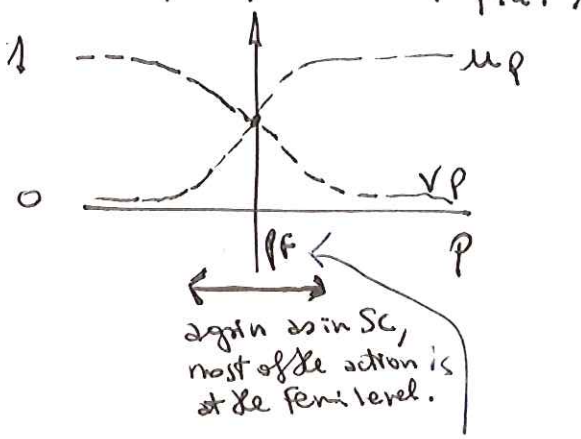
The eigenvector will have the form $\begin{pmatrix} u_p \\ -v_p \end{pmatrix}$ with $u_p^2 + v_p^2 = 1$.

↑ it means $u_p c_p^+ |0\rangle - v_p c_{p+q}^+ |\downarrow\rangle$

As in BCS, let us propose

$$u_p^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_p}{|E_p|}\right)$$

$$v_p^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_p}{|E_p|}\right)$$



T/2 at half filling.

The condition of eigenvector is

$$\begin{pmatrix} \varepsilon_p - \Delta \\ -\Delta & -\varepsilon_p \end{pmatrix}\begin{pmatrix} u_p \\ -v_p \end{pmatrix} = E_p \begin{pmatrix} u_p \\ -v_p \end{pmatrix}$$

or $\varepsilon_p u_p + \Delta v_p$ should be $E_p u_p$,
and $-\Delta u_p + \varepsilon_p v_p$ should be $-E_p v_p$.

But $\varepsilon_p u_p + \Delta v_p = u_p\left(\varepsilon_p + \Delta \frac{v_p}{u_p}\right) = u_p\left(\varepsilon_p + \Delta\sqrt{\frac{|E_p| - \varepsilon_p}{|E_p| + \varepsilon_p}}\right) =$

$$= u_p\left(\varepsilon_p + \Delta\sqrt{\frac{(|E_p| - \varepsilon_p)^2}{|E_p|^2 - \varepsilon_p^2}}\right) = u_p\left(\varepsilon_p + \Delta\sqrt{\frac{(|E_p| - \varepsilon_p)^2}{\Delta^2}}\right) = u_p\left[\varepsilon_p + (|E_p| - \varepsilon_p)\right]$$

$$= u_p |E_p| \quad \text{O.K.}$$

and

$$-\Delta u_p + \varepsilon_p v_p = (-v_p)\left(+\Delta\frac{u_p}{v_p} - \varepsilon_p\right) = (-v_p)\left(\Delta\sqrt{\frac{\varepsilon_p + |E_p|}{-\varepsilon_p + |E_p|}} - \varepsilon_p\right) =$$

$$= (v_p)\left[\Delta\sqrt{\frac{(E_p+\varepsilon_p)^2}{|E_p|^2-\varepsilon_p^2}}-\varepsilon_p\right] = (v_p)\left[\Delta\sqrt{\frac{(E_p+\varepsilon_p)^2}{\Delta^2}}-\varepsilon_p\right] = (v_p)|E_p|.$$

Then $\begin{pmatrix} u_p \\ -v_p \end{pmatrix}$ is indeed eigenvector, with eigenvalue $+\sqrt{\varepsilon_p^2+\Delta^2} = |E_p|$.

The other one will be $\begin{pmatrix} v_p \\ u_p \end{pmatrix}$ ← with eigenvector $-|E_p|$. which is orthogonal to the previous one. There is no need to verify that it is since just showing the orthogonality to the previous eigenvector is here enough. Indeed

$$(u_p - v_p)\begin{pmatrix} v_p \\ u_p \end{pmatrix} = 0 .$$

The operators "γ" corresponding to eigenvectors are

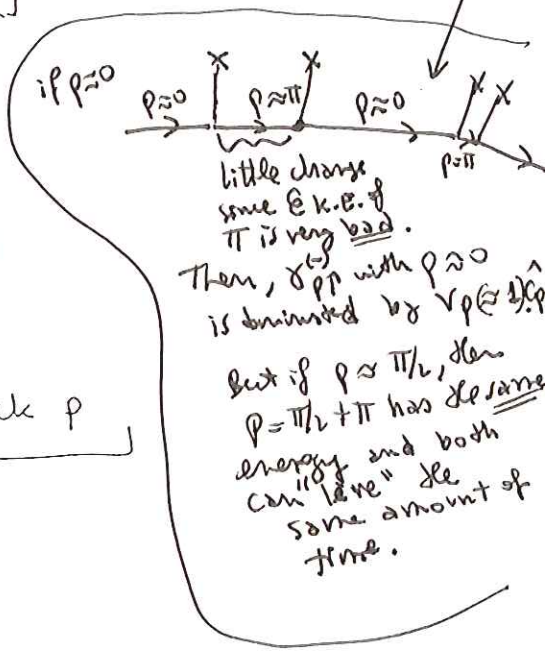
eigenstates are mixtures of 2 types of electrons!

$$\hat{\gamma}^{(+)}_{p\uparrow} = u_p \hat{C}_{p\uparrow} - v_p \hat{C}_{p+Q\uparrow} \quad \leftarrow \text{Eigenvalue } |E_p|$$

$$\hat{\gamma}^{(-)}_{p\uparrow} = v_p \hat{C}_{p\uparrow} + u_p \hat{C}_{p+Q\uparrow} \quad \leftarrow \quad " \quad -E_p|$$

or schematically

$$\begin{pmatrix} \hat{\gamma}^{+}_{p\uparrow} \\ \hat{\gamma}^{-}_{p\uparrow} \end{pmatrix} = \begin{pmatrix} u_p & -v_p \\ v_p & u_p \end{pmatrix}\begin{pmatrix} \hat{C}_{p\uparrow} \\ \hat{C}_{p+Q\uparrow} \end{pmatrix}$$



The Hamiltonian corresponding to block p is now:

$$\left(\gamma^{\dagger(+)}_{p\uparrow},\ \gamma^{\dagger(-)}_{p\uparrow}\right)\begin{pmatrix}|E_p| & 0\\ 0 & -|E_p|\end{pmatrix}\begin{pmatrix}\gamma^{(+)}_{p\uparrow}\\ \gamma^{(-)}_{p\uparrow}\end{pmatrix} =$$

$$= |E_p|\left(\gamma^{\dagger(+)}_{p\uparrow}\gamma^{(+)}_{p\uparrow} - \gamma^{\dagger(-)}_{p\uparrow}\gamma^{(-)}_{p\uparrow}\right)$$

where $|E_p| = +\sqrt{\varepsilon_p^2 + \Delta^2}$.

$$\hat{H} = \sum_{\substack{p\in \\ 1/2\,BZ \\ \sigma}} |E_p|\left(\gamma^{\dagger(+)}_{p\sigma}\gamma^{(+)}_{p\sigma} - \gamma^{\dagger(-)}_{p\sigma}\gamma^{(-)}_{p\sigma}\right)$$

Now, for spin down we simply change $-\Delta \to \Delta$ in the Hamiltonian block. In such a case we propose $\begin{pmatrix}u_p\\ v_p\end{pmatrix}$

and we get

$$\begin{pmatrix}\varepsilon_p & \Delta\\ \Delta & -\varepsilon_p\end{pmatrix}\begin{pmatrix}u_p\\ v_p\end{pmatrix} = E_p\begin{pmatrix}u_p\\ v_p\end{pmatrix}$$

or $\quad \varepsilon_p u_p + \Delta v_p$ should be $E_p u_p$,

$\Delta u_p - \varepsilon_p v_p$ should be $E_p v_p$.

$$\varepsilon_p u_p + \Delta v_p = u_p\left(\varepsilon_p + \Delta\frac{v_p}{u_p}\right) = u_p\left(\varepsilon_p + \Delta\sqrt{\frac{|E_p|-\varepsilon_p}{|E_p|+\varepsilon_p}}\right) =$$

$$= u_p\left(\varepsilon_p + \Delta\frac{\sqrt{(|E_p|-\varepsilon_p)^2}}{\sqrt{|E_p|^2-\varepsilon_p^2}}\right) = u_p\left(\varepsilon_p + \Delta\sqrt{\frac{(|E_p|-\varepsilon_p)^2}{\Delta^2}}\right) =$$

$$= u_p|E_p|.$$

An orthogonal vector is $\begin{pmatrix}v_p\\ -u_p\end{pmatrix}$

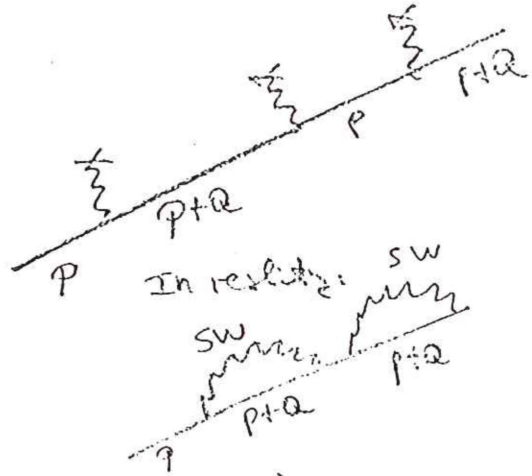
and thus the eigenoperators are:

$$\boxed{\begin{aligned} \hat{\gamma}^{(+)}_{p\downarrow} &= u_p \hat{C}_{p\downarrow} + v_p \hat{C}_{p+Q\downarrow} \\ \hat{\gamma}^{(-)}_{p\downarrow} &= v_p \hat{C}_{p\downarrow} - u_p \hat{C}_{p+Q\downarrow} \end{aligned}}$$

← eigenvalue $|E_p|$

← eigenvalue $-|E_p|$

The ground state is then:



$$\prod_{p \in \text{reduced BZ}} \gamma^{+(-)}_{p\uparrow} \gamma^{+(-)}_{p\downarrow} |0\rangle =$$

$$= \prod_{p \in \text{reduced BZ}} \left(v_p C^+_{p\uparrow} + u_p C^+_{p+Q\uparrow}\right)\left(v_p C^+_{p\downarrow} - u_p C^+_{p+Q\downarrow}\right)|0\rangle$$

↖ $\prod C^+_{p\uparrow} C^+_{p\downarrow} |0\rangle$ is just one of a zillion states!!

The state $C^+_{p\uparrow} C^+_{p\downarrow} |0\rangle$ has chance v_p^2

" $C^+_{p+Q\uparrow} C^+_{p+Q\downarrow} |0\rangle$ " " u_p^2

" $C^+_{p\uparrow} C^+_{p+Q\downarrow} |0\rangle$ " " $u_p v_p$

" $C^+_{p+Q\uparrow} C^+_{p\downarrow} |0\rangle$ " " $u_p v_p$

If $\Delta = 0$, $v_p = 1$ in the reduced BZ
and $u_p = 0$ " " " ".

If $\Delta \neq 0$ but small, then $v_p \gg u_p$ and the state $C^+_{p\uparrow} C^+_{p\downarrow} |0\rangle$ dominates although the rest have a nonzero chance specially near the boundary of the reduced B.Z., where $\varepsilon_p = 0$.

} same as in BCS.