

# COOPER PAIRING IN “EXOTIC” FERMI SUPERFLUIDS: AN ALTERNATIVE APPROACH

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1. Anisotropic Cooper pairing (textbook version)

Can still use fundamental ansatz (I. 1)

$$\Psi_N(\mathbf{r}_1\sigma_1 \dots \mathbf{r}_N\sigma_N) = n \cdot \mathcal{A} \cdot \varphi(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2)\varphi(\mathbf{r}_3\sigma_3\mathbf{r}_4\sigma_4)\dots\varphi(\mathbf{r}_{N-1}\sigma_{N-1}\mathbf{r}_N\sigma_N)$$

same  $\varphi!$

normalization      antisymmetrizer

and still require

$$\varphi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \varphi(\mathbf{r}_1 - \mathbf{r}_2; \sigma_1 \sigma_2) \leftarrow \text{i.e. COM at rest}$$

but now allow  $\varphi$  to be nontrivial functions of  $\sigma$ 's and  $\hat{r}_{12}$ .

However, because of  $\mathcal{A}$  (Pauli principle)  $S = 0 \Leftrightarrow f(\mathbf{r}_1 - \mathbf{r}_2)$  even,  $S = 1 \Leftrightarrow f(\mathbf{r}_1 - \mathbf{r}_2)$  odd.

Even-parity case is simple generalization of BCS:

$$\Psi_N = \mathcal{N} \left( \sum_k c_k a_{k\uparrow}^+ a_{-k\downarrow}^+ \right)^{N/2} |vac\rangle \quad c_k = c_{-k} = f(|\mathbf{k}|, \hat{\mathbf{k}})$$

$\Rightarrow$  generalized gap equation

$$\Delta_k = \sum_{k'} V_{kk'} \Delta_{k'} / 2E_{k'} \quad E_{k'} \equiv (E_k^2 + |\Delta_k|^2)$$

in general (in 3D) gap has nodes at 2 or more points on F.S.



Odd-parity case: must now pair spins to form  $S = 1$ . Description of general case (e.g.  ${}^3\text{He} - B$ ) complicated, but simplifies for ESP ( ${}^3\text{He} - A, \text{Sr}_2\text{RuO}_4$ ). In this case proper description is equal spin pairing ( $\uparrow\uparrow$  and  $\downarrow\downarrow$ , no  $\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$ )

$$\varphi(\mathbf{r}_1 - \mathbf{r}_2; \sigma_1 \sigma_2) = f_{\uparrow\uparrow}(\mathbf{r}_1 - \mathbf{r}_2) | \uparrow\uparrow \rangle + e^{i\varphi} f_{\downarrow\downarrow}(\mathbf{r}_1 - \mathbf{r}_2) | \downarrow\downarrow \rangle$$

$$\Rightarrow \Psi_N = \mathcal{N} \left( \sum_k c_{k\uparrow} a_{k\uparrow}^+ a_{-k}^+ + e^{i\varphi} c_{k\downarrow} a_{k\downarrow}^+ a_{-k\downarrow}^+ \right)^{N/2} |vac\rangle \quad (\uparrow !)$$

but in most TQC contexts usually adequate to replace by

$$\Psi_N = \Psi_{\frac{N}{2}\uparrow} \Psi_{\frac{N}{2}\downarrow}, \quad \Psi_{\frac{N}{2}\uparrow} = \mathcal{N}_{\uparrow} \left( \sum_k c_k a_{k\uparrow}^+ a_{-k\uparrow}^+ \right)^{N/4} |vac\rangle \text{ (etc.)}$$

From now on, concentrate on single spin population (e.g.  $\uparrow$ ) so omit  $\uparrow$ 's and let  $N/2 \rightarrow N$  (i.e.  $N$  is number of "relevant" particles),  $\Psi_{N/2,\uparrow} \rightarrow \Psi_N$

Thus, at first sight,

$$\Psi_N = \mathcal{N} \left( \sum_k c_k a_k^+ a_{-k}^+ \right)^{N/2} |vac\rangle \quad c_k = -c_{-k} \quad \text{(Pauli)}$$

$\uparrow$ : State  $\mathbf{k} = 0$  has no partner! (contrast even-parity case, ( $0 \uparrow 0 \downarrow$ )), hence, strictly correct odd-parity GSWF for an odd number ( $2N + 1$ ) of particles is

$$\Psi_N = \mathcal{N} \left( \sum_{\mathbf{k} \neq 0} c_k a_k^+ a_{-k}^+ \right)^{N/2} a_0^+ |vac\rangle$$



(We will usually implicitly subtract off this odd particle in the accounting)

Most interesting case (especially in 2D) is when  $c_k$  is (nontrivially) **complex**. Important example ( ${}^3\text{He} - A, \text{Sr}_2\text{RuO}_4(?)$ ) is  **$p + ip$  state**:

$$c_k = f(|\mathbf{k}|) \exp i\varphi_k \quad \leftarrow \angle \text{ of } \mathbf{k} \text{ on Fermi surface}$$

In this case, pair wave function  $F_k$  is of form

$$F_k = \frac{c_k}{1 + |c_k|^2} = \frac{\Delta_k}{2E_k} \quad \Delta_k = |\Delta_k| \exp i\varphi_k$$

(so in 2D, no nodes). Thus, if we write

$$|\Delta_k|_{|k|=k_F} \equiv \Delta_0 k_F ,$$

then on and near F.S.,

$$\Delta_k = \Delta_0 (k_x + ik_y) \quad (\text{hence, “}p + ip\text{”})$$

However, from symmetry of gap equation (with  $V_{kk'} = V_{k-k'}$ )

$$\Delta_k = - \sum_{k'} V_{k-k'} \Delta_{k'} / 2E_{k'}$$

$$(E_k \equiv (\epsilon_k^2 + |\Delta_k|^2)^{1/2} = f(|\mathbf{k}|))$$

$\Delta_k$  must have same symmetry for **all**  $|k|$  (down to  $|k| \rightarrow 0$ ). Does it also have same dependence on  $|k|$ ? (i.e. is  $|\Delta_k| \propto |k|$ ? If potential  $V(r)$  can be Taylor-expanded, yes – usually assumed in literature. Thus, usual assumption is

$$\Delta_k = \Delta_0 (k_x + ik_y), \quad \forall \mathbf{k} \quad (\text{including } |k| \rightarrow 0).$$

For future simplicity, write for 2D  $p + ip$  state

$$\hat{\Omega}^\dagger \equiv \mathcal{N}' \sum_k |c_k| e^{i\varphi_k} a_k^+ a_{-k}^+$$

so that

$$\Psi_N^{p+ip} = (\Omega^\dagger)^{N/2} |vac\rangle$$

The 2D  $p + ip$  state has several intriguing properties:

1. Since by direct calculation  $[\hat{L}_z, \hat{\Omega}^\dagger] = \hbar\Omega^\dagger$

we have

$$\hat{L}_z |\Psi_N\rangle = \frac{N\hbar}{2} |\Psi_N\rangle$$

2. Nevertheless, if we take the limit  $|c_k| \rightarrow \theta(k_F - k)$ , we find

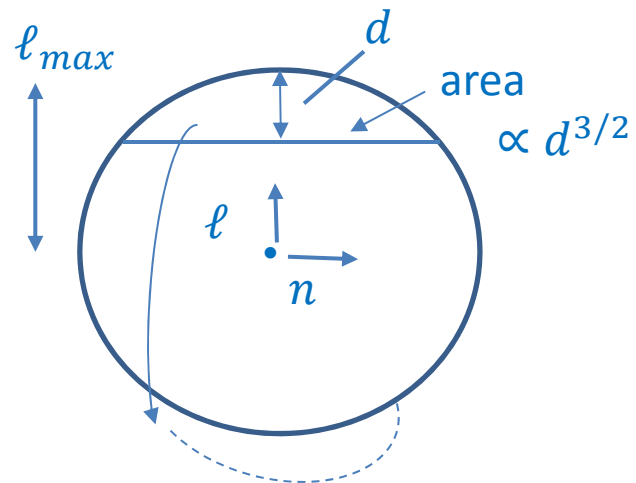
$$\begin{aligned} \Psi_N &= \left( \sum_{k < k_F} e^{i\varphi_k} a_k^+ a_{-k}^+ \right)^{N/2} |vac\rangle \\ &= \prod_{k < k_F} (e^{i\varphi_k} a_k^+ a_{-k}^+) |vac\rangle \\ &\equiv \left( \prod_{k < k_F} e^{i\varphi_k} \right) \prod_{k < k_F} a_k^+ a_{-k}^+ |vac\rangle \equiv \left( \prod_{k < k_F} e^{i\varphi_k/2} \right) |FS\rangle \end{aligned}$$

So since an overall phase factor is physically irrelevant,  $\hat{L}_z |\Psi_N\rangle = 0!$

Relevant observation:  
 how much energy does  
 it cost to polarize  
 Fermi sea to ang.  
 momentum  $N\hbar/2$ ?

Answer:  $O(N^{1/3})!$

(Moment of inertia  
 is not extensive)



Possible resolution of apparent inconsistency  
 of 1 and 2 (M. Stone):

In a finite system of dimension  $R$  as  $\Delta \rightarrow 0$ ,  
 Cooper-pair radius  $\xi \sim \hbar v_F / \Delta$  eventually  
 becomes  $> R$ . So, for  $\xi \ll R$   $L \sim N\hbar/2$ , for  
 $\xi \gg R$   $L \sim 0$ ?

3. Behavior of “molecular” wave function  $\varphi$  at large  
 $|\mathbf{r}_1 - \mathbf{r}_2|$ :

By inverting the general relation  $F_k = \frac{c_k}{1+|c_k|^2}$  and

substituting the equilibrium value of  $F_k, \Delta_k/2E_k,$

we obtain for  $k < k_F$  ( $\epsilon_k < \mu$ ) the relation

$$c_k = \frac{\Delta_k/2E_k}{\left(1 - \frac{|\epsilon_k - \mu|}{E_k}\right)}$$

which in the limit  $\epsilon_k \rightarrow 0$  reduces to  $\mu / 4\Delta_k^*$  ( $+0(\Delta^2 / \mu^2)$ ). Thus provided  $|\Delta(k)| \propto |k|$  for  $|k| \rightarrow 0$  as assumed,

$$c_k = \frac{\text{const}}{k_x - ik_y} \quad \text{as } k \rightarrow 0$$

Thus the F. T., the “molecular wave function”  $\varphi(\mathbf{r})(\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2)$ , behaves at large differences as

$$\varphi(r) \sim z^{-1} \quad (z \equiv x + iy)$$

and for these distances the many body GSWF has the “Pfaffian” form

$$\Psi_N \sim Pf \left\{ \frac{1}{z_i - z_j} \right\} \quad \leftarrow \text{Moore - Read form for } \nu = 5/2 \text{ QHE}$$



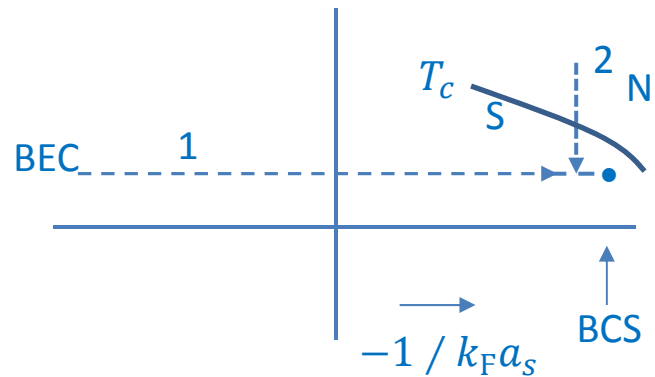
## 2. Anisotropic Cooper pairing: alternative approach

AC 2.8

The ground state of a  $p + ip$  Fermi superfluid looks “natural” when reached by path 1, much less so when matched by 2, since

(a)  $\Delta L$  at  $T_c \sim N$

(b) Cooper instability affects only states near Fermi surface, not far down in Fermi sea. So consider the ansatz

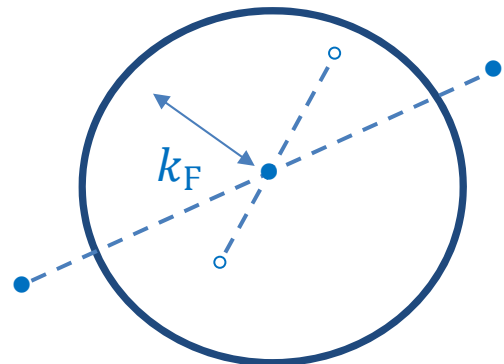


$$\Psi_N^{alt} \sim n \left( \sum_{k > k_F} c_k a_k^+ a_{-k}^+ \right)^M \left( \sum_{k < k_F} d_k a_{-k} a_k \right)^M |FS\rangle$$

(M  $\ll$  N)

where  $d_k$  is related to the  $c_k$  of the textbook approach (call it  $c_k^{(0)}$ ) by

$$d_k = \left( c_k^{(0)} \right)^{-1}$$



This reproduces the “standard” value of  $\langle n_k \rangle$ , since the number of holes in state  $k < k_F$  is  $\frac{|d_k|^2}{1+|d_k|^2}$ :

$$\langle n_k \rangle = 1 - \frac{|d_k|^2}{1 + |d_k|^2} = \frac{|c_k^{(0)}|^2}{1 + |c_k^{(0)}|^2}$$

It also reproduces the value of  $\langle a_k^+ a_{-k}^+ a_{-k'} a_{k'} \rangle$  for  $|\mathbf{k}|, |\mathbf{k}'|$  both above or both below  $k_F$ , but not for (e.g.)  $k > k_F, k' < k_F$ .

However this can be remedied by a small modification of  $\Psi_N$ :



put  $\Omega_+^\dagger \equiv \sum_{k > k_F} c_k a_k^+ a_{-k}^+$ ,  $\Omega_-^\dagger \equiv \sum_{k < k_F} d_k a_{-k} a_k$  and write

$$\Psi_N^{alt} \equiv \sum_M k_M (\Omega_+^\dagger \Omega_-^\dagger)^M |FS\rangle, k_M \text{ slowly varying in phase as } f(M)$$

(one possible implementation:

$$\Psi_N^{(alt)} \sim \int d\varphi (\exp i\varphi/2 \cdot \Omega_+^\dagger + \exp -i\varphi/2 \cdot \Omega_-^\dagger)^{N/2} |FS\rangle$$

then both  $\langle n_k \rangle$  and  $\langle a_k^+ a_k^+ a_{-k'} a_{k'} \rangle$  same for all  $k, k'$  (to order  $N^{-1/3}$ )

as in textbook approach  $\left( F_k (k < k_F) = \frac{d_k^*}{1+|d_k|^2} = \frac{c_k^{(0)}}{1+|c_k^{(0)}|^2} \right) \Rightarrow$

energy/particle of 2 states identical in thermodynamic limit.

At first sight  $\Psi_N^{alt}$  is just a rewriting of  $\Psi_N$  in different notation, as in the s-wave case. However,

$$[L_z, \Omega_+^\dagger] = \hbar \Omega_+^\dagger \quad \text{but} \quad [L_z, \Omega_-^\dagger] = -\hbar \Omega_-^\dagger$$

$$\Rightarrow \hat{L}_z |\Psi_N^{(alt)}\rangle = 0 ! \quad (+0(\Delta/E_F)^2 \text{ due to shift of } \mu \text{ in } S \text{ phase})$$

So ... which is right,  $\Psi_N$  or  $\Psi_N^{(alt)}$  (or maybe a hybrid wave function)?

A possible answer: both, or neither! The MBGS may be

**degenerate** within terms of relative order  $N^{-1/3}$  in thermodynamic limit.

Note:  $\Psi_N^{(alt)}$  almost certainly corresponds to a quite different behavior of  $\varphi(r)$  in the limit  $r \rightarrow \infty$ . Plausibly (but not proved): the modification to  $\varphi(r)$  from its  $N$  -state value  $\propto r^{-3}$ .



### 3. Fermionic quasiparticles: the textbook approach (BCS (isotropic) case)

Recall: in BCS formalism, even-no-parity (PNC) GS is written in form

$$\Psi_{\text{BCS}} = \prod_k (u_k + v_k a_{k\uparrow}^+ a_{-k\downarrow}^+) |vac\rangle.$$

$$\equiv \prod_k \Phi_k, \Phi_k \equiv u_k |00\rangle_k + v_k |11\rangle_k$$

$$u_k = u_{-k}, v_k = v_{-k}, u_k \text{ real}$$

We make standard Bogoliubov-Valatin transformation:

$$\alpha_{k\sigma}^+ = u_k a_{k\sigma}^+ - \sigma v_k^* a_{-k,-\sigma}$$

So (e.g.)

$$\alpha_{k\uparrow}^+ = u_k a_{k\uparrow}^+ - v_k^* a_{-k\downarrow}$$

and so

$$\begin{aligned} a_{k\uparrow}^+ |\Phi_k\rangle &\equiv (u_k a_{k\uparrow}^+ - v_k^* a_{-k\downarrow}) (u_k + v_k a_{k\uparrow}^+ a_{-k\downarrow}^+) |GS\rangle \\ &= u_k^2 a_{k\uparrow}^+ |vac\rangle + |v_k|^2 a_{k\uparrow}^+ |GS\rangle \\ &\quad \uparrow \text{ACR's!} \\ &\equiv \alpha_{k\uparrow}^+ |GS\rangle \equiv |1,0\rangle \end{aligned}$$

Similarly the operator

$$\alpha_{-k\downarrow}^+ \equiv u_k a_{-k\downarrow}^+ + v_k^* a_{k\uparrow}$$

when applied to the BCS groundstate, generates the state  $|01\rangle_k$ .

However, from the four operators  $a_{k\uparrow}^+, a_{k\uparrow}^*, a_{-k\downarrow}^+, a_{-k\downarrow}$  one can generate two other linearly independent (orthogonal) combinations:

$$\beta_{k\uparrow} \equiv v_k a_{k\uparrow}^+ + u_k a_{-k\downarrow}$$

$$\beta_{-k\downarrow} \equiv v_k a_{-k\downarrow}^+ - u_k a_{k\uparrow}$$

Applying these to the BCS groundstate gives, *e.g.*,

$$\begin{aligned} \beta_{k\uparrow} |\Phi_k\rangle &\equiv (v_k a_{k\uparrow}^+ + u_k a_{-k\downarrow})(u_k + v_k a_{k\uparrow}^+ a_{-k\downarrow}^+) |\text{GS}\rangle \\ &= v_k u_k a_{k\uparrow}^+ |\text{vac}\rangle - u_k v_k a_{k\uparrow}^+ |\text{GS}\rangle \equiv 0 \end{aligned}$$

and similarly for  $\beta_{k2}$ . So  $\beta_{k1}$  and  $\beta_{k2}$  are **pure annihilators**. At first sight this looks trivial, since  $\beta_{k\uparrow}$  is just the H.C. of  $\alpha_{-k\downarrow}^+$ , *i.e.*  $\alpha_{-k\downarrow}$ , and we are all used to the fact that the  $\alpha$ 's annihilate the ground state. But it's worth noting for future reference...



To summarize, in simple BCS theory the simplest MB energy eigenstates can be expressed in the form of a tensor product of occupation states  $\Phi_k$  referring to the pair of plane-wave states  $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ . The (even-numbered-parity) “ground pair” state is

$$\Phi_k^{GP} = u_k |00\rangle + v_k |11\rangle$$

There is a second “completely-paired” (even-numbered parity) state orthogonal to  $\Phi_k^{GP}$ , :

$$\Phi_k^{EP} = -v_k^* |00\rangle + u_k |11\rangle$$

which can in fact be generalized by successive application of  $\alpha_{k\uparrow}^+$  and  $\alpha_{-k\downarrow}^+$

The odd-number-parity energy eigenstates are

$$|10\rangle \equiv \alpha_{k\uparrow}^+ |\Phi_k^{GP}\rangle \quad \text{and} \quad |01\rangle \equiv \alpha_{-k\downarrow}^+ |\Phi_k^{GP}\rangle$$

while the operators  $\beta_{k\uparrow} \equiv \alpha_{-k\downarrow}$  and  $\beta_{-k\downarrow} \equiv \alpha_{k\uparrow}$  annihilate  $\Phi_k^{GP}$

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All the above analysis generalizes straightforwardly to the anisotropic case, including the  $(p + ip)$  state. (irrespective of whether we use the textbook or alternative approach\*).

\*In the latter,  $\Phi_k$  is simply  $|u_k|e^{-i\varphi_k}|00\rangle + |v_k||11\rangle$ .



So far, so good... But what if our Hamiltonian is more general:

$$\hat{H} = \sum_{\sigma\sigma'} \int dr \left( -\frac{\hbar^2}{2m} \delta_{\sigma\sigma'} \psi_{\sigma}^{\dagger}(\mathbf{r}) \nabla^2 \psi_{\sigma'}(\mathbf{r}) + U_{\sigma\sigma'}(\mathbf{r}) \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}(\mathbf{r}) \right) \\ + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \iint dr dr' V_{\alpha\beta\gamma\delta}(\mathbf{r}, \mathbf{r}') \psi_{\alpha}^{\dagger}(\mathbf{r}) \psi_{\beta}^{\dagger}(\mathbf{r}') \psi_{\gamma}(\mathbf{r}') \psi_{\delta}(\mathbf{r}) ?$$

We can still use our general definition of a “completely paired”  $N(=even)$  – particle state:

same!

$$\Psi_N = \mathcal{N} \cdot \mathcal{A} \cdot \{ \varphi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \varphi(\mathbf{r}_3\sigma_3, \mathbf{r}_4\sigma_4) \dots \varphi(\mathbf{r}_{N-1}\sigma_{N-1}, \mathbf{r}_N\sigma_N) \} \\ \equiv \mathcal{N}' \left( \sum_{\sigma\sigma'} \iint dr dr' \varphi(\mathbf{r}\sigma, \mathbf{r}'\sigma') \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}^{\dagger}(\mathbf{r}') \right)^{N/2} |vac\rangle$$

Theorem: can always find complete orthonormal set  $n, \bar{n}$  (i.e.  $\langle n, \bar{n}' \rangle = 0$ ,  $\langle n | n' \rangle = \delta_{nn'}$ ,  $\langle \bar{n}, \bar{n}' \rangle = \delta_{\bar{n}\bar{n}'}$ ) such that

$$\varphi(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \sum_n c_n \chi_n(r\sigma) \chi_{\bar{n}}(r'\sigma')$$

Thus, can write any completely paired state in the form

$$\Psi_N = \mathcal{N}'' \left( \sum_m c_m a_m^{\dagger} a_{\bar{m}}^{\dagger} \right)^{N/2} |vac\rangle$$

As long as we deal only with the even-number-parity states, we can continue the analogy to BCS:

$$\bar{\Psi}_{\text{BCS}} = \prod_m \Phi_m^{GP}, \quad \Phi_m^{GP} \equiv u_m |00\rangle + v_m |11\rangle, \quad |00\rangle \equiv |00\rangle_{m\bar{m}}, \text{ etc.}$$

$$c_m \equiv v_m/u_m, \quad |u_m|^2 + |v_m|^2 = 1$$

and the “excited-pair” state is given by

$$\Phi_m^{EP} = -v_m^* |00\rangle + u_m |11\rangle \quad (c_m \rightarrow -c_m^{*-1})$$

This is an energy eigenstate if  $\Phi_m^{GP}$  is, since  $\langle n_m \rangle \rightarrow 1 - \langle n_m \rangle$  and  $F_m \rightarrow -F_m$ .

In the BCS case we found the values of the  $c_k$ 's (or equivalently of the quantities  $\langle n_k \rangle$  and  $F_k$ ) by minimizing the sum of the single – particle and pairing terms in  $\langle \hat{H} \rangle$ . Can we do the same here? Since the functions  $\chi_n, \chi_{\bar{n}}$  are unknown a priori, our calculation should also find them. Suppose we write

$$U_m(\mathbf{r}) \equiv U_m \chi_m(\mathbf{r}\sigma), \quad V_m(\mathbf{r}) \equiv V_m \chi_{\bar{m}}(\mathbf{r}\sigma)$$

and minimize the s.p. + pairing terms with respect to the functions  $U_m(\mathbf{r}\sigma), V_m(\mathbf{r}\sigma)$ , subject to the orthogonality constraints. ( $(U_m, U_{m'}) \sim \delta_{mm'}$ , etc.). The resulting equations are, formally, exactly the standard BdG equations (see below) but with **much stronger orthogonality constraints**. So we can obtain an explicit solution this way only in special cases (e.g.  $\bar{m} = \text{TR of } m$ ).



Now let's turn to the odd-number-parity states. By exact analogy with the BCS case, the combinations

$$\beta_m \equiv v_m a_m^+ + u_m a_{\bar{m}}$$

$$\beta_{\bar{m}} \equiv v_m a_{\bar{m}}^+ - u_m a_m$$

are pure annihilators:  $\beta_m |\Psi_N\rangle = \beta_{\bar{m}} |\Psi_N\rangle = 0$  Note that any linear combination of PA's is itself a PA! Moreover the states

$$\alpha_m^+ \equiv u_m a_m^+ - v_m^* a_{\bar{m}} \equiv (\beta_{\bar{m}})^\dagger$$

$$\alpha_{\bar{m}}^+ \equiv u_m a_{\bar{m}}^+ + v_m^* a_m \equiv (\beta_m)^\dagger$$

create the states  $|1,0\rangle_m$  and  $|0,1\rangle_m$  respectively

$|1,0\rangle_m \equiv$  occupied,  $\bar{m}$  empty, etc.) and  $\alpha_m^+ \alpha_{\bar{m}}^+$  generates the "excited pair" state  $\Phi_m^{EP}$ . However, these two states are **not in general energy eigenstates**. This is fairly obvious, since when written in the (basis of the  $\chi_m$  and  $\chi_{\bar{m}}$  even the single-particle term  $\hat{H}$  is nondiagonal. So the odd-parity energy eigenstates must be linear combinations of the states  $|1,0\rangle_m$  and  $|0,1\rangle_m$ :

$$\gamma_i^\dagger = \sum_m (\lambda_{im} \alpha_m^+ + \mu_{im} \alpha_{\bar{m}}^+)$$

How to find these linear combinations? Standard method is mean-field (BdG) approach: in spirit of BCS, factorize potential term in Hamiltonian:

$$V \psi_\alpha^\dagger(r) \psi_B^\dagger(r') \psi_\gamma(r') \psi_\delta(r) \rightarrow \left\langle \psi_\alpha^\dagger(r) \psi_\beta^\dagger(r') \psi_\gamma(r') \psi_\delta(r) \right\rangle + \left\langle \psi_\gamma(r') \psi_\delta(r) \right\rangle \psi_\alpha^\dagger(r) \psi_\beta^\dagger(r')$$

and define

$$\Delta_{\alpha\beta}(r, r') \equiv \sum_{\gamma\delta} V_{\alpha\beta\gamma\delta}(r, r') \langle \psi_\gamma(r') \psi_\delta(r) \rangle$$





Then the effective mean-field Hamiltonian is bilinear in  $\psi$  and  $\psi^\dagger$ :

$$\hat{H}_{mf} = \sum_{\alpha\beta} \int dr \left( \psi_\alpha^\dagger(r) \hat{H}_o \psi_\beta(r) \right) + \frac{1}{2} \sum_{\alpha\beta} \iint dr dr' \left\{ \Delta_{\alpha\beta}(\mathbf{r}, \mathbf{r}') \psi_\alpha^\dagger(r) \psi_\beta^\dagger(r') + H.C. \right\}$$

where the quantity  $\langle \psi_\gamma(r') \psi_\delta(r) \rangle$  occurring in  $\Delta_{\alpha\beta}$  must eventually be determined self-consistently. We now seek the creation operators of odd-parity energy eigenstates in the form

$$\gamma_i^\dagger = \int dr \{ u(r) \psi^\dagger(r) + v(r) \psi(r) \}$$

with the normalization constraint

$$\int |u(r)|^2 + |v(r)|^2 dr = 1$$

in words, we create an extra particle with wave function  $u(r)$  **and an extra hole** with wave function  $v(r)$ . Demanding that

$$[\hat{H}_{mf}, \gamma_i^\dagger] = E_i \gamma_i^\dagger$$

yields the famous Bogoliubov-de Gennes (BdG) equations, which in general, because of the spin degree of freedom, are  $4 \times 4$ : here I give for simplicity the version for a single spin species (but keep the spatial “nonlocality”):



$$\hat{H}_o u_i(\mathbf{r}) + \int \Delta(\mathbf{r}, \mathbf{r}') v_i(\mathbf{r}') dr' = E_i u_i(\mathbf{r})$$

$$\int \Delta^*(\mathbf{r}, \mathbf{r}') u_i(\mathbf{r}') dr' - \hat{H}_o^* v_i(\mathbf{r}) = E_i v_i(\mathbf{r})$$

or schematically

$$\begin{pmatrix} \hat{H}_o & \Delta \\ \Delta & -\hat{H}_o^* \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

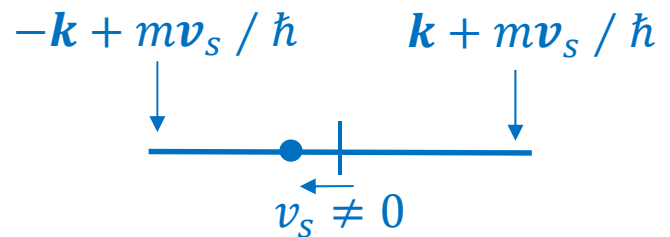
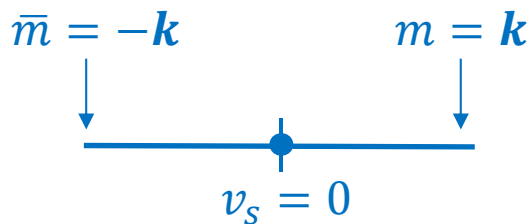
While the  $u$ 's do not in general by themselves form an orthonormal set, the spinors  $(u, v)$  do, *i.e.*

$(u_i, u_j) + (v_i, v_j) = \delta_{ij}$  (generated by equations themselves). Hence the set of  $\gamma_i^\dagger$  form a complete set of anticommuting Fermi operators, with  $\gamma_i |\Psi_{\text{BCS}}\rangle = 0$ .

It is often pointed out in the literature that if  $\begin{pmatrix} u_i \\ v_i \end{pmatrix}$  solves the BdG equations with energy eigenvalue  $E_i$ , then  $\begin{pmatrix} -v_i^* \\ u_i^* \end{pmatrix}$  solves them with eigenvalue  $-E_i$ , and so one says that this combination creates a “negative-energy state”. But this is illusory: the corresponding operator (call it  $\tilde{\gamma}_i^\dagger$ ) is actually a combination of pure annihilators and hence itself simply **a pure annihilator** (in fact, with a  $\pi$  rotation of  $v$  relation to  $u$ , it is just  $\gamma_i$  ).

Problems with the MF-BdG approach:

(a) Galilean invariance: (simple BCS problem)



Rest frame of condensate

$$\alpha_m^+ = u_k a_{k\uparrow}^+ - v_k^* a_{-k\downarrow}$$

$$P = \hbar(|u_k|^2 \mathbf{k} - |v_k|^2 (-\mathbf{k}))$$

$$= \hbar \mathbf{k} \sqrt{\phantom{x}}$$

$$(\equiv \mathbf{P} - \mathbf{P}_0)$$



Total momentum of  
groundstate (= 0)

Frame moving with velocity  
 $v_s$  w.r.t. condensate:

$$(\alpha_m^+)' = u_k a_{k+mv_s/\hbar}^+ - v_k^* a_{-k+mv_s/\hbar}$$

$$(\mathbf{P} - \mathbf{P}_0)' = \hbar(|u_k|^2 \mathbf{k} + mv_s/\hbar)$$

$$- |v_k|^2 (-\mathbf{k} + mv_s/\hbar))$$

$$= \hbar \mathbf{k} + (|u_k|^2 - |v_k|^2) m v_s$$

But: Galilean invariance requires simply

$$(\mathbf{P} - \mathbf{P}_0)' = (\mathbf{P} - \mathbf{P}_0) + m v_s !!$$

note discrepancy **depends on  $u_k, v_k$** , hence cannot be fixed simply  
by involving “spontaneously broken  $U(1)$  symmetry”.



Solution: when creating “hole” component of odd-parity state,

**MUST ADD A COOPER PAIR!**

thus, correct “Bog QP” creation operator is

$$\alpha_m^+ = u_m a_m^+ - v_m^* a_{\bar{m}} \hat{C}^+ \quad \left( \hat{C}^+ \equiv \mathcal{N} \sum_m c_m a_m^+ a_{\bar{m}}^+ \right)$$

For condensate at rest, changes nothing (still have  $(\mathbf{P} - \mathbf{P}_o) = \hbar \mathbf{k}$ ).  
But for condensate moving, adds an extra  $2 |v_k|^2 m v_s$ , so that

$$\begin{aligned} (\mathbf{P} - \mathbf{P}_o)' &= \hbar \left\{ \begin{array}{l} |u_k|^2 (\mathbf{k} + m \mathbf{v}_s / \hbar) - |v_k|^2 (-\mathbf{k} + m \mathbf{v}_{-s} / \hbar) + \\ 2 |v_k|^2 m \mathbf{v}_s / \hbar \end{array} \right\} \\ &= \hbar \mathbf{k} + m \mathbf{v}_s = (\mathbf{P} - \mathbf{P}_o) + m \mathbf{v}_s \quad \text{as required.} \end{aligned}$$

- (6) NMR of Majorana fermions (M.A. Silaev, PRB **84** 144508 (2011)): consistent calculation based on MF Hamiltonian  $\rightarrow$  spectral weight in longitudinal resonance absorption above Larmor frequency. (independent of dipole coupling constant  $g_D$ )

Problem: violates sum rule! (for  $g_D = 0$ ,  $\int \omega \chi''(\omega) d\omega = 0$ , and for nonzero  $g_D$ ,  $\propto g_D$ )

Solution: need to consider response also of added Cooper pair (E. Taylor et al., arXiv:1412.7153)

Moral: In any situation where Cooper pairs are behaving “nontrivially,”

**MUST ENFORCE PARTICLE NUMBER CONSERVATION!**

