Topological Superfluids: Majorana Fermions

The subject of topological superfluids, though they werel not originally called by that name, actually antedates that of topological insulators, and has played a major role in the attempt to implement topological quantum computation (see lectures 25 and 28). Crudely speaking, the analogy with TI's goes as follows: in a crystalline solid with spin-orbit coupling, the single-particle energy eigenstates are hybridized quantum superpositions of two different levels of the original Hamiltonian (that without SOI). If the hybridizing SOI has a suitable form and magnitude, the system will be a topological insulator, and in that case one inevitably finds, at the surface, $E = 0$ excitations which are a superposition of the two bands with equal weight (see lecture 22). In the case of a Fermi superfluid, the "unhybridized" Hamiltonian is the kinetic energy, so that the two "bands" of single-particle excitations are the particles and the holes, and at this stage there is no energy gap (corresponding to $M = 0$ in the "toy model" of lecture 22). The role of the hybridizing term is played by the"off-diagonal field" in the BCS theory. When this is taken into account the single-particle eigenstates are hybridized quantum superpositions of a "particle" and a "hole" state [1]; the energy gap is now generally speaking nonzero in the bulk. However, if the off-diagonal field has an appropriate form and magnitude, we may as in the TI case find $E = 0$ excitations at a surface, or more generally in regions where the off-diagonal field has sharp discontinuities (e.g. at a vortex). Similarly to the TI case, these $E = 0$ excitations (and, sometimes, the nonzero-k branch derived from them) are an equal superposition of a particle and a hole, they have very exotic properties (in particular, they are their own antiparticles, and in the case of a metal have no net charge); they are called $Majorana$ $fermions$. Thus the analogy with the case of a TI is most direct in the context of the excitations at a surface or other singularity, and less so in the context of the bulk.

We now give a brief account of the "orthodox" approach to topological Fermi superfluids [2] Since it turns out that systems which form Cooper pairs in a spin singlet state (such as the electrons in a classic BCS superconductor) cannot show interesting topological effects, we may as well specialize right away to the case of spin triplet pairing. In the simplest case of such pairing (which is believed to be realized in the A phase of superfluid ^3He and possibly in some superconductors) the spin axes can be chosen so that only parallel-spin particles are paired ($\uparrow\uparrow, \downarrow\downarrow$) ("equal-spin-pairing (ESP) states"), and to a first approximation we can treat the $\uparrow\uparrow$ and $\downarrow\downarrow$ pairs as independent systems so that the spin index drops out of the problem. Thus in the following discussion we shall for simplicity treat the case of (fictitious) "spinless" fermions.

The generic "particle-conserving" BCS ansatz for N spinless fermions (N even) moving

[1] At least according to the standard presentations: c.f. however below.

[2] See the chapters by T. Hughes in the Bernevig book.

in free space is

$$\Psi_N = \left(\sum_{\boldsymbol{k}} c_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a^\dagger_{-\boldsymbol{k}}\right)^{N/2} |\mathrm{vac}\rangle, \text{ where } c_{\boldsymbol{k}} = -c_{-\boldsymbol{k}} \text{ (from antisymmetry)} \tag{1}$$

In the literature, it is more common to use the PNC (particle non-conserving) form:

$$\Psi_{\mathrm{BCS}} = \prod_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a^\dagger_{-\boldsymbol{k}})|\mathrm{vac}\rangle, \ u_{\boldsymbol{k}} = u_{-\boldsymbol{k}}, \ v_{\boldsymbol{k}} = -v_{-\boldsymbol{k}} \tag{2}$$

with

$$u_{\boldsymbol{k}} \equiv \frac{1}{(1+|c_{\boldsymbol{k}}|^2)^{1/2}}, \ v_{\boldsymbol{k}} \equiv \frac{c_{\boldsymbol{k}}}{(1+|c_{\boldsymbol{k}}|^2)^{1/2}} \tag{3}$$

so that $|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 \equiv 1$, $c_{\boldsymbol{k}} = v_{\boldsymbol{k}}/u_{\boldsymbol{k}}$.
Two important quantities in BCS theory are

$$\langle n_{\boldsymbol{k}}\rangle = |v_{\boldsymbol{k}}|^2, \ F_{\boldsymbol{k}} \equiv \langle a_{-\boldsymbol{k}} a_{\boldsymbol{k}}\rangle_{\mathrm{BCS}} = u^*_{\boldsymbol{k}} v_{\boldsymbol{k}} = \frac{c_{\boldsymbol{k}}}{1+|c_{\boldsymbol{k}}|^2} \tag{4}$$

The Fourier transform of $F_{\boldsymbol{k}}$, $F(\boldsymbol{r})$ ($\equiv \langle\hat\psi(0)\hat\psi(\boldsymbol{r})\rangle_{\mathrm{BCS}}$) plays the role of the wave function of the Cooper pairs.

In standard BCS ("mean-field") theory, one minimizes the sum of the kinetic energy $\langle T\rangle = \sum_{\boldsymbol{k}} (\epsilon_{\boldsymbol{k}} - \mu)\langle n_{\boldsymbol{k}}\rangle$ and the "pairing" part of the potential energy

$$\langle V_{\mathrm{pair}}\rangle = \sum_{\boldsymbol{k}\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} \langle a^\dagger_{\boldsymbol{k}} a^\dagger_{-\boldsymbol{k}} a_{-\boldsymbol{k}'} a_{\boldsymbol{k}'}\rangle \qquad \big(V_{\boldsymbol{k}\boldsymbol{k}'} \equiv \langle \boldsymbol{k},\ -\boldsymbol{k}|V|\boldsymbol{k}',\ -\boldsymbol{k}'\rangle\big) \tag{5}$$

By making the"mean-field" ansatz (which for the "truncated" potential energy given by eqn. (5) can be shown to be exact in the thermodynamic limit) $< a^+_k a^+_{-k} a_{-k'}, a_{k'} >=$ $< a^+_k a^+_{-k} > \cdot < a_{-k'} a_{k'} > \equiv F^*_k F_{k'}$

Then the pair wavefunction $F_{\boldsymbol{k}}$ satisfies the Schrödinger-like equation:

$$2E_{\boldsymbol{k}} F_{\boldsymbol{k}} = -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} F_{\boldsymbol{k}'} \tag{6}$$

with

$$E_{\boldsymbol{k}} \equiv \frac{|\epsilon_{\boldsymbol{k}} - \mu|}{(1-4|F_{\boldsymbol{k}}|^2)^{1/2}} \equiv E_{\boldsymbol{k}}[F_{\boldsymbol{k}}] \tag{7}$$

which is a disguised form of the BCS gap equation:

$$\begin{aligned} \Delta_{\boldsymbol{k}} &= -\textstyle\sum_{\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} \Delta_{\boldsymbol{k}'}/2E_{\boldsymbol{k}'} \\ E_{\boldsymbol{k}} &= \sqrt{(\epsilon_{\boldsymbol{k}} - \mu)^2 + |\Delta_{\boldsymbol{k}}|^2} \end{aligned} \tag{8}$$

Note that the gap equation refers to the Cooper pairs (condensate). However, in the spatially uniform case $E_{\boldsymbol{k}} \equiv \sqrt{(\epsilon_{\boldsymbol{k}}-\mu)^2+|\Delta_{\boldsymbol{k}}|^2}$ also represents the energy of excitation of single quasiparticle of momentum $\boldsymbol{k}$: in the PNC formalism

$$\Psi_0 = \prod_{\boldsymbol{k}>0} \left(u_{\boldsymbol{k}}|00\rangle_{\boldsymbol{k}} + v_{\boldsymbol{k}}|11\rangle_{\boldsymbol{k}}\right) \equiv \prod_{\boldsymbol{k}>0} \Phi_{\boldsymbol{k}}^{(0)} \tag{9}$$

$$\Psi^{k0} = \prod_{\boldsymbol{k}\neq\boldsymbol{k}_0} \Phi_{\boldsymbol{k}}^{(0)} \cdot |01\rangle_{\boldsymbol{k}_0} \qquad (or \ \ldots|10\rangle_{\boldsymbol{k}_0}) \tag{10}$$

where $|01\rangle_{\boldsymbol{k}}$ means the state with $\boldsymbol{k}$ empty and $-\boldsymbol{k}$ occupied, etc.

In 2D, a possible p-wave solution of gap equation is

$$F_{\boldsymbol{k}} = (k_x+ik_y)f(|\boldsymbol{k}|)\big(\equiv (p_x+ip_y)f(|\boldsymbol{p}|), \text{ hence "}p+ip\text{" }\big) \tag{11}$$

then also $\Delta_{\boldsymbol{k}} = (k_x+ik_y)g(|\boldsymbol{k}|)$, $E_{\boldsymbol{k}} = h(|\boldsymbol{k}|)$ ($\hat{\boldsymbol{k}}-$indep.) $\neq 0$, $\forall\boldsymbol{k}$.

It is important to note that the energetics is determined principally by the form of $F_{\boldsymbol{k}}$ close to Fermi energy ($|\epsilon_{\boldsymbol{k}}-\mu| \lesssim \Delta_0 \leftarrow\equiv |\Delta_{\boldsymbol{k}}|_{\boldsymbol{k}=\boldsymbol{k}_{\rm F}}$). But for TQC applications, we may need to know $F_{\boldsymbol{k}}$ very far from the Fermi surface ($k\to 0$ and/or $k\to\infty$). Note that in most real-life cases, (^3He-A and Sr_2RuO_4) we have

$$\Delta_0 \ll \mu \qquad\qquad (\text{"BCS limit"}) \tag{12}$$

but this need not be true a priori, and in fact it seems likely that the case $\Delta_o \sim \mu$ will be realized in the not too distant future in an ultracold alkali Fermi gas having a p-wave resonance. We will discuss the $(p+ip)$ Fermi superfluid in detail in lecture 28.

Bogoliubov-de Gennes (BdG) equations

In the simple spatially uniform case, a simple relation exists between the "completely paired" state of $2N$ particles and the $(2N+1)$-particle states ("quasiparticle excitations")– the BCS wavefunction is product of states $(\boldsymbol{k},-\boldsymbol{k})$, the excitations involve breaking single pair as in eqn. (10). In the general case no such simple relationship exists: nevertheless, the BdG equations enable us to relate $(2N+1)$-particle states to $(2N)$-particle GS. (They do not tell us directly about the $(2N)$-particle GS itself). The standard (PNC) approach goes as follows: The exact Hamiltonian is

$$\hat{H}-\mu\hat{N} = \int d\boldsymbol{r}\psi^\dagger(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\nabla^2+U(\boldsymbol{r})-\mu\right) + \iint d\boldsymbol{r}d\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')V(\boldsymbol{r}-\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) \tag{13}$$

where $U(\boldsymbol{r})$ is the single-particle potential. In PE term, we make the generalized mean-field approximation:

$$\psi^\dagger(\boldsymbol{r'})\psi^\dagger(\boldsymbol{r})V(\boldsymbol{r}-\boldsymbol{r'})\psi(\boldsymbol{r'})\psi(\boldsymbol{r}) \to \Delta(\boldsymbol{r},\ \boldsymbol{r'})\psi^\dagger(\boldsymbol{r'})\psi^\dagger(\boldsymbol{r}) + H.C. \tag{14}$$

where

$$\Delta(\boldsymbol{r},\ \boldsymbol{r'}) \equiv \int V(\boldsymbol{r}-\boldsymbol{r'})\langle\psi(\boldsymbol{r'})\psi(\boldsymbol{r})\rangle \quad (=\text{c-number}) \tag{15}$$

So:

$$\hat{H}-\mu\hat{N} = \int d\boldsymbol{r}\hat{\psi}^\dagger(\boldsymbol{r})\hat{H}_0\hat{\psi}(\boldsymbol{r}) + \left\{\iint d\boldsymbol{r}d\boldsymbol{r'}\Delta(\boldsymbol{r},\boldsymbol{r'})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r'}) + \text{H.c.}\right\} \tag{16}$$

which is a bilinear form and can be diagonalized

In this (PNC) formalism, the GS is a superposition of even-N states. Similarly, the excitations are superpositions of odd-N states and are generated by operators of the form (operating on the GS)

$$\gamma_n^\dagger = \int d\boldsymbol{r}\left\{u_n(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}) + v_n(\boldsymbol{r})\psi(\boldsymbol{r})\right\} \tag{17}$$

with (positive) energies E_n (so $\hat{H}-\mu\hat{N} = \sum_n E_n\gamma_n^\dagger\gamma_n + \text{const.}$)

To obtain the eigenvalues E_n and eigenfunctions $u_n(\boldsymbol{r})$, $v_n(\boldsymbol{r})$ of the MF Hamiltonian, we need to solve the equation

$$[\hat{H}-\mu\hat{N}, \gamma_n^\dagger] = E_n\gamma_n^\dagger \tag{18}$$

Explicitly, this gives the BdG equations

$$\hat{H}_0 u_n(\boldsymbol{r}) + \int \Delta(\boldsymbol{r},\boldsymbol{r'})v_n(\boldsymbol{r'})d\boldsymbol{r'} = E_n u_n(\boldsymbol{r}) \tag{23a}$$

$$\int \Delta^*(\boldsymbol{r},\boldsymbol{r'})u_n(\boldsymbol{r'})d\boldsymbol{r'} - \hat{H}_0^* v_n(\boldsymbol{r}) = E_n v_n(\boldsymbol{r}) \tag{23b}$$

$$\left(\hat{H}_0 \equiv -\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}) - \mu\right)^{\ddagger}$$

General properties of solutions of BdG equations:

1. For $E_n \neq E_{n'}$, the spinors $\binom{u_n(\boldsymbol{r})}{v_n(\boldsymbol{r})}$ are mutually orthogonal, i.e., we can take

$$(u_n,\ u_{n'}) + (v_n,\ v_{n'}) = \delta_{nn'} \qquad \left((f,\ g) \equiv \int f^*(\boldsymbol{r})g(\boldsymbol{r})\,d\boldsymbol{r}\right) \tag{24}$$

‡Note that in absence of magnetic vector potential, $\hat{H}_0^* = \hat{H}_0$.

2. If $\binom{u}{v}$ is a solution with energy E_n, then $\binom{v^*}{-u^*}$ is a solution with energy $-E_n$. For $E_n \neq 0$ the negative-energy solutions are conventionally taken to describe the "filled Fermi sea."

3. Under special circumstances, it may be possible to find a solution corresponding to $E_n = 0$ *and* $u_n(\boldsymbol{r}) = v_n^*(\boldsymbol{r})$. In this case

$$\begin{aligned}\hat{\gamma}_n &\equiv \int d\boldsymbol{r}\{u_n^*(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}) + v_n^*(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\} \\ &= \int d\boldsymbol{r}\{v_n(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}) + u_n(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\} \equiv \hat{\gamma}_n^\dagger\end{aligned} \tag{25}$$

   i.e., the "particle" is its own antiparticle! Such a situation is said to describe a *Majorana fermion* (MF). (Note: this can only happen when the paired fermions have parallel spin, otherwise particle and antiparticle would differ by their spin. This is why superconductors with spin singlet pairing cannot sustain Majorana fermions.)

The above conclusions prima facie rely heavily on the BdG equations, which in turn rest on the assumption of "spontaneously broken U(1) gauge symmetry". So we now need to raise the question: Can we do without this assumption?

The answer turns out to be yes. Recall the result for a translationally invariant system in simple BCS theory: (up to normalization), for even N, PC $\to \Psi_N = \left[\sum_{\boldsymbol{k}} c_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger\right]^{N/2} |\text{vac}\rangle$. If we select the pair of states $(\boldsymbol{k}, -\boldsymbol{k})$, this can be written

$$\Psi_N = \tilde{\Psi}_N^{(\boldsymbol{k})}|00\rangle_{\boldsymbol{k}} + c_{\boldsymbol{k}}\tilde{\Psi}_{N-k}^{(\boldsymbol{k})}|11\rangle_{\boldsymbol{k}} \tag{26}$$

where

$$\tilde{\Psi}_N^{(\boldsymbol{k})} \equiv \left(\sum_{\boldsymbol{k}'\neq\boldsymbol{k}} c_{\boldsymbol{k}'} a_{\boldsymbol{k}'}^\dagger a_{-\boldsymbol{k}'}^\dagger\right)^{N/2} |\text{vac}\rangle$$

or with normalization

$$\Psi_N = u_{\boldsymbol{k}}^* C^\dagger \tilde{\Psi}_{N-z}^{(\boldsymbol{k})}|00\rangle_{\boldsymbol{k}} + v_{\boldsymbol{k}}^*\tilde{\Psi}_{N-k}^{(k)}|11\rangle_{\boldsymbol{k}} \quad (|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1)$$

where

$$C^\dagger \equiv \mathcal{N}\left(\sum_{\boldsymbol{k}'\neq\boldsymbol{k}} c_{\boldsymbol{k}} a_{\boldsymbol{k}'}^\dagger a_{-\boldsymbol{k}'}^\dagger\right)$$

turns the *normalized* state $\Psi_{N-1}^{(\boldsymbol{k})}$ into the *normalized* state $\Psi_N^{(\boldsymbol{k})}$.

Now consider the $N+1$-particle states (odd total particle number). A simple ansatz for such a state is the (normalized) state

$$|N+1:\boldsymbol{k}\rangle = \tilde{\Psi}_N^{(\boldsymbol{k})}|10\rangle_{\boldsymbol{k}} \qquad \text{(or } \tilde{\Psi}_N^{(\boldsymbol{k})}|01\rangle_{\boldsymbol{k}}) \tag{27}$$

This is obtained from the expression (26) by the prescription

$$|N+1:\boldsymbol{k}\rangle = \left(u_{\boldsymbol{k}}a_{\boldsymbol{k}}^{\dagger} + v_{\boldsymbol{k}}a_{-\boldsymbol{k}}C^{\dagger}\right)\Psi_N \equiv \hat{\alpha}_{\boldsymbol{k}}^{\dagger}\Psi_N \tag{28}$$

Unsurprisingly, this state turns out to be an energy eigenstate with energy (relative to $E_0(N)+\mu$) of $E_{\boldsymbol{k}} \equiv \sqrt{(\epsilon_{\boldsymbol{k}}-\mu)^2+|\Delta_{\boldsymbol{k}}|^2}$ Note that one can form another expression of this type, namely

$$\hat{\beta}_{\boldsymbol{k}}^{\dagger} \equiv v^* a_{\boldsymbol{k}}^{\dagger} - u_{\boldsymbol{k}}^* a_{-\boldsymbol{k}}C^{\dagger} \tag{29}$$

$$\text{such that} \qquad \hat{\beta}_{\boldsymbol{k}}^{\dagger}\Psi_N \equiv 0$$

i.e., $\hat{\beta}_{\boldsymbol{k}}^{\dagger}$ is a pure annihilator. An arbitrary operator of the form $\lambda a_{\boldsymbol{k}}^{\dagger} + \mu a_{-\boldsymbol{k}}$ can be expressed as a linear combination of $\hat{\alpha}_{\boldsymbol{k}}^{\dagger}$ and $\hat{\beta}_{\boldsymbol{k}}^{\dagger}$. For each 4-D Hilbert space $(\boldsymbol{k},-\boldsymbol{k})$ there are 2 quasiparticle creation operators and 2 pure annihilators.

Generalization to non-translationally-invariant case

Let's assume, for the moment, that the even-N groundstate is perfectly paired, i.e., that

$$\Psi_N(\equiv|N:0\rangle) = \mathcal{N}\left[\iint d\boldsymbol{r}d\boldsymbol{r'}\,K(\boldsymbol{r}\boldsymbol{r'})\psi^{\dagger}(\boldsymbol{r})\psi^{\dagger}(\boldsymbol{r'})\right] \tag{30}$$

where $K(\boldsymbol{r'})$ is some antisymmetric function. Then there exists a theorem[4] that we can always find an orthonormal set $\{m,\,\overline{m}\}$ such that Ψ_N can be written

$$\Psi_n = \mathcal{N}\cdot\left(\sum_m c_m a_m^{\dagger}a_{\overline{m}}^{\dagger}\right)^{N/2}|\text{vac}\rangle \qquad (\text{i.e. } (m,m') = (\overline{m},\overline{m}') = \delta_{mm'},\ (m,\overline{m}')=0) \tag{31}$$

We could now proceed by analogy with the translation-invariant case by constructing the quantity $\tilde{\Psi}_N^{(m)} \equiv \left(\sum_{m'\neq m} c_m a_{m'}^{\dagger}a_{\overline{m}'}^{\dagger}\right)^{N/2}|\text{vac}\rangle$, etc. Then if we define $c_m = v_m/u_m$ as in that case, the operators $\hat{\beta}_m^{\dagger} \equiv v_m^* a_m^{\dagger} - u_m^* a_{\overline{m}}$ are pure annihilators (as of course are any linear combinations of them). However, in general, in contrast

[4] See e.g., Yang, RMP **34**, 694 (1962) lemma in Appendix A.

with the translation-invariant case, states of the form $|N_1 : m\rangle = \tilde{\Psi}_N^{(m)}|01\rangle_m$ are not energy eigenstates. The true $N+1$-particle energy eigenstates are superpositions:

$$\begin{aligned} |N+1 : E_n\rangle &= \sum_m q_m(E_n)|N+1 : E_m\rangle + (m \to \overline{m}) \\ &\sum_m |q_m(E_n)|^2 + (m \to \overline{m}) = 1 \end{aligned} \tag{32}$$

Equivalently, we can write

$$|N+1 : E_n\rangle = \left\{ \sum_m (\tilde{u}_m a_m^\dagger + \tilde{v}_m a_{\overline{m}} C^\dagger) + (m \to \overline{m}) \right\} |\Psi_N\rangle \tag{33}$$

$$\equiv \int \Big[u(\boldsymbol{r})\psi^\dagger + v(\boldsymbol{r})\psi(\boldsymbol{r})C^\dagger \Big] \; |\Psi_N\rangle \qquad (\tilde{u}_m \equiv q_m u_m, \; \tilde{v}_m \equiv q_m v_m)$$

which (apart from the PC factor $C^\dagger$) is exactly the form postulated in the BdG approach. The functions $u(\boldsymbol{r})$ and $v(\boldsymbol{r})$ are now determined by solving the BdG equations exactly as in the standard approach. But note we never had to relax particle conservation!

Nature of "Majorana Fermions"

In the standard approach, the BdG equations are equivalent to the statement that $[\hat{H}_{\text{BdG}}, \gamma_n^\dagger] \; |\Psi_N\rangle = E_n \gamma_n^\dagger |\Psi_N\rangle$. For $E_n > 0$ the interpretation is unambiguous: $\gamma_n^\dagger|\Psi_N\rangle$ is an $N+1$-particle energy eigenstate with energy $(\mu+)E_n$ ("Dirac-Bogoliubov fermion"). But we know that if $(u, \; v)$ is a solution with $E_n > 0$, then $(v^*, \; -u^*)$ is a solution with energy eigenvalue $-E_n$. These negative energy solutions are usually interpreted in terms of the "filled Dirac sea."

However, the above equation is entirely compatible with the statement that $\gamma_n^\dagger|\Psi_N\rangle \equiv 0$! Hence, in the present PC approach, we interpret the "negative energy" $\gamma_n^\dagger$'s as pure annihilators. There must be exactly as many pure annihilators as there are DB fermion states. Suppose there exists a DB fermion with $E = 0$, and wavefunction (u, v) satisfying the BdG equations. The corresponding pure annihilator $\beta_0^\dagger$ automatically satisfies them, also with $E = 0$ (indeed any E!). Then let $\alpha_0^\dagger$ create the $E = 0$ DB fermion, and consider $\gamma_0^\dagger = e^{i\pi/4}(\alpha_0^\dagger + i\beta_0^\dagger)$. The wavefunction (u, v) corresponding to $\gamma_0^\dagger|\Psi_N\rangle$ obviously satisfies the BdG equations with $E = 0$, and moreover satisfies $u(\boldsymbol{r}) = v^*(\boldsymbol{r})$. Hence it conforms exactly to the definition of a "Majorana fermion." A second MF is generated by $e^{i\pi/4}(\alpha_0^\dagger - i\beta_0^\dagger)$.

Conclusion: In the PC representation, a "Majorana fermion" is nothing but a quantum superposition of a real "Dirac-Bogoliubov" fermion ($N+1$)-particle energy eigenstate) and a pure annihilator.

Consider in particular the case where $\alpha_0^\dagger = \alpha_1^\dagger + i\alpha_2^\dagger$ with 1 and 2 referring to spatially distant positions. Then the two MF's will each be localized, at 1 and 2 respectively. Or putting it the other way around: any pair of (localized) MF solutions can be combined to give a (delocalized, "split") DB fermion. This of course raises the question: Can we be sure that there will always be an even number of MF solutions? The answer turns out to be yes, although the general proof is not trivial. In simple cases such as the Kitaev quantum wire the statement can be explicity verified, see below.

Illustration: An (ultra-)toy model

Consider N (=even) spinless fermions that can occupy (a) a "bath" of states that need not be specified in detail, or (b) two specific states 0, 1 ("system"). We use a notational convention such that whenever the number of particles in the "system" changes by $+2(-2)$, the operator $C(C^\dagger$ is applied to the bath so as to conserve particle number. Then the effect of the bath is to supply to the effective (BdG-type) Hamiltonian of the system a term of the form

$$\Delta a_0^\dagger a_1^\dagger + \text{H.c.} \tag{34}$$

There will also be in general a "tunnelling" term, of the form

$$t a_0^\dagger a_1 + \text{H.c.} \tag{35}$$

and a term of the form $U_0 a_0 a_0 + U_1 a_1^\dagger a_1$, which we will set = 0. Let's make the special choice

$$\Delta = it \tag{36}$$

and measure energies in units of t. Then

$$\hat{H}_{\text{BdG}} = (a_1^\dagger a_0 - i a_1^\dagger a_0^\dagger) + \text{H.c.} \tag{37}$$

The GS is easily found to be

$$\psi_0 = \frac{1}{\sqrt{2}}(1 + i a_1^\dagger a_0^\dagger)|\text{vac}\rangle \tag{38}$$

or more accurately

$$\psi_0 = \frac{1}{\sqrt{2}}(1 + i a_1^\dagger a_0^\dagger \, \hat{C})|\text{vac}\rangle \tag{39}$$

where $|\text{vac}\rangle \equiv$ (no particles in system, N in bath).

Consider now the linear combinations of the operators $a_0^\dagger,\ a_1^\dagger,\ a_0,\ a_1$: The operators

$$\widehat{\Omega}_1 \equiv \frac{1}{\sqrt{2}}(a_1^\dagger - i a_0),\ \widehat{\Omega}_2 \equiv \frac{1}{\sqrt{2}}(a_0^\dagger - i a_1) \tag{40}$$

are pure annihlators. The operator

$$\widehat{\prod}_1 \equiv \frac{1}{2}(a_1^\dagger + ia_0 - a_0^\dagger + ia_1) \tag{41}$$

when acting on ψ_0 creates the "+" state $\psi_+ = \frac{1}{\sqrt{2}}(a_1^\dagger + a_0^\dagger)|\text{vac}\rangle$ with energy 1 and the operator

$$\widehat{\prod}_2 \equiv \frac{1}{2}(a_1^\dagger + ia_0 - a_0^\dagger + ia_1) \tag{42}$$

creates the "−" state $\psi_- = \frac{1}{\sqrt{2}}(a_1^\dagger - a_0^\dagger)|\text{vac}\rangle$ The ψ_- state has zero energy relative to the GS.
The 2 MF's are linear combinations of the pure annihilators and the zero-energy DB fermion state ψ_-:

$$\widehat{M}_0 \equiv -\widehat{\prod}_- + \widehat{\Omega}_1 + \widehat{\Omega}_2 = a_0^\dagger - ia_0 \tag{43}$$

$$\widehat{M}_1 \equiv +\widehat{\prod}_- + \widehat{\Omega}_1 + \widehat{\Omega}_2 = a_1^\dagger - ia_1 \tag{44}$$

In this ultra-toy model, the effects of the MF's is not particularly spectacular, because the question of spatial localization does not arise.

... so let's go on:

A slightly less trivial model: The Kitaev 1D quantum wire

Consider a linear array of n sites (the "system") coupled to a large superfluid "bath", so that there are $N(\gg n)$ particles in total. In the mean-field approximation the most general Hamiltonian of a system of spinless electrons has the form, for nearest-neighbour coupling only.

$$\hat{H} = \sum_{j=0}^{n-1} U_j a_j^\dagger a_j - \sum_{j=1}^{n-1}(t_j a_{j-1}^\dagger a_j + H.c.) + \sum_{j=1}^{n-1}(\Delta_j a_{j-1}^\dagger a_j^\dagger \hat{C} + H.c.) \tag{45}$$

Eqn. (45) may be viewed as the nearest we can get to a 1D version of the $(p + ip)$ mean-field Hamiltonian. Let us make the very special choice.

$$U_j = 0, \Delta_j = -it_j \leftarrow\equiv -iX_j, \qquad X_j > 0 \tag{46}$$

Then the Hamiltonian becomes

$$\hat{H} = \sum_{j=1}^{n-1} X_j \hat{K}_j \tag{47}$$

where

$$\hat{K}_j \equiv (a^\dagger_{j-1} + ia_{j-1})(a_j + ia^\dagger_j) \tag{48}$$

Note the absence of a $\hat{K}_0$ term.

Note:

(a) $\hat{K}_j$ is Hermitian

(b) $\hat{K}_j^2 = 1$

(c) The $\hat{K}_j$'s are mutually commuting

(d) $\prod_{j=0}^{n-1} \hat{K}_j$ = number parity

Properties (a) - (c), with the Hamiltonian (47), imply that the ground state must satisfy the conditions

$$\hat{K}_j|\psi_0\rangle = |\psi_0\rangle, j = 1, 2, ..., n-1 \tag{49}$$

$$E_0 = -\sum_{j=1}^{n-1} X_j \tag{50}$$

The explicit form of GSWF is

$$|\psi_0\rangle = \mathcal{N} \cdot \prod_{j=1}^{n-1}(1 + \hat{K}_j)|\text{vac}\rangle \tag{51}$$

e.g. for $n = 4$,

$$|\psi_0\rangle = N \cdot \{1 + i(a_0^\dagger a_1^\dagger + a_1^\dagger a_2^\dagger + a_2^\dagger a_3^\dagger - a_0 -^\dagger a_2^\dagger - a_1^\dagger a_3^\dagger + \mathrm{a}_0^\dagger \mathrm{a}_3^\dagger(\times\hat{C}) \tag{52}$$

$$-a_0^\dagger a_1^\dagger a_2^\dagger a_3^\dagger(\times\hat{C}^2)\}|\text{vac}\rangle \tag{53}$$

Notice that the term $a_0^+ a_3$ produces entanglement between the sites 0 and 3, despite the fact that there is no direct interaction between them. This state of affairs is very characteristic of topologically interesting superfluid states.

Note: The GSWF of the whole "universe" (system + bath) can be written in the form $\Psi_0 = (\hat{\Lambda} + \hat{C})^{N/2}$ where $\hat{\Lambda} \equiv \sum_{l=1}^{n/2} c_l \alpha_l^\dagger \alpha_{\bar{l}}^\dagger$ ($\alpha_l^\dagger \equiv \sum_j q_{lj} a_j^\dagger$) but it is not entirely trivial to determine the constants[5] c_l and q_{lj}.

Excited states From the $2n$ $a_j^\dagger$ and a_j it must be possible to form n DB fermion creation operators and n pure annihilators. If we assume that for $j \neq 0$ the "link" j is associated with one DB creator $\hat{\Pi}_j$ and one annihilator $\hat{\Omega}_j$, then we must have

$$[\hat{K}_j, \hat{\Pi}_j] = +\hat{\Pi}_j, \qquad (\text{and } [\hat{K}_j, \hat{\Pi}_{j'}] = 0 \text{ for} j \neq j') \tag{56}$$

This is satisfied by the operator

$$\hat{\Pi}_j = \frac{1}{2}[(a_{j-1}^\dagger + ia_{j-1}) + (a_j^\dagger - ia_j)] \tag{57}$$

Hence, $\hat{\Pi}_j$ creates a DB fermion with energy (relative to the GS) X_j. The corresponding annihilator is $\hat{\Omega}_j \equiv \frac{1}{2}[(a_{j-1}^\dagger + ia_{j-1}) - (a_j^\dagger - ia_j)]$

However, we are still missing one DB creation operator and one pure annihilator. Clearly these have to be associated with the "missing" link $(n-1) - 0$. In fact, consider

$$\hat{\Pi}_0 \equiv \frac{1}{2}[(a_{n-1}^\dagger + ia_{n-1}) + (a_0^\dagger - ia_0)] \tag{58}$$

This may be verified explicitly to create an $(N+1)$-particle energy eigenstate which is *degenerate* with the groundstate. The corresponding pure annihilator is

$$\hat{\Omega}_0 \equiv \frac{1}{2}[(a_{n-1}^\dagger + ia_{n-1}) - (a_0^\dagger - ia_0)] \tag{59}$$

If now we consider the operators

$$\hat{M}_0 \equiv \frac{1}{\sqrt{2}}(\hat{\Pi}_0 + \hat{\Omega}) = \frac{1}{\sqrt{2}}(a_{n-1}^\dagger + ia_{n-1}) \tag{60}$$

$$\hat{M}_n \equiv \frac{1}{\sqrt{2}}(\hat{\Pi}_0 + \hat{\Omega})) = \frac{1}{\sqrt{2}}(a_0^\dagger + ia_0) \tag{61}$$

these generate $Majorana\ fermions$ localized on sites $n-1$ and 0 separately.

[5]For $n = 4$ the solution is

$$\alpha_1^\dagger = \frac{1}{2}\sum_{j=0}^{3} e^{ij\pi/4}\alpha_j^\dagger, \alpha_1^\dagger = \frac{1}{2}\sum_{j=0}^{3} e^{-ij\pi/4}\alpha^\dagger, \alpha_2^\dagger = \frac{1}{2}\sum_{j=0}^{3} e^{3ij\pi/4}\alpha_j^\dagger, \tag{54}$$

$$\alpha_2^\dagger = \frac{1}{2}\sum_{j=0}^{3} e^{3ij\pi/4}\alpha^\dagger, c_1 = i(1-\sqrt{2}), c_2 = i(1+\sqrt{2}) \tag{55}$$

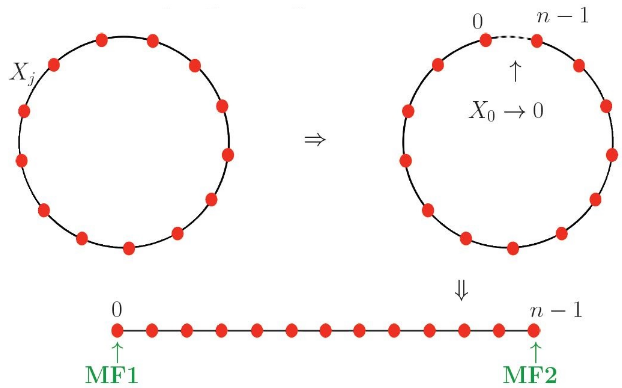

Fig. 1

An intuitive way of generating MF's in the Kitaev quantum wire is the following: Start with the wire bent into a loop and with all X_j's nonzero, so that the sum in eqn. (50) now includes $j = 0$.

At this point we have a set of n DB fermions, one associated with each link and created by the operator $\hat{\Pi}_j$. Now imagine gradually turning down one particular X_j, say X_o; when $X_o \to$, the link between the sites 0 and $n-1$ is "broken", i.e. nothing depends on the state of this link. Given that, we can now physically break the link and unbend the ring into a linear wire. But what has happened to the operator $\hat{\Pi}_o$, which created an excitation (an extra fermion) on this link? It must have been "split" into the two terms $a^+_{n-1} + ia_{n-1}$ and $a^+_o - ia_o$ which are localized at the two ends of the wire; when combined with the corresponding pure annihilators these generate $E = 0$ solutions of the BdG equations, i.e. Majorana fermions, which are localized at the ends.

THE SEARCH FOR MAJORANA FERMIONS:

<u>"INDUCED" P-WAVE SUPERCONDUCTIVITY</u>

While $(p + ip)$ Fermi superfluids are believed to tolerate MF's on their boundaries and vortices, there is a problem: the only currently realized bulk $(p + ip)$ Fermi superfluids are

(a) $^3He-$ A (difficult / impossible to prepare in 2D form)

(b) Sr_2RuO_4 (Majoranas believed to occur on half-quantum vortices, but no obvious "control parameter").

So: do Majoranas occur elsewhere?

Kane + Fu 2008: s-wave superconductor with vortex on top of TI (topological insulator)

Sau et al, Alicea (2010): s-wave superconductor with vortex on top of semiconducting nanowire with strong spin-orbit coupling.

Lutchyn *et al.*, Oreg *et al.*, (2010): no vortex needed in s-wave superconductor!

Possible design:

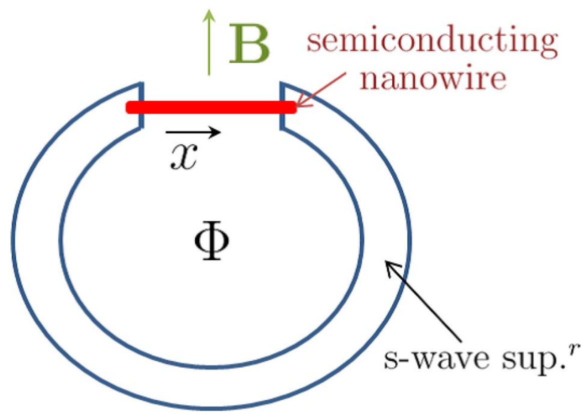

Fig. 2

The general principle[6]:

1. In semiconductor, strong Rashba spin-orbit coupling

$$\hat{H}_R = \alpha \sigma_y p_x \tag{62}$$

dominates at small p, orients spin ⊥'r to $\boldsymbol{p}$. ⇒

2. Magnetic field $\boldsymbol{B}$ ⊥'r σ opens gap $E_z = g\mu_B B$ at crossing point:

Hybridized states are "s-p mixed", i.e.

$$\varphi + (\mathbf{k}) = \begin{pmatrix} A_\uparrow(k) \\ A_\downarrow(k) \cdot \mathbf{k_x} + \mathbf{ik_y} \end{pmatrix}, \qquad \varphi - (\mathbf{k}) = \begin{pmatrix} B_\uparrow(k) \cdot \mathbf{k_x} + \mathbf{ik_y} \\ B_\downarrow(k) \end{pmatrix} \tag{63}$$

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[6]Alicea, PRB 81, 125318 (2010)

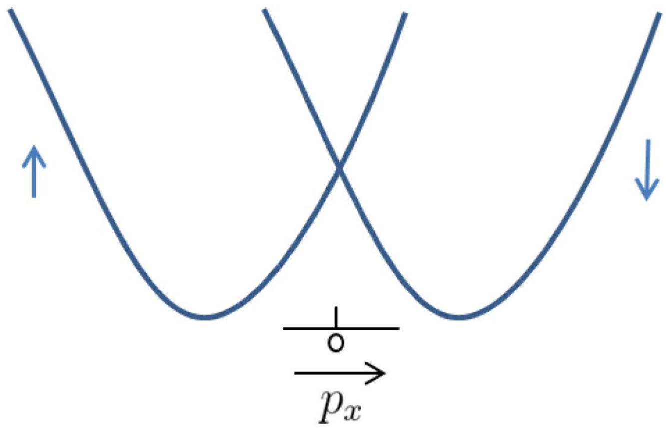

Fig. 3

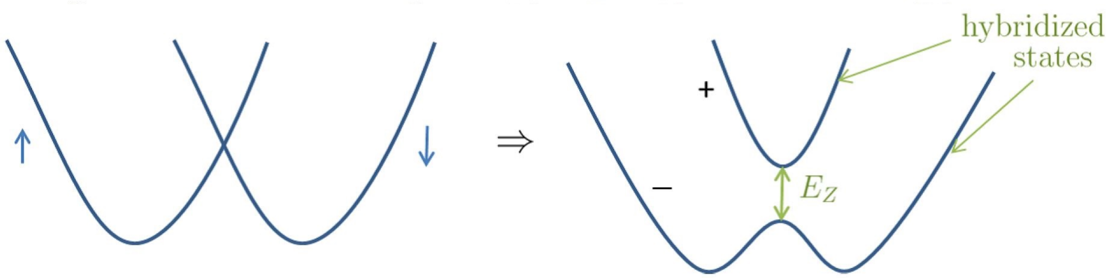

Fig. 4

(3) Introduce pair field from s-wave superconductor:

$$\begin{aligned}
\hat{H}_{SC} &= \int \Delta(\boldsymbol{r})\psi_\uparrow^\dagger(\boldsymbol{r})\psi_\downarrow^\dagger(\boldsymbol{r}) + \text{ H.c.} \\
&= \int d\boldsymbol{k}\{\Delta_\pm(k)\psi_+^\dagger(\boldsymbol{k})\psi_-^\dagger(\boldsymbol{k}) + \Delta_{--}(\boldsymbol{k})\psi_-^\dagger(\boldsymbol{k})\psi_-^\dagger(-\boldsymbol{k}) \\
&\qquad + \Delta_{++}(\boldsymbol{k})\psi_+^\dagger(\boldsymbol{k})\psi_+^\dagger(-\boldsymbol{k})\} \\
\Delta_{+-}(\boldsymbol{k}) &= f(|k|) \quad \text{(boring)} \\
\Delta_{--}(\boldsymbol{k}) &= g(|k|)(\hat{\boldsymbol{k}}_x + i\hat{\boldsymbol{k}}_y) \quad \text{induced p-wave!}
\end{aligned}$$

(4) Now tune μ (chemical potential) to lie in gap and assume $\Delta \ll E_z$: then the band drops out and we get pure p-wave superconductivity in lower band! ($\cong$ generalized Kitaev quantum wire.)

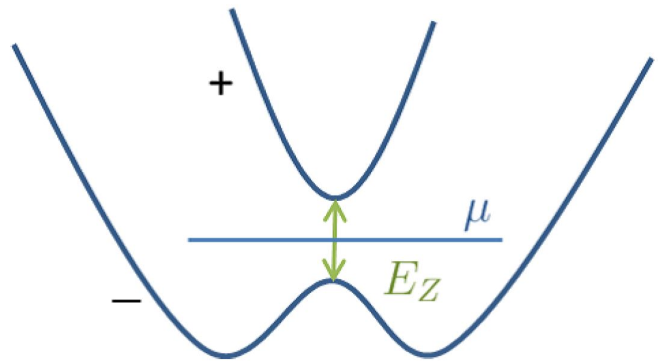

Fig. 5

Prediction for Majoranas (Lutchyn *et al.*, Oreg *et al.*):
critical quantity is

$$C_0 \equiv \mu^2 + \Delta_0^2 - E_z^2 \tag{64}$$

which can be made $x - dependent$. For $C_0 > 0$ we are in "trivial" phase, for $C_0 < O$ in "topological" phase. Majoranas are predicted to form at the boundary (if any) between the trivial and topological phases.

(Additional prediction is dependence of current through nanowire on phase drop in superconductor across wire: 4π periodicity $\to$ periodicity in flux is $\frac{h}{e}$).

EVIDENCE FOR MAJORANA FERMIONS IN SEMICONDUCTOR/SUPERCONDUCTOR NANOWIRE STRUCTURES:

(Mourik et al., Science 336, 1003 (2012)

Expt. arrangement (schematic):

Existence of topological phase requires

$$E_z > (\Delta^2 + \mu^2)^{1/2} \tag{65}$$

Majoranas predicted to sit at the two points where

$$E_z^2 = \Delta^2 + \mu^2 \tag{66}$$

Expt. probes only the one at the N end.
Raw data: $\partial I/\partial V$ as $f(B, V_g, \Delta, ...)$. Crucial observation:

very stable ZBP in $\partial I/\partial V$ at V=0

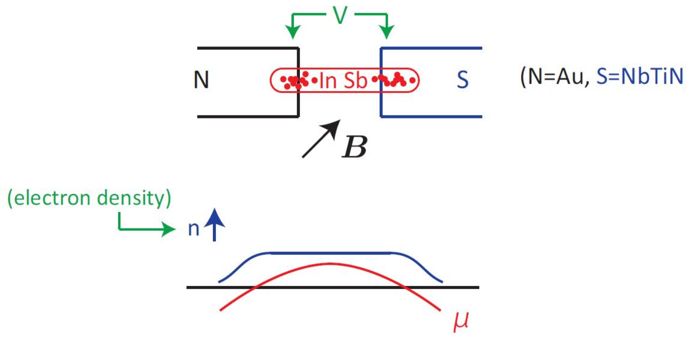

Fig. 6

unmovable by large changes in B, V_g, ... requires nonzero Δ,
vanishes when direction of $\boldsymbol{B}$ along ($\leftarrow$ spin-orbit field) ......
$\Rightarrow$ Majorana?