The quest for Majorana fermions

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based in part on joint work with
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$\uparrow$: $p+ip$ Fermi superfluids only (not e.g. QHE)

Reminder: simple BCS theory (spatially uniform system):

relax particle conservation and study "interesting" states given by

$$\Psi = \prod_k \Phi_k$$

where Φ_k is a state vector in 4D "occupation" space of $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)$ spanned by

$$|00\rangle_k \equiv |\text{vac}\rangle_k, \quad |1\,0\rangle \equiv a^+_{k\uparrow}|\text{vac}\rangle_k,$$

$\uparrow$
empty

$$|0\,1\rangle_k \equiv a^+_{-k\downarrow}|\text{vac}\rangle_k, \quad |1\,1\rangle_k \equiv a^+_{k\uparrow}\, a^+_{-k\downarrow}|\text{vac}\rangle_k$$

$\uparrow$
doubly occupied

Even-number-parity groundstate is special case

$$\Psi^{(\text{even})}_{\text{BCS}} = \prod_k \Phi^{(0)}_k, \qquad \Phi^{(0)}_k \equiv u_k|0\,0\rangle_k + v_k|1\,1\rangle_k$$

$$\equiv (u_k + v_k a^+_{k\uparrow} a^+_{-k\downarrow})|\text{vac}\rangle_k$$

Simplest odd-number-parity states ("Bogoliubov quasiparticles") generated by operating on $\Psi_{\mathrm{BCS}}^{(\mathrm{even})}$ with operators

$$\alpha_{k\uparrow}^{+} \equiv u_k a_{k\uparrow}^{+} - v_k a_{-k\downarrow} \qquad \alpha_{k\uparrow}^{+} \Phi_k^{(0)} = |1\ 0\rangle_k$$

$$\alpha_{-k\downarrow}^{+} \equiv u_k a_{-k\downarrow}^{+} + v_k a_{k\uparrow} \qquad \alpha_{-k\downarrow}^{+} \Phi_k^{(0)} = |0\ 1\rangle_k$$

However, there are 4 possible linearly independent combinations of $a_{k\uparrow}^{+}$, $a_{-k\downarrow}^{+}$, $a_{k\uparrow}$, $a_{-k\downarrow}$. What are the other two?

Ans:

$$\left.\begin{aligned} \beta_{k\uparrow}^{+} &\equiv v_k a_{k\uparrow}^{+} + u_k a_{-k\downarrow} \\ \beta_{-k\downarrow}^{+} &\equiv -v_k a_{-k\downarrow}^{+} + u_k a_{k\uparrow} \end{aligned}\right\} \text{"pure annihilators"}$$

$$\beta_{k\uparrow}^{+}\ \Phi_k^{(0)} = \beta_{-k\downarrow}^{+}\ \Phi_k^{(0)} = \underset{\substack{\uparrow \\ \text{null vector}}}{|0\rangle} \qquad (\text{not } |\text{vac}\rangle_k\ !)$$

In this simple case, $\beta_{k\uparrow}^{+} \equiv \alpha_{-k\downarrow}$ and $\beta_{-k\downarrow}^{+} \equiv \alpha_{k\uparrow}$, so not usually "remarked on". However…

More general paired state of a Fermi superfluid

Theorem (Yang): any "completely paired" even-number-parity state can always be written in the form

$$\Psi_{\text{c.p.}}^{(\text{even})} = \prod_n \Phi_n^{(i)} \, ,$$

where $\Phi_n^{(i)}$ is a state vector in the 4D "occupation" space of $(n, \bar{n})$ where n and $\bar{n}$ together make up a complete orthonormal set.

In particular the even-parity groundstate can be written in form

$$\Psi_{\text{gs}}^{(\text{even})} = \prod_n \Phi_n^{(0)} \, , \qquad \Phi_n^{(0)} \equiv u_n |0\ 0\rangle_n + v_n |1\ 1\rangle_n$$

$$\equiv (u_n + v_n a_n^+ a_{\bar{n}}^+) |\text{vac}\rangle_n$$

We can then define pure annihilators similarly to the BCS case:

$$\left.\begin{aligned} \beta_n^+ &\equiv u_n a_n^+ + v_n a_{\bar{n}} \\ \beta_{\bar{n}}^+ &\equiv -v_n a_{\bar{n}}^+ + u_n a_n \end{aligned}\right\} \quad \beta_n^+ \ \Phi_n^{(0)} = \beta_{\bar{n}}^+ \ \Phi_n^{(0)} = |0\rangle$$

↑ null vector

However, consider the states created by the operators (analogous to $\alpha_{k\uparrow}^{+}$, $\alpha_{-k\downarrow}^{+}$ in BCS)

$$\alpha_n^{+} \equiv u_n a_n^{+} - v_n a_{\bar{n}} \qquad\qquad \alpha_n^{+}\Phi_n^{(0)} \equiv |1\ 0\rangle_n$$

$$\alpha_{\bar{n}}^{+} \equiv u_n a_{\bar{n}}^{+} + v_n a_n \qquad\qquad \alpha_{\bar{n}}^{+}\Phi_n^{(0)} \equiv |0\ 1\rangle_n$$

While those are odd-number-parity states, they are not in general energy eigenstates! To obtain energy eigenstates we must use linear combinations of the α_n^{+} and $\alpha_{\bar{n}}^{+}$:

$$\gamma_i^{\dagger} = \sum_n (\lambda_{in}\alpha_n^{+} + \mu_{in}\alpha_{\bar{n}}^{+})$$

and find the coefficients in μ_{in} by minimizing the total energy in the $(n, \bar{n})$ basis. The result is just the Bogoliubov-de Gennes (BdG) equations written in this basis. However, it is more conventional to use the coordinate basis.

Bogoliubov-de Gennes (BdG) equations

note: BdG equations don't tell us about either the even-parity groundstate, or the odd-parity excited states, as such: rather they tell us about the relation between them.

Prescription for generating odd-parity states ("Bogoliubov quasiparticles") from even-parity groundstate

$$\Psi_i^{(\text{odd})} = \gamma_i^\dagger \Psi_{\text{c.p.}}^{(\text{even})},$$ in spinless case,

$$\gamma_i^\dagger \equiv \int d\boldsymbol{r} \left\{ u_i(\boldsymbol{r}) \underset{\text{creation}}{\hat{\psi}^\dagger(r)} + v_i(r) \underset{\text{annihilation}}{\hat{\psi}(r)} \right\}$$

$$\left(\int |u_i(r)|^2 + |v_i(r)|^2 dr = 1 \right)$$

where $u_i(r)$ and $v_i(r)$ solve the BdG equations: $[\hat{\mathrm{H}}, \gamma_i^\dagger] = \mathrm{E}_i \gamma_i^\dagger$ or explicitly

$$\begin{pmatrix} \hat{\mathrm{H}}_0 & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{\mathrm{H}}_0^* \end{pmatrix} \begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix} = \mathrm{E}_i \begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix} \qquad (*)$$

here $\hat{\mathrm{H}}_0 \equiv \left(-\frac{\hbar^2}{2m} \nabla^2 - \mu \right) + \mathrm{U}_{\text{ext}}(r)$

and Δ is an integral operator:

$$\hat{\Delta}(r)v(r) \equiv \int \Delta\,(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r}')d\boldsymbol{r}', \quad \Delta(\boldsymbol{r},\boldsymbol{r}') \equiv V(\boldsymbol{r}-\boldsymbol{r}')\langle\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}')\rangle$$

Note: formally, if the spinor $\begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix}$ satisfies (*) with eigenvalue $\mathrm{E}_i > 0$, then the spinor $\begin{pmatrix} v_i^*(r) \\ -u_i^*(r) \end{pmatrix}$ (not necessarily the H.c. of any γ_i^+) satisfies (*) with $-\mathrm{E}_i$. So the “state” $\begin{pmatrix} v_i^*(r) \\ -u_i^*(r) \end{pmatrix}$ is sometimes said to represent a “negative-energy state”. This is misleading: the operator in question is just a pure annihilator.

(note that any linear combination of pure annihilators is itself a pure annihilator).

Majorana zero modes (MZM)

Formally, a MZM is defined as a solution γ_0^+ to the BdG equations which satisfies $\gamma_0^+ = \gamma_0$ (and is localized in at least one dimension). This immediately implies

(a) that "particles" and "holes" have the same spin
(b) that $u_0(r) = v_0^*(r)$
(c) that $\mathrm{E}_i = 0$

Where might we find such a beast?

Typically, in a parallel-spin-paired (or spinless) "topological superconductor" at point where order parameter varies substantially in space.

Possible examples:

(a) bulk (^{3}He-A, Sr_2RuO_4, $FeTe_{0.55}Se_{0.45}$, UTe_2…): at (half-quantum)* vortices
(b) induced (semiconductor-superconductor hybrids with strong spin-orbit coupling): at boundary between "trivial" and "topological" phases.

In both cases, calculation based on BdG equations shows that a MZM solution exists.

*because on full-quantum (Abrikosov) vortices get 2 MZM solutions = 1 Bogoliubov fermion

But what **is** a "Majorana fermion" (or MZM)?

Clue: it is a solution of

$$\left[\hat{\mathrm{H}}_{\mathrm{BdG}}, \gamma_0^\dagger\right]|\Psi_0\rangle = 0 \cdot \gamma_0^\dagger \; |\Psi_0\rangle$$

But this has two possible interpretations when applied to the even-parity GS:

(i) $\gamma_0^\dagger$ creates an odd-parity state with energy 0 relative to the GS.

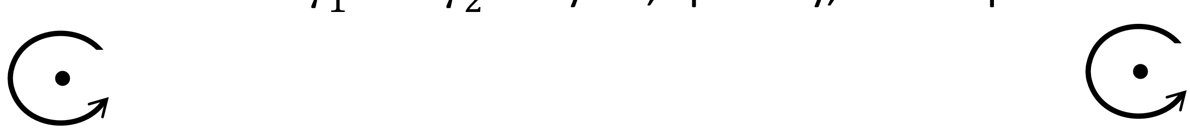
(ii) $\gamma_0^\dagger$ simply annihilates the GS (i.e. $\gamma_0^\dagger|\Psi_0\rangle = \underset{\substack{\uparrow \\ \text{null vector}}}{|0\rangle}$)

Neither (i) alone nor (ii) alone satisfies $\gamma_0^\dagger = \gamma_0$. But a linear combination of them can! Thus,

a Majorana fermion is simply a quantum superposition of a zero-energy (Bogoliubov) fermion and a pure annihilator.

If so, then by putting 2 MZM's together $\left(\alpha^+ = \frac{1}{2}\left(\gamma_1^\dagger + i\gamma_2^\dagger\right)\right)$ we can eliminate the pure-annihilator component and generate a real Bogoliubov fermion with zero energy. (Fortunately, MBS solutions always come in pairs).

But… solutions $\gamma_1^\dagger$ and $\gamma_2^\dagger$ may be, spatially, miles apart!



$\gamma_1^\dagger$ $\gamma_2^\dagger$

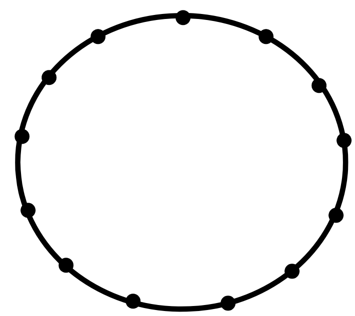
single Bogoliubov fermion!

Are we sure that these "delocalized" Bogoliubov fermions (DBF's) really exist?'
(cf. e.g. wormhole solutions of equations of GR)

In particular: does existence of a solution to BdG equations guarantee that there exist an even-parity and odd-parity state related by this solution?

In at least one "toy model", yes!

<u>1D Kitaev quantum wire</u> (KQW)
1D ring, n sites



$$\hat{H} = \sum_j \mathrm{U}_j \, a_j^+ a_j - \sum_j \left(t_j a_{j-1}^+ a_j^+ + \mathrm{H.c.} \right)$$

on-site

single-particle hopping

$$+ \sum_j \left(\Delta_j a_{j-1}^+ a_j^+ + \mathrm{H.c.} \right)$$

pair creation

With special choice $\mathrm{U}_j = 0$, $\Delta_j = -it_j \equiv -iX_j$, becomes

$$\hat{H} = -\sum_j X_j \hat{K}_j \qquad \text{with} \qquad \hat{K}_j \equiv \left(a_{j-1}^+ + i a_{j-1} \right) \cdot \left(a_j + i a_j^+ \right)$$

↑

note refers to bonds not sites

Can solve explicitly for even-parity GS

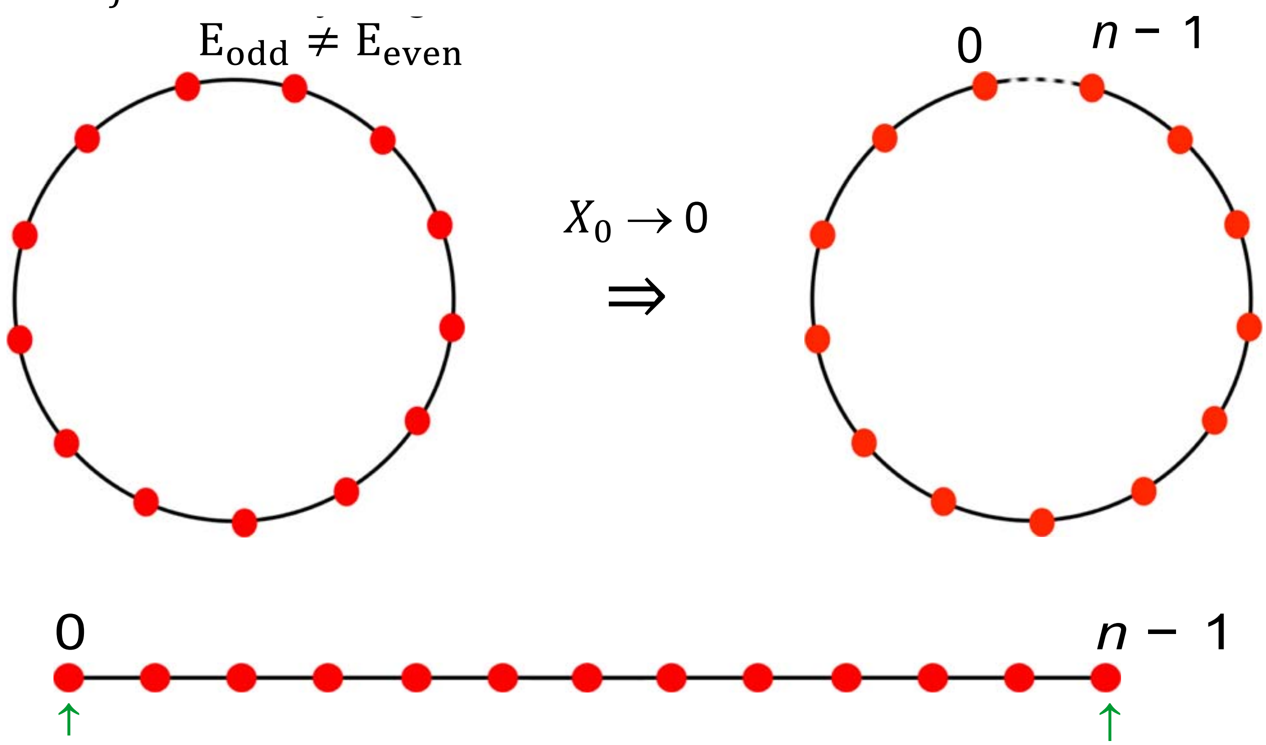
$$\Psi_0 = (\text{normalization}) \prod_{j=1}^{n-1} \left(1 + \hat{K}_j\right) |\text{vac}\rangle \qquad \mathrm{E}_0 = -\sum_{j=1}^{n-1} X_j$$

Simplest odd-parity states obtained by "turning over" bond j, with excitation energy $2X_j$.

Now, what happens if one of the X_j (say X_0) $\rightarrow$ 0?

all $X_j \neq 0$ $\qquad\qquad$ $\mathrm{E}_{\text{odd}} = \mathrm{E}_{\text{even}}$

$\mathrm{E}_{\text{odd}} \neq \mathrm{E}_{\text{even}}$



MZM1 $\qquad\qquad$ MZM2

<u>single</u> delocalized Bogoliubov fermion!

(Extensions to (quasi-) 2D …)

But… is the "pure-annihilator" component really disposed of?

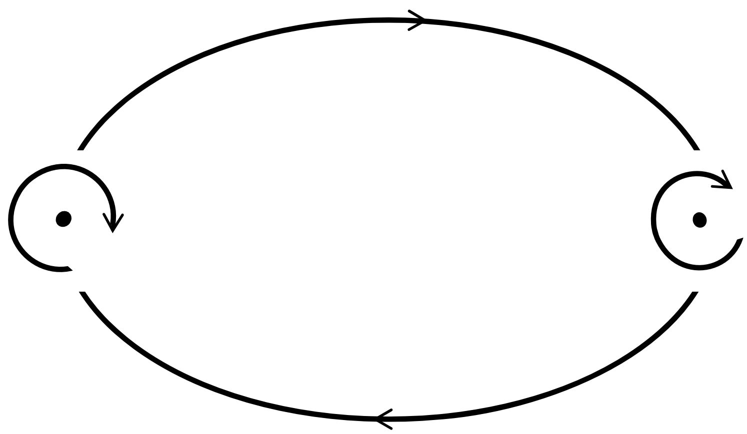
Why are these "delocalized" Bogoliubov fermions (DBF's) so interesting? (in particular for topologically protected quantum computing)?

(1) Local undetectability:
recall that within "standard" BdG scheme,

$$\gamma_i^\dagger \equiv \int d\boldsymbol{r}\left\{u_i(r)\hat{\psi}^\dagger(r) + v_i(r)\hat{\psi}(r)\right\}$$

so if $|v_i(r)|^2 = |u_i(r)|^2$, no extra particle density associated with the MZM solutions or with the DBF's built from them $\Rightarrow$ "invisible" by any local probe.

(2) Braiding:



If 2 vortices without MZM's on them exchanged, Berry phase = 0 (or $2n\pi$)
What if a single DBF (=2 MZM's) is split between them?
Then (Ivanov, 2001)

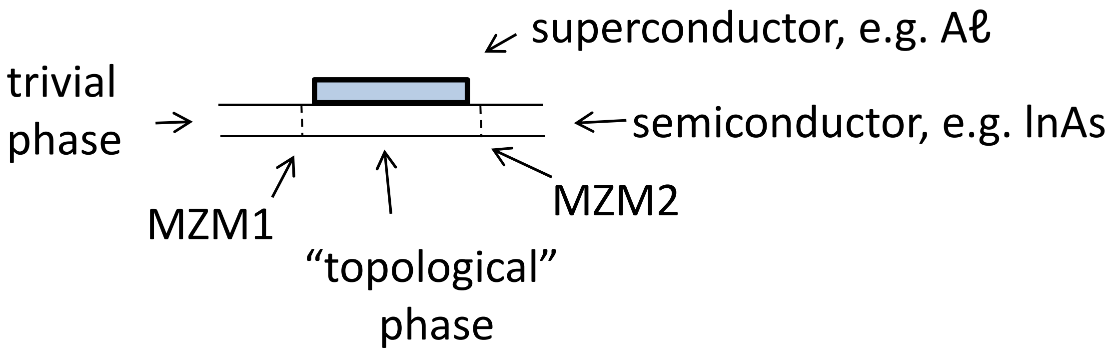
Berry phase $= \pi/2$

$\Rightarrow$ MZM's behave as Ising anyons $\Rightarrow$ possibility of (partially) topologically protected quantum computation.

The experimental situation

a. Superconductor-semiconductor hybrids*

The general idea:



by combining spin-orbit interaction and (appropriately oriented) magnetic field, can induce in InAs "1D *p+ip*" Cooper pairing of ↑↑ spins only (so similar to KQW)

↑
Kitaev 1D
quantum wire

MZM's predicted to occur at boundaries between "topological" and "trivial" phases.

*Lutchyn et al. Nature Reviews/Materials **3**, 52 (2018)

Diagnostics of a MZM:

1. Zero-bias anomaly (ZBA) in conductance G(v) with strength confidently predicted to be $2e^2/h$ at T=0. (total Andreev reflection)

2. Periodicity of various quantities, e.g. Coulomb

   blockade, changes from $\underset{h/2e}{\underset{\uparrow}{\Phi_0}}$ to $\underset{h/e}{\underset{\uparrow}{2\Phi_0}}$

3. "Fractional Josephson effect" (~ special case of (2))
   ("$2\pi \rightarrow 4\pi$")

Since 2012, many experiments.

Problem: "what else could it be?" – quite a lot!

Main evidence for MZM is robustness of effects against

variation of parameters.

But in any case, 1D system so no possibility of braiding.

Experimental situation, cont.

b. Bulk quasi-2D Superconductors.

Prediction: (single) MZM's should occur on half-quantum vortices in "$p+ip$" superconductor.

SRO

Candidates: (^{3}He-A), Sr_2RuO_4, $FeTe_{0.55}Se_{0.45}$, UPt_3, UTe_2 …

To date, only claim* of observation of MZM is in $FeTe_{0.55}Se_{0.45}$ (topological insulator $\Rightarrow$ superconductor, surface states)

Most researched: Sr_2RuO_4 (SRO)

Majority belief until ~ April 2019: pairing state of SRO is "Γ_5" (↑↑ and ↓↓ spins with common nonzero orbital angular momentum, analogous to ^{3}He-A). This state breaks TRI, seemed consistent with most experiments and should sustain MZM's on half-quantum vortices (for which evidence)

Cat thrown among pigeons: UCLA experiment† April 2019. Apparently cannot be Γ_5! Most plausible hypothesis:

↑↑ and ↓↓ spins each have nonzero, but opposite angular momentum ("$\Gamma_1 - \Gamma_4$")

Such a state does not break TRI overall, but does break it for each spin population separately $\Rightarrow$ in half-quantum vortices, MZM's can still occur!

Can we find "smoking-gun evidence for MZM's? (NSF Grand Challenge…)

*Wang et al., Science **362**, 333 (2018)
† Pustogow et al., arXiv 1904.00047

An all-pervasive problem in the theory of MZM's:

> 99% of literature is based on (naïve form of) BdG equations.

In turn, BdG equations rest on assumption of SBU(1)S

↑

spontaneously broken
U(1) symmetry

The problem: SBU(1)S is a myth!

lead → ← lead

↑

superconductor

reduced
density matrix ⟶ $\rho_{N,N}$ nonzero for more than one value of n
of S

However, $\rho_{NN'}$ = 0 for N ≠N'!

Effect of taking particle number conservation seriously

With assumption of SBU(1)S ← spontaneously broken U(1) symmetry

standard formula for creation of Bogoliubov quasiparticle from even-parity groundstate $|\Psi_0\rangle \sim \hat{C}^{N/2}|vac\rangle$ is

$$\psi_u = (u_k a^{+}_{k\uparrow} - v_k a_{-k\downarrow})|\Psi_0\rangle$$

or more generally (BDG) ⟵ Bogoliubov-de Gennes

$$\psi_u = \gamma^{\dagger}|\Psi_0\rangle$$

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

This does not conserve particle number. Remedy:

$$\gamma^{\dagger} = \int \{u(r)\hat{\psi}^{\dagger}(r) + v(r)\hat{\psi}(r)\underset{\uparrow}{\hat{C}}\}\, dr$$

creates extra Cooper Pair

Question 1: Is the "extra" pair the same as those in the even-parity GS?

Question 2: Irrespective of answer to 1,

does it matter?

Conjecture: for “usual” case (e.g. Andreev bound state in S-wave superconductor), effect is nonzero but probably small.

but for case where Cooper pairs have “interesting” properties (e.g. intrinsic angular momentum) effect may be qualitative.

The crunch case: Majorana fermions in ($p+ip$) Fermi superfluid (Sr_2RuO_4?): does extra Cooper pair change results of “standard theory (e.g. Ivanov 2001) qualitatively?

-the $64K (actually $6.4M!) question…

Back to the Ivanov problem

According to Ivanov, if we have paired vortices j and $j+1$ and we interchange them, then

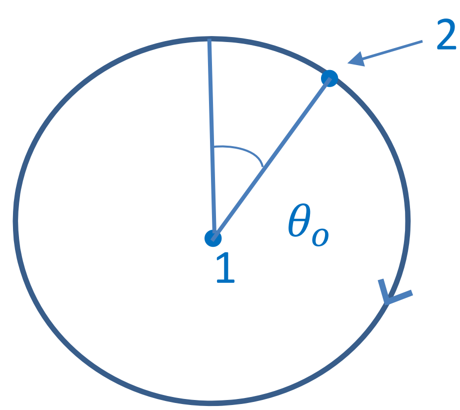
if no Majoranas, $\varphi_B = 0$

if two Majoranas, $\varphi_B = \pi/2$

It is more convenient to consider encirclement of $j(\text{at } \boldsymbol{r}=0)$ by $j+1$. So in our language, Ivanov's prediction for this operation is

even-number-parity states:
$\varphi_B = 0$

odd-number-parity states:
$\varphi_B = \pi$



Can we recover this prediction?

We use the fundamental result that since $\Psi_N(\theta_i) = \Psi_N\{\theta_i - \theta_o\}$,

$$\varphi_B = 2\pi\langle L_z\rangle.$$

particle-nonconserving

(a) In the PNC approach (taken by Ivanov) for the odd-number-parity state

$$\langle L_z \rangle = \frac{1}{4}\left(\ell_{u_1} + \ell_{u_2} + \ell_{v_1} + \ell_{v_2}\right)$$

($\ell_{u1} \equiv$ ang. momentum of "particle" component of Majorana in vortex 1, etc.)

However, since $u_1^*(r) = v_1(r), \ell_{u_1} = -\ell_{v_1}$ (etc.) $\Rightarrow \langle L_z \rangle = 0$. Thus, within PNC approach we have for the odd-number-parity state (mod. 2π)

$\varphi_B = 0$ different from Ivanov's result!

particle-conserving

(b) In the PC approach, the $v-$ component of the Majorana is associated with creation of one extra Cooper pair. Hence

$$\langle L_z \rangle = \frac{1}{4}\left(\ell_{u_1} + \ell_{v_1} + \ell_c + \ell_{u_2} + \ell_{v_2} + \ell_c\right) = \frac{1}{2}\ell_c$$

where ℓ_c is the total angular momentum associated with the addition of an extra Cooper pair. If we assume that this "extra" Cooper pair is the same as those in groundstate, this is just $\Omega_1 + \Omega_2 + \ell_{\text{int}}$

vortex 1 vortex 2 relative a.m.

And since $\ell_{\text{int}} = 1$, and $\Omega_1 + \Omega_2 = 0$ or 2, ℓ_c is always an odd integer and thus

$\varphi_B = \pi$ recovering Ivanov's result

↑: when we let (say) $u_1 \to v_1$ and thus add a Cooper pair, does that pair "feel" the effects of the angular momentum around the distant vortex 2?

Conclusions

1. The “tried and true” methods of standard condensed matter theory (e.g. the BdG equations) have served us well for 60 years in their traditional context. In a quantum-information context we may need to rethink them from scratch.

2. In thinking about “Majorana zero modes” the analogy with particle physics confuses more than it illuminates.

3. Particularly in thinking about possible applications of MZM’s to topologically protected quantum computation, essential to take into account the “extra” Cooper pair.