TM

TOPOLOGICAL SUPERCONDUCTIVITY:

IS THE MEAN-FIELD APPROACH ADEQUATE?

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joint work with Yiruo Lin
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Theses and questions in this talk:

Theses:

1. For 50 years, almost all theoretical work on inhomogenous Fermi superfluids, including work on “topological superconductors” has been based on the solution of the BdG (mean-field) Hamiltonian, which in turn is justified by appeal to the idea of “spontaneously broken U(1) gauge symmetry” (SBGS)

2. There is no physical justification for the idea of SBGS, and hence none for the use of the BdG Hamiltonian (at least without considerable caution).

3. Moreover, simple examples show that it can lead to physically incorrect conclusions.

4. This is because in the cases of interest the response of the Cooper pairs cannot be ignored.

Questions:

How does correction of this error affect “established” results on topological superconductors? In particular, in the case of Majorana fermions, does it affect

(a) their existence?

(b) their braiding properties?

(c) their undetectability by local probes?

“Spontaneously broken gauge symmetry”

Claim: An isolated superconductor with an even number of particles need not be in an eigenstate of total particle number N, rather it may be described by the particle-nonconserving (PNC) wave function

$$\Psi_{\mathrm{PNC}}^{(\mathrm{even})} = \sum_N C_N \Psi_{2N} \ \ , C_N \sim \exp iN\varphi$$

so that $\langle \hat{\psi}\hat{\psi} \rangle \sim \sum_N C_{N+1}^* \, C_N \sim$ const. $\exp i\varphi \neq 0$. Then it is consistent to construct odd-parity states i by the BdG prescription: e.g. for parallel-spin pairing.

$$\Psi_{\mathrm{PNC}}^{(\mathrm{odd}_i)} = \int dr \{ u_i(\boldsymbol{r}) \hat{\psi}^\dagger(\boldsymbol{r}) + v_i(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) \} \left| \Psi_{\mathrm{PNC}}^{(\mathrm{even})} \right\rangle \equiv \gamma_i^\dagger \left| \Psi_{PNC}^{(\mathrm{even})} \right\rangle$$

where the spinors $\left(u_i(r), v_i(r)\right)$ are normalized eigenfunctions of the particle-nonconserving mean-field (BdG) Hamiltonian.

Claimed analogy between topological (e.g. $p + ip$) superconductor (TS) and topological insulator (TI):

Single-particle Hamiltonian: $\hat{H}_{sp} = \begin{pmatrix} \mathcal{H}_z & \mathcal{H}_\perp \\ \mathcal{H}_\perp & \mathcal{H}_z \end{pmatrix}$

	TI	TS
"single-particle" basis	$\begin{pmatrix} s \text{ band} \\ p \text{ band} \end{pmatrix}$	$\begin{pmatrix} \text{particle} \\ \text{hole} \end{pmatrix}$
diagonal field $\mathcal{H}_z$	s - p splitting	kinetic + external potential energies
off-diagonal field $\mathcal{H}_\perp$	spin-orbit coupling	order parameter $\Delta(r, r')$
in presence of spatial inhomogeneity	edge states (experimental status well-confirmed)	Majoranas (experimental status controversial)

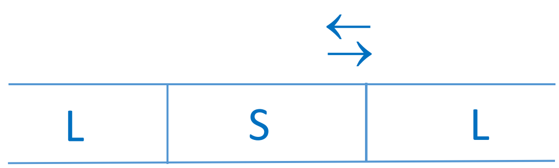
The \$64K question:

WHY SHOULD WE BELIEVE ALL THIS?

"You hear a lot of things in life
and some of them ain't true:
there's many things the Danube is;
the Danube IS NOT blue"
-Anon

"Blue" Danube ⇄ "spontaneously broken" U(1) symmetry?

Justification no. (1): Particle no. is not conserved (e.g. leads)



However: total particle no. (S + L) is still conserved. Reduced density matrix $\rho_{NN'}$ of S is obtained by tracing over L, so while diagonal elements ρ_{NN} are nonzero for more than one N, still have $\rho_{NN'}$=0 for $N \neq N'$. No go!

Justification no. (2): (Anderson, 1958)

Write $\Psi_{\text{PNC}}^{(\text{even})} \sim \Psi(\varphi)$, then

$$\frac{1}{2\pi}\int_0^{2\pi} \Psi(\varphi) \exp iN_0\varphi d\varphi = \Psi_{PC}(N_0)$$

↑
particle-conserving w.f. for $2N_0$ particles

Fine for even-parity states by themselves (also for odd-parity ones by themselves), but:

problem is relation of odd-parity states to even-parity ones.

Justification no. (3):

OK, strictly speaking when I add hole component of Bogoliubov quasiparticle I should add extra Cooper pair to make up particle number. But this can't matter, since this pair distributes itself over the whole volume and thus in the thermodynamic limit its effect must be negligible.

WRONG!

Failure of BdG/MF: a trivial (but apparently not well-known) example:

Consider an even-number-parity BCS superfluid at rest (so $P_0 = 0$)

↑ total momentum

Now create a single fermionic quasiparticle in state **k**:

For this, the appropriate BdG qp creation operator $\gamma_i^\dagger$ turns out to be

$$\gamma_i^\dagger = u_k a_{k\uparrow}^\dagger + v_k a_{-k\downarrow}, \qquad u_k \equiv \frac{1}{2}(1 + \frac{\epsilon_k}{E_k}), v_k \equiv \frac{1}{2}(1 - \frac{\epsilon_k}{E_k})$$

$$E_k \equiv \left(\epsilon_k^2 + |\Delta_k|^2\right)^{1/2}$$

The total momentum $\boldsymbol{P}_f$ of the (odd-number-parity) many-body state created by γ_i is

standard textbook result ↓

$$\boldsymbol{P}_f = |u_k|^2(\hbar\boldsymbol{k}) - |v_k|^2(-\hbar\boldsymbol{k}) = (|u_k|^2 + |v_k|^2)\hbar\boldsymbol{k} \equiv \hbar\boldsymbol{k}$$

$$\text{so } \Delta\boldsymbol{P}_f \equiv \boldsymbol{P}_f - \boldsymbol{P}_o = \hbar\boldsymbol{k}$$

Now consider the system as viewed from a frame of reference moving with velocity $-\boldsymbol{v}$, so that the condensate COM velocity is v. Since the pairing is now between states with wave vector $q + mv/\hbar$ and $-q + mv/\hbar$, intuition suggests (and explicit solution of the BdG equations confirms) that the form of $\gamma_f^\dagger$ is now

$$\gamma_f^\dagger = u_k a_{\mathbf{k}+\mathbf{mv}/\hbar,\uparrow}^\dagger + v_k a_{-\mathbf{k}+\mathbf{mv}/\hbar,\downarrow} \leftarrow nb.not\ \ a_{-(\mathbf{k}+\mathbf{mv}/\hbar,\downarrow)}!$$

Thus the added momentum is

$$\Delta\boldsymbol{P}'_f = |u_k|^2(\hbar\boldsymbol{k} + m\boldsymbol{v}) - |v_k|^2(-\hbar\boldsymbol{k} + m\boldsymbol{v}) = \hbar\boldsymbol{k} + (|u_k|^2 - |v_k|^2)m\boldsymbol{v}$$

Recap: $BdG \rightarrow \Delta P_f' = \hbar \boldsymbol{k} + (|u_k|^2 - |v_k|^2) m\boldsymbol{v}$

However, by Galilean invariance, for any given condensate number N,

$$\boldsymbol{P}_0' = \boldsymbol{P}_o + Nm\boldsymbol{v}, \boldsymbol{P}_f' = \boldsymbol{P}_f + (N+1)m\boldsymbol{v}$$
$$\Rightarrow \Delta \boldsymbol{P}_f' \equiv \boldsymbol{P}_f' - \boldsymbol{P}_0' = \Delta \boldsymbol{P}_f + m\boldsymbol{v} = \hbar \boldsymbol{k} + m\boldsymbol{v}$$

and this result is independent of N (so invoking "spontaneous breaking of U(1) symmetry" in GS doesn't help! – we can still consider the average $\Delta \boldsymbol{P}_f'$)

So:

$$\begin{cases} BdG \Rightarrow \Delta P'_f = \hbar \boldsymbol{k} + (|u_k|^2 - |v_k|^2) m\boldsymbol{v} \\ GI \rightarrow \Delta \boldsymbol{P}'_f = \hbar \boldsymbol{k} + m\boldsymbol{v} \end{cases}$$

(GI: Galilean invarance)

What has gone wrong?

Solution: Conserve particle no.! (and take the extra Cooper pair seriously)

When condensate is at rest, correct expression for fermionic correlation operator $\gamma_i^\dagger$ is

$$\gamma_i^\dagger = u_k a_{k\uparrow}^\dagger + v_{-k\downarrow} a \hat{C}_{(0)}^\dagger$$

← creates extra Cooper pair (with COM velocity 0)

Because condensate at rest has no spin/momentum/spin current …, the addition of $\hat{C}_{(0)}^\dagger$ has no effect. However: when condensate is moving

$$\gamma_f^\dagger = u_k a_{\boldsymbol{k}+m\boldsymbol{v}/\hbar,\uparrow}^\dagger + v_k a_{-\boldsymbol{k}\downarrow+m\boldsymbol{v}/\hbar} \hat{C}_{(\boldsymbol{v})}^\dagger$$

← Cooper pair with COM velocity $\boldsymbol{v}$|

$$\Delta \boldsymbol{P}'_f = |u_k|^2(\hbar \underline{\boldsymbol{k}} + m\underline{\boldsymbol{v}}) - |v_k|^2(-\hbar \underline{\boldsymbol{k}} + m\underline{\boldsymbol{v}}) + |v_k|^2 2m\underline{\boldsymbol{v}}$$
$$= (|u_k|^2 + |v_k|^2)(\hbar \underline{\boldsymbol{k}} + m\underline{\boldsymbol{v}}) = \hbar \underline{\boldsymbol{k}} + m\underline{\boldsymbol{v}}$$

in accordance with GI argument

So, moral is:

Whenever Cooper pairs (CP's) (order parameter) has nontrivial degrees of freedom, must add extra CP to hole component of Bogoliubov quasiparticle (and take it seriously).

But by definition, in a TS the CP's do have nontrivial degree of freedom! (e.g. in $p+ip$, internal angular momentum)

Thus must write for all fermionic quasiparticles (including Majoranas)

$$\gamma_i^\dagger = \int d\boldsymbol{r}\,\{u_i(r)\hat{\psi}^\dagger(\boldsymbol{r}) + v_i(r)\hat{\psi}(\boldsymbol{r})C^\dagger\}|\Psi$$

↑ CP creation operator

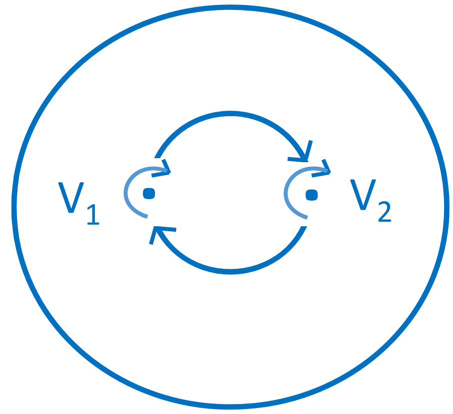
What are consequences for

(a) existence of Majorana fermions (MF's)
(b) braiding properties of MF's
(c) local undetectability of MF's?

As to (a): Majorana solutions $\left(u(\boldsymbol{r}), v(\boldsymbol{r})\right)$ still exist but are no longer self-conjugate. This probably doesn't matter too much for the physics (e.g. still get solutions on vortices in $(p+ip)$ TS).

(b) What is effect of particle number conservation on braiding of Majorana fermions?

The Ivanov problem:



2 vortices V_1 and V_2, which either are both "empty" ("e") or each carry a single Majorana fermion (i.e. total of a single DB fermion) ("M")

↑ Dirac-Bogoliubov

Under (say) clockwise exchange, define Berry phases $\Delta\varphi_e, \Delta\varphi_M$ and relative Berry phase

$$\Delta\varphi_{\text{rel}} \equiv \Delta\varphi_M - \Delta\varphi_e$$

Question: What is $\Delta\varphi_B$?

Ivanov's answer *: $\Delta\varphi_{\text{rel}} = \pi/2$

This result is fundamental to the whole proposal for topological quantum computing in $(p + ip)$ Fermi superfluids.

*D. A. Ivanov, PRL **86**, 268 (2001)

Theorem (Y-R Lin): under exchange,

$$\Delta\varphi = \pi\langle L_z\rangle \quad (\text{mod. } \pi)$$

$$\Rightarrow \Delta\varphi_{rel} = \pi\langle \Delta L_z\rangle \quad (\text{mod. } \pi)$$

So: what is $\langle \Delta L_z\rangle$ **?**

↑
difference in angular
momentum between states
e and M.

(1) Standard mean-field approach:

Since (for V_1 and V_2 parallel) either both MF's have angular momentum 0 or both ± 1, added DB fermion created by $\gamma_1 + i\gamma_2$ has $\langle \Delta L_z \rangle = 0 \text{ or } 1 \ \Rightarrow$

$$\Delta\varphi_{\text{rel}} = \pi \qquad (\text{mod. } \pi)$$

In contradiction to Ivanov.

(↑: what happens for V_2 antiparallel to V_1?)

(2) Particle-conserving approach:

Crucial point: In the situation considered ($p + ip$ TS with 2 parallel vortices V_1 and V_2) a CP has (a) COM angular momentum, 1 with respect to V_1 (b) COM angular momentum 1 with respect to V_2 (c) internal (relative) angular momentum 1. Hence the total angular momentum added by a CP is

$$L_{CP} = 3$$

However, the CP is added only to the hole component of the MF wave function, which has a weight of exactly ½. Hence $\langle \Delta L_z \rangle$ =3/2, so by Lin's theorem,

$$\Delta\varphi_{\text{rel}} = 3\pi/2 \sim (-)\pi/2$$

just as in Ivanov's calculation! (unlikely to be accident…)

(c) Does requirement of particle number conservation affect nondetectability of MF's by local probes?

Standard argument (mean-field):

$$\gamma^{\dagger} = \int d\boldsymbol{r} \left\{ u(r)\hat{\psi}^{\dagger}(r) + v(r)\hat{\psi}(r) \right\}, \qquad u(\boldsymbol{r}) = v^{*}(\boldsymbol{r})$$

$$\Delta N \equiv \int_{V_M} \delta\rho(r) dr = \int dr \left\{ |u(r)|^2 - |v(r)|^2 \right\} \equiv 0$$

Volume of "vortex core" (region occupied by MF)

Correction for particle number conservation:

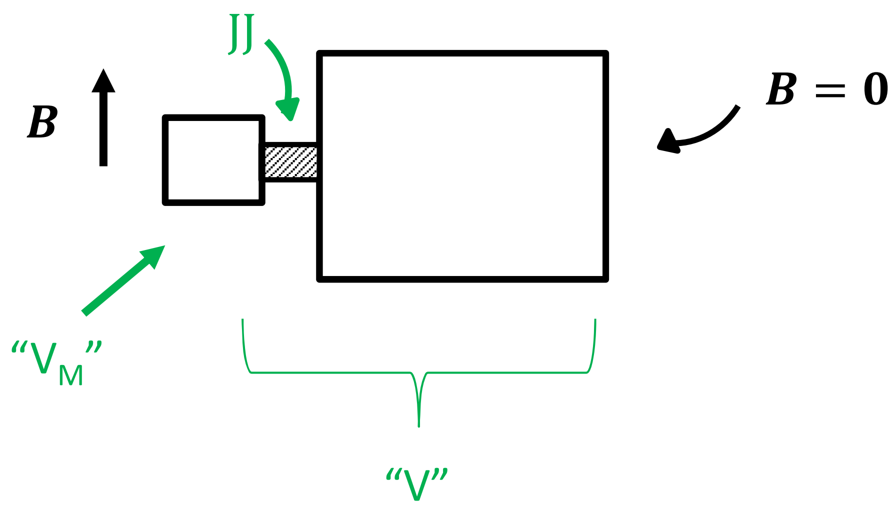
$$\gamma^{\dagger} = \int dr \left\{ u(r)\hat{\psi}^{\dagger}(r) + v(r)\hat{\psi}(r) C^{\dagger} \right\}$$

however, claim:

extra Cooper pair is spread over whole volume, so contribution to ΔN is $0(V_M/V)$ and vanishes in thermodymamic limit. (but already suggests power-law not exponential effect!)

Question: Is this true?

To examine, consider ultra-toy "Zeeman-Josephson" model: simple BCS superconductor in "Cooper-Pair box"

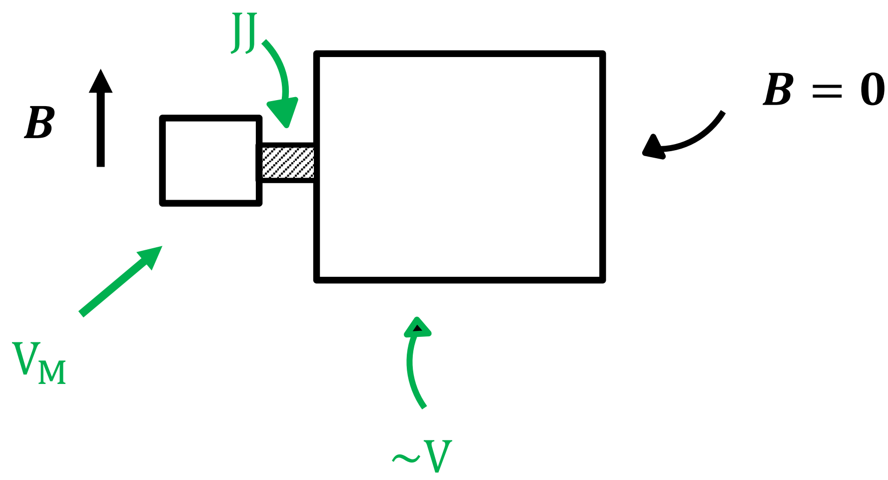


in even-no.-parity GS, some average number $\langle n \rangle_e$ of particles in $\mathrm{V_M}$.
in lowest odd-parity state, **B** localizes one spin-↑ quasiparticle in $\mathrm{V_M}$.:
average number of particles in V_M is $\langle n \rangle_o$. : $\Delta\langle n \rangle \equiv \langle n \rangle_o - \langle n \rangle_e$.

Mean-field (BdG) theory would say $\Delta\langle n \rangle = \mathrm{V_M} / \mathrm{V}$
(since $\Delta N_{tot} = +1$)

$64K question: Is this right?

"Zeeman-Josephson" problem:



Standard "Cooper pair box" ("transmon") Hamiltonian: if $\hat{n}$ is no. of Cooper pairs transferred from V to V_M

$$\hat{H} = E_c(\hat{n} - n_g)^2 - E_J \cos\hat{\varphi} \leftarrow \text{phase drop of Cooper pairs across junction}$$

↑ capacitance energy

↑ "offset charge"

↑ Josephson tunnelling energy

Crucial point: in limit $V = \infty$, V_M finite, $E_c \nrightarrow 0$.
Note "mean-field" description equivalent to $E_J \to \infty$. In this limit, assume $\Delta\langle n\rangle = V_M/V$; since in this limit $\Delta\langle n\rangle = n_g$, "effective" $n_g = V_M/V$.

Hellman-Feynman theorem:

$$\Delta\langle n\rangle = n_g + \frac{1}{2E_c}\frac{\partial E_o}{\partial n_g} \qquad E_o = \text{(even-parity) GS energy}$$

$E_o(n_g)$ is calculated in original transmon paper*: $\Rightarrow$

$$\Delta\langle n\rangle = n_g\,(\,1 - const.\,(E_J/E_c)^2\,exp - \underbrace{\sqrt{2E_J/E_c}}\,) \sim n_g \sim \mathrm{V_M/V}$$

$\uparrow$

$\nrightarrow\infty$ in thermodynamic limit

$\Delta\langle n\rangle = n_g$ would be "unobservable", so

"detectability" $\sim\Delta\langle n\rangle - n_g \sim$ const. $(\mathrm{V_M/V})\;\; exp - \sqrt{2E_J|E_c}$

$\sim\mathrm{V_M/V}$

$\uparrow$

power-law not exponential

suggests (but does not prove) that also for M.F.'s

"undetectability" is power-law not exponential in system dimensions.

Moral: Much more work needed!

*J. Koch et al., Phys. Rev. A **76**, 042319 (2007)