Topological classification of three-dimensional superconductors with interactions beyond mean field

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Ordinary BCS superconductors

- Bogolyubov-de Gennes Hamiltonian

\[ H = \sum_{p,\sigma} \xi(p) a_{p\sigma}^\dagger a_{p\sigma} + \sum_p \left( \Delta^* a_{-p\downarrow} a_{p\uparrow} + \Delta a_{p\uparrow}^\dagger a_{-p\downarrow}^\dagger \right) \]

- Nambu representation

\[
\hat{H} = \frac{1}{2} \sum_p \hat{\psi}_p^\dagger H(p) \hat{\psi}_p, \quad \hat{\psi}_p = \begin{pmatrix} \hat{a}_{p\uparrow} \\ \hat{a}_{p\downarrow} \\ \hat{a}_{-p\downarrow}^\dagger \\ -\hat{a}_{-p\uparrow}^\dagger \end{pmatrix}
\]

where \( \mathcal{T} \) is the time reversal operation

\[
H(p) = \begin{pmatrix} \xi(p) & \Delta \\ \Delta^* & -\xi(p) \end{pmatrix}
\]

(each entry is, actually, a 2 \( \times \) 2 matrix: a number times the identity matrix)
Triplet superconductor/superfluid

- General form of the Hamiltonian

\[ H(p) = \begin{pmatrix} \xi(p) & \Delta_\alpha(p) \cdot \sigma^\alpha \\ \Delta_\alpha(p)^* \cdot \sigma^\alpha & -\xi(p) \end{pmatrix} \]

- \( \Delta_\alpha \) are odd functions of \( p \)

- \( \alpha = x, y, z \)

- Superfluid \(^3\)He-B

\[ \Delta_\alpha(p) = \frac{\Delta}{p_F} W_{\alpha \beta} p_\beta \]

- complex number

- real orthogonal matrix (mapping between the orbital and spin spaces)

- e.g. \( W_{\alpha \beta} = \delta_{\alpha \beta} \)

- fully gapped: \( \Delta \) does not vanish on the Fermi sphere

- time reversal invariant (if \( \Delta \) is purely imaginary)

- Time reversal symmetry

\[ \mathcal{T} : \quad \Delta_\alpha(p) \mapsto -\Delta_\alpha^*(p) \]
Topology of a gapped TRI superconductor

- Gap function on the Fermi sphere: 
  \[ \Delta_\alpha = i |\Delta| f_\alpha(p) \]

  \[ f : S^2 \to S^2 \]

  Fermi sphere \quad \text{unit sphere in the spin space}

- Topological invariant: \( \nu \in \mathbb{Z} \) (reduced to \( \mathbb{Z}_{16} \) in the presence of interactions)

  For pairing near the Fermi sphere, \( \nu = \text{deg} f \)

  For example, if \( f_\alpha(p) = \pm p_\alpha / p_F \), then \( \nu = \pm 1 \)

- More generally, consider both \( \xi(p) = \frac{p^2}{2m} - \mu \) and \( \Delta(p) \)

  \[ \xi(p), \quad \varepsilon = \sqrt{\xi^2 + \Delta^2} \]

  \( \mu > 0, \quad \nu = \pm 1 \)

  \( \mu < 0, \quad \nu = 0 \)
Characterizing the difference between phases

- Hamiltonian near the phase transition

  When $\mu$ is small, the pairing occurs near $p = 0$, therefore the $\frac{p^2}{2m}$ term may be neglected

  \[
  H(p) \approx \begin{pmatrix}
  -\mu & iu \sigma^\alpha \\
  -iu p_\alpha \sigma^\alpha & \mu
  \end{pmatrix}
  \]

  \[
  \begin{align*}
  \mu > 0 & \Rightarrow \nu = 1 \\
  \mu < 0 & \Rightarrow \nu = 0
  \end{align*}
  \]

- Field-theoretic description

  \[
  \hat{H} = \int \hat{\Psi}^T \left( \begin{pmatrix}
  0 & u\sigma^\alpha \\
  -u\sigma^\alpha & 0
  \end{pmatrix} \frac{\partial}{\partial x^\alpha} + \begin{pmatrix}
  -\mu & 0 \\
  0 & \mu
  \end{pmatrix} \right) \hat{\Psi} \, dx
  \]

  Different phases ($\nu = 1$ vs. $\nu = 0$) are characterized by different mass terms, while the kinetic term is fixed.

  We will introduce a general formalism of this kind, which is suitable for all gapped systems of free fermions.
Majorana formalism (for discrete systems)

- Hamiltonian in terms of creation and annihilation operators

\[ \hat{H} = \sum_{j,k} h_{jk} \hat{a}_j^{\dagger} \hat{a}_k + \sum_{j,k} (\Delta_{jk} \hat{a}_j \hat{a}_k + \Delta_{jk}^* \hat{a}_k^{\dagger} \hat{a}_j^{\dagger}) \]

spin (if any) is included in the index \( j \)

- Majorana operators:

\[ \hat{c}_{2j-1} = \hat{a}_j + \hat{a}_j^{\dagger}, \quad \hat{c}_{2j} = \frac{\hat{a}_j - \hat{a}_j^{\dagger}}{i} \]

- Complete problem in terms of the Majorana operators

\[ \hat{H} = \frac{i}{4} \sum_{j,k} A_{jk} \hat{c}_j \hat{c}_k , \quad \text{where} \quad \hat{c}_k \hat{c}_l + \hat{c}_l \hat{c}_k = 2\delta_{kl}, \quad \hat{c}_k^{\dagger} = \hat{c}_k \]
Majorana formalism for continuous systems

- Hamiltonian:

\[ \hat{H} = \frac{i}{4} \int \eta^T \left( \sum_{j=1}^{n} \Gamma_{\mu} \partial_{\mu} + M \right) \eta \, dx \]

(Any gapped free-fermion phase has a representative of this form)

\[ \Gamma_{\mu} \text{ is real symmetric, } \Gamma_{\mu} \Gamma_{\nu} + \Gamma_{\nu} \Gamma_{\mu} = 2\delta_{\mu\nu} \]

\[ M \text{ is real skew-symmetric} \]

\[ M^2 = -1 \]

\[ M \Gamma_{\mu} = -\Gamma_{\mu} M \]

\[ \Gamma_1, \ldots, \Gamma_n \text{ are fixed} \]

Different phase are characterized by different \( M \)
Example: Majorana wire \((n = 1)\)

- Discrete version:
  \[
  \hat{H} = \frac{i}{2} \left( u \sum_{j=1}^{m} \hat{c}_{2j-1} \hat{c}_{2j} + v \sum_{j=1}^{m-1} \hat{c}_{2j} \hat{c}_{2j+1} \right)
  \]

- Continuum limit:
  \[
  u = 1 - w, \quad v = 1 + w \quad \text{where} \ w \ll 1
  \]
  \[
  \hat{H} = \frac{i}{4} \int \eta^T \left( \sum_{j=1}^{n} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial x} + \begin{pmatrix} 0 & w \\ -w & 0 \end{pmatrix} \right) \eta \, dx
  \]

  In this equation, we may set \(w = \pm 1\) (because there is no lattice)

- Different phases
  
  Trivial: \(w < 0\); \hspace{1cm} \text{Nontrivial:} \ w > 0 \ .
Full classification for $n = 0$

- General form of matrix $M$ (recall that $M^2 = -1$ w.l.o.g.):
  \[
  M = S \begin{pmatrix}
  0 & 1 \\
  -1 & 0 \\
  \ddots & \ddots \\
  0 & 1 \\
  -1 & 0 
  \end{pmatrix}
  S^{-1}
  \]
  $S \in \text{O}(2m)$
  $M \in \text{O}(2m)/\text{U}(m)$

- Classifying space of 0-dimensional states:
  \[
  \mathcal{F}_0^{(\text{free})} = \text{O}/\text{U}
  \]
  (A set that is homotopy equivalent to the set of ground states of all gapped free-fermion Hamiltonians)

- Topological invariant: $\text{Pf } M \in \mathbb{Z}_2$
  (describes the connected components of $\mathcal{F}^{(\text{free})}$)

$\text{Pf } M = +1$ — even number of particles
$\text{Pf } M = -1$ — odd number of particles
  \{ counting particles in the ground state \}
Full classification in all dimensions
(of gapped free-fermion systems without any symmetry)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\mathcal{F}_n^{(\text{free})}$</th>
<th>$\pi_0(\mathcal{F}_n^{(\text{free})})$</th>
<th>examples</th>
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<td>O/U</td>
<td>$\mathbb{Z}_2$</td>
<td>even/odd number of particles</td>
</tr>
<tr>
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<td>O</td>
<td>$\mathbb{Z}_2$</td>
<td>Majorana wire</td>
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<td>$\mathbb{Z}$</td>
<td>$p_x + ip_y$ superconductor</td>
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<tr>
<td>7</td>
<td>U/Sp</td>
<td>0</td>
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Time reversal symmetry

- General form:
  \[ T(\hat{c}_j) = \sum_k T_{jk} \hat{c}_k \]
  \[ T(i) = -i \]
  for continuous systems, replace \( \hat{c}_j \) with \( \hat{\eta}_j(x) \)

- Conventional TR symmetry: \( T^2 = -1 \)
  \[ T(\hat{a}_{j\uparrow}) = \hat{a}_{j\downarrow} \]
  \[ T(\hat{a}_{j\downarrow}) = -\hat{a}_{j\uparrow} \]
  \[ T \left( \begin{array}{c}
  \hat{c}_{2j-1,\uparrow} \\
  \hat{c}_{2j-1,\downarrow} \\
  \hat{c}_{2j,\uparrow} \\
  \hat{c}_{2j,\downarrow}
  \end{array} \right) = T \left( \begin{array}{cccc}
  0 & 0 & 1 & 0 \\
  0 & 0 & 0 & -1 \\
  -1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0
  \end{array} \right) \left( \begin{array}{c}
  \hat{c}_{2j-1,\uparrow} \\
  \hat{c}_{2j-1,\downarrow} \\
  \hat{c}_{2j,\uparrow} \\
  \hat{c}_{2j,\downarrow}
  \end{array} \right) \]

- Unconventional TR symmetry: \( T^2 = 1 \)
  \[ T(\hat{c}_l) = \hat{c}_l \]
  or \( T(\hat{c}_l) = -\hat{c}_l \)
  (for spinless systems)
Application to 3D superconductors (finally!)

- General form of the Hamiltonian

\[ \hat{H} = \frac{i}{4} \int \eta^T \left( \sum_{j=1}^{3} \Gamma_\mu \partial_\mu + M \right) \eta \, dx \]

\[ \Gamma_1 = \sigma^x \otimes I \otimes I, \quad \Gamma_2 = \sigma^z \otimes I \otimes I, \quad \Gamma_3 = (i\sigma^y) \otimes (i\sigma^y) \otimes I \]

\[ M = (i\sigma^y) \otimes (\sigma^x \otimes m + \sigma^z \otimes m') \]

- TR symmetry:

\[ T = (i\sigma^y) \otimes \sigma^z \otimes I \quad \text{(anticommutes with } \Gamma_\mu \text{)} \]

\[ \mathcal{T}(M) = -TMT^{-1} \quad \mathcal{T}(M) = M \quad \Rightarrow \quad M = (i\sigma^y) \otimes \sigma^x \otimes m \]

- Topological invariant

\[ m \text{ is a real symmetric matrix with eigenvalues } \pm 1 \]

\[ \nu = \text{(number of } +1 \text{ eigenvalues)} - \text{(number of } -1 \text{ eigenvalues)} \]
Main question

Is $\nu$ well-defined in the presence of interactions? In other words,

Can a $\nu = 0$ state be continuously changed into a $\nu \neq 0$ state?

(The intermediate states may include interparticle interactions, but the energy gap must never close.)

Claim: In the presence of interaction, $\nu$ is defined modulo 16.

- The $\nu = 16$ phase is connected to the trivial phase by a continuous path. (Shown by explicit construction.)
- If $\nu \not\equiv 0 \pmod{16}$, then there is no continuous path.
  - One has to consider all possible quantum states with suitable restrictions: an exact definition is needed.
  - The question can be reduced to the classification of cross sections of a certain fibration up to homotopy (a typical homotopy theory problem).
Related (somewhat simpler) question

The boundary between different phases supports gapless modes. Can those modes be suppressed by suitable interactions without breaking the TR symmetry or creating a topological order?

- Effective boundary theory

\[ \hat{H} = \frac{i}{4} \int \eta^T \left( \sum_{j=1}^{2} \Gamma_\mu \partial_\mu \right) \eta \, dx \]

\[ \Gamma_1 = \sigma^x \otimes I, \quad \Gamma_2 = \sigma^z \otimes I \]

- Possible mass term

\[ M = (i\sigma^y) \otimes m, \quad \text{where} \ m \ \text{is a real symmetric} \ \nu \times \nu \ \text{matrix} \]

- However,

\[ \mathcal{T}(m) = -m \]

If \( m \neq 0 \), then the symmetry is broken
Dynamic surface mass terms

• Key idea: Let \( m = m(x, t) \) fluctuate (as a quantum Bose field)

• Claim: Ergodic, symmetry non-breaking dynamics can be arranged (using a suitable \( \sigma \)-model) *if there are no topological obstructions*

• Example of a topological obstruction (for \( \nu = 1 \))

If \( m > 0 \) then \( \mathcal{T}(m) < 0 \). There is no continuous path between \( m \) and \( \mathcal{T}(m) \) in the space of nondegenerate mass terms.
The second obstruction (for $\nu = 2$)

- Resolving the previous obstruction

Let $m = \sigma^z$ be an admissible value of the dynamic mass term. Then $\mathcal{T}(m) = -\sigma^z$

Path from $m$ to $\mathcal{T}(m)$:

$$p_1(\theta) = (\cos \theta) \sigma^z + (\sin \theta) \sigma^x,$$
where $\theta \in [0, \pi]$.

- New obstruction: No way to interpolate between $p_1$ and $(\mathcal{T}(p_1))^{-1}$

In the real space:

- space of nondegenerate real symmetric $2 \times 2$ matrices
- gapless vortex
Further steps

• For $\nu = 4$, the obstruction corresponds to a soft-core soliton

• For $\nu = 8$, one can define a $\sigma$-model with the target space $S^3$

\[ m(x, t) = \sum_{k=1}^{4} u_k(x, t) m_k, \quad \text{where} \quad u \in S^3, \quad \text{i.e.} \quad \sum_{k=1}^{4} u_k^2 = 1 \]

\[ m_1 = \sigma^z \otimes I \otimes I, \quad m_2 = \sigma^x \otimes I \otimes I, \]

\[ m_3 = (i\sigma^y) \otimes (i\sigma^y) \otimes I, \quad m_4 = (i\sigma^y) \otimes \sigma^x \otimes (i\sigma^y) \]

– The model is TR invariant if we assume that $\mathcal{T}(u) = -u$

– $m(x, t)$ is nondegenerate because $m_j m_k + m_k m_j = 2\delta_{jk}$

However, the system is gapless due to a nontrivial WZW term

• For $\nu = 16$, the WZW term vanishes, which can be shown by extending the target space to $S^5$. The system is fully gapped.
Nontriviality of the $\nu = 8$ phase

- There could be a different, gapped $\sigma$-model for $\nu = 8$.
  
  It would correspond to a map $f$ from $S^5$ to the space of nondegenerate real symmetric matrices of size $8 \times 8$ such that $f(-u) = -f(u)$.

- Reduction to a homotopy theory problem
  
  Each value of $\nu$ corresponds to a cross section of a certain fibration over the classifying space of the symmetry group: $B\mathbb{Z}_2 = \mathbb{R}P^\infty$.

- Algebraic tools
  
  Atiah-Hirzebruch spectral sequence

- Result
  
  The $\nu = 0$ and $\nu = 8$ sections are not fiber-wise homotopic.
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