Antiferomagnetism and triplet superconductivity in Bechgaard salts

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Outline

• Introduction. Phase diagram of Bechgaard salts

• New experimental tests of triplet superconductivity

• Antiferomagnet to triplet superconductor transition in quasi 1d systems. SO(4) symmetry

• Implications of SO(4) symmetry for the phase diagram. Comparison to (TMTSF)$_2$PF$_6$

• Experimental test of SO(4) symmetry
Bechgaard salts

Stacked molecules form 1d chains

Evidence for triplet superconductivity in Bechgaard salts

• Strong suppression of $T_c$ by disorder
  Choi et al., PRB 25:6208 (1982)
  Tomic et al., J. Physique 44: C3-1075 (1982)

• Superconductivity persists at fields exceeding the paramagnetic limit
  \[ \mu_B H_p = \frac{\Delta_0}{\sqrt{2}} = 1.2 k_B T_c \]
  Lee et al., PRL 78:3555 (1997)
  Oh and Naughton, cond-mat/0401611

• No suppression of electron spin susceptibility below $T_c$. NMR Knight shift study of $^{77}$S in (TMTSF)$_2$PF$_6$
  Lee et al, PRL 88:17004 (2002)
P-wave superconductor without nodes

Order parameter

\[ \langle c_{-p\alpha}c_{p\beta} \rangle = (\sigma_2 \bar{\sigma})_{\alpha\beta} \bar{\Psi}(p) \]

\[ \bar{\Psi}(\bar{p}) = \hat{b} p_x \]

Specific heat in (TMTSF)$_2$PF$_6$

Nuclear spin lattice relaxation rate in (TMTSF)$_2$PF$_6$

For (TMTSF)$_2$ClO$_4$ similar behavior has been observed by Takigawa et.al. (1987)

Typically this would be attributed to nodal quasiparticles (nodal line)

This work: $T^3$ behavior of $1/T_1$ due to spin waves
Spin waves in triplet superconductors

Spin wave: d-vector rotates in space

Dispersion of spin waves

Full spin symmetry

Easy axis anisotropy
Spin anisotropy of the triplet superconducting order parameter

Spin anisotropy in the antiferromagnetic state:

\[ \Delta H = \delta J_z \sum_{\langle ij \rangle} S_i^z S_j^z \]
\[ \delta J_z = 10^{-4} J = 0.01 \text{ K} \]

Easy direction for the superconducting order parameter is along the b axis.

Assuming the same anisotropy in the superconducting state

\[ \frac{\omega_0}{\Delta_0} = 2(\delta J_z N_0 v_0)^{1/2} \log\left(\frac{1.14 \omega_{BOS}}{T_c}\right) \]

Easy direction for the superconducting order parameter is along the b axis

\[ \vec{\Psi}(\vec{p}) = \hat{b} p_x \]

For Bechgaard salts we estimate

\[ \omega_0 / 2\pi \sim 1 \text{ GHz} \]
Contribution of spin waves to $1/T_1$

Experimental regime of parameters $\omega_N << \omega_0 << T$

Moriya relation: $\omega_N$ -- nuclear Larmor frequency

$$\frac{1}{T T_1} = \int d^d q |A_q|^2 \frac{\chi''_1(q, \omega_N)}{\omega_N}$$

Creation or annihilation of spin waves does not contribute to $T_1^{-1}$

Scattering of spin waves contributes to $T_1^{-1}$
Contribution of spin waves to $1/T_1$

\[ \int d^d q \chi''_{zz}(q, \omega_N) \sim \int d\epsilon_1 d\epsilon_2 \rho(\epsilon_1)\rho(\epsilon_2) \left( n_B(\epsilon_1) - n_B(\epsilon_2) \right) \delta(\epsilon_1 - \epsilon_2 - \omega_N) \]

$\rho(\epsilon)$ is the density of states for spin wave excitations. Using $T >> \omega_N$

\[ \int d^d q \chi''_{zz}(q, \omega_N) \sim \int d\epsilon \rho^2(\epsilon) (-\omega_N) \frac{\partial n_B(\epsilon)}{\partial \epsilon} \]

For $T >> \omega_0$ we can take $\rho(\epsilon) \sim \epsilon^{d-1}$ where $d$ is the dimension

This result does not change when we include coherence factors.
For small fields, $T_1^{-1}$ depends on the direction of the magnetic field. For point-like hyperfine interaction, $1/T_1 \sim \sin^2 \theta$.

- When $T >> \omega_0$, we have $T^3$ scaling of $T_1^{-1}$ in $d=2$.
- When $T << \omega_0$, we have exponential suppression of $T_1^{-1}$.

These predictions of the spin-wave mechanism of nuclear spin relaxation can be checked in experiments.
Spin-flop transition in the triplet superconducting state

S=1 \quad S_z=0 \quad | \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle \quad \hat{\Psi} \parallel \hat{z}

S=1 \quad S_x=0 \quad | \uparrow \uparrow \rangle - | \downarrow \downarrow \rangle \quad \hat{\Psi} \parallel \hat{x}

S=1 \quad S_y=0 \quad | \uparrow \uparrow \rangle + | \downarrow \downarrow \rangle \quad \hat{\Psi} \parallel \hat{y}

At B=0 start with \( \hat{\Psi} \parallel \hat{z} \) (easy axis). For \( \vec{B} \parallel \hat{z} \) this state does not benefit from the Zeeman energy.

For \( B > B_{\text{crit}} \) the order parameter flops into the xy plane.

\[
|\Psi\rangle = \alpha | \uparrow \uparrow \rangle + \beta | \downarrow \downarrow \rangle
\]

This state can benefit from the Zeeman energy without sacrificing the pairing energy.

For Bechgaard salts we estimate \( H_{\text{flop}} \approx 300 \ G \).
Field and direction dependent Knight shift in UPt$_3$

Tau et al., PRL 80:3129 (1998)
Competition of antiferomagnetism and triplet superconductivity in Bechgaard salts
Coexistence of superconductivity and magnetism

Interacting electrons in 1d

Interaction Hamiltonian

Phase diagram

SDW (CDW) TSC (SS)

CDW (SS) SS (CDW) SS

SDW/TSC transition at $K_\rho=1$.
This corresponds to

$2g_2 = g_1$
Symmetries

Spin SO(3)$_S$ algebra

\[ [S_\alpha, S_\beta] = i\epsilon_{\alpha\beta\gamma} S_\gamma \]

SO(3)$_S$ is a good symmetry of the system

\[ [\mathcal{H}, S_\alpha] = 0 \]

Isospin SO(3)$_I$ symmetry

\[ \theta^\dagger = \sum_k \left( a^\dagger_{Rk\uparrow} a^\dagger_{R-k\downarrow} - a^\dagger_{Lk\uparrow} a^\dagger_{L-k\downarrow} \right) \quad \quad Q = \frac{1}{2} \sum_{k\sigma} \left( a^\dagger_{Rk\sigma} a_{Rk\sigma} + a^\dagger_{Lk\sigma} a_{Lk\sigma} \right) \]

\[ I_x = \frac{1}{2}(\theta^\dagger + \theta) \quad I_y = \frac{1}{2i}(\theta^\dagger - \theta) \quad I_z = Q \]

\[ [I_a, I_b] = i\epsilon_{abc} I_c \]

We always have charge U(1) symmetry

\[ [\mathcal{H}, I_z] = 0 \]

When $K_p = 1$, U(1) is enhanced to SO(3)$_I$ because

\[ [\mathcal{H}, I_{\pm}] = 0 \]
SO(4) = SO(3)_S x SO(3)_I symmetry. Unification of antiferromagnetism and triplet superconductivity.

Order parameter for antiferromagnetism: \( \vec{N} \)

Order parameter for triplet superconductivity: \( \vec{\Psi} \)

\[
Q_{a\alpha} = \begin{pmatrix}
\text{Re } \Psi_x & \text{Im } \Psi_x & N_x \\
\text{Re } \Psi_y & \text{Im } \Psi_y & N_y \\
\text{Re } \Psi_z & \text{Im } \Psi_z & N_z \\
\end{pmatrix}
\]

\( Q_{a\alpha} \) transforms as a vector under spin and isospin rotations.

\[
[ S_\alpha, Q_{b\beta} ] = i \epsilon_{\alpha\beta\gamma} Q_{b\gamma}
\]

\[
[ I_a, Q_{b\beta} ] = i \epsilon_{abc} Q_{c\gamma}
\]
Ginzburg-Landau free energy

\[ F = \frac{1}{2} |\nabla \bar{\Psi}|^2 + \frac{1}{2} (\nabla \bar{N})^2 + \frac{r_1}{2} |\bar{\Psi}|^2 + \frac{r_2}{2} \bar{N}^2 + u_1 (|\bar{\Psi}|^2)^2 + u_3 |\bar{\Psi}|^2 + 2v_1 |\bar{\Psi}|^2 \bar{N}^2 + 2v_2 |\bar{N} \bar{\Psi}|^2 + u_2 (\bar{N}^2)^2 \]

SO(4) symmetry requires

\[ r_1 = r_2 \quad u_2 - u_3 = u_1 \quad u_2 - 2u_3 = v_1 \quad v_2 = 2u_3 \]

SO(4) symmetric GL free energy

\[ F = \frac{1}{2} (\nabla Q_{\alpha \alpha})^2 + \frac{r}{2} Q_{\alpha \alpha}^2 + \tilde{u}_1 Q_{\alpha \alpha} Q_{\alpha \alpha} Q_{b \beta} Q_{b \beta} + \tilde{u}_2 Q_{\alpha \alpha} Q_{b \alpha} Q_{a \beta} Q_{b \beta} \]

Weak coupling analysis

\[ \tilde{u}_1 = \frac{21 \zeta(3)}{16\pi^2 v_f T^2} \quad \tilde{u}_2 = -\frac{7 \zeta(3)}{8\pi^2 v_f T^2} \]
Role of interchain hopping
GL free energy. Phase diagram

\[ F = \frac{1}{2} |\nabla \Psi|^2 + \frac{1}{2} (\nabla N)^2 + \frac{r_1}{2} |\Psi|^2 + \frac{r_2}{2} N^2 + (\tilde{u}_1 + \frac{\tilde{u}}{2})(|\Psi|^2)^2 \]
\[ + \frac{\tilde{u}_2}{2} |\Psi|^2 + 2\tilde{u}_1 |\Psi|^2 N^2 + 2\tilde{u}_2 |N\Psi|^2 + (\tilde{u}_1 + \tilde{u}_2)(N^2)^2 \]

Unitary TSC for \( \tilde{u}_2 < 0 \). TSC order parameter
\[ \Psi = e^{i\theta} \vec{n} \]

First order transition between AF and TSC
Unitary TSC and AF. Thermal fluctuations

Extend spin SO(3) to SO(N). Do large N analysis in d=3

- First order transition between normal and triplet superconducting phases (analogous result for $^3\text{He}$: Bailin, Love, Moore (1997))
- Tricritical point on the normal/antiferromagnet boundary
Triplet superconductivity and antiferromagnetism. Phase diagram

First order transition becomes a coexistence region

Phase diagram of Bechgaard salts

Experimental test of quantum SO(4) symmetry

\( \Theta \) operator rotates between AF and TSC orders

<table>
<thead>
<tr>
<th>Operator</th>
<th>Charge</th>
<th>Spin</th>
<th>Momentum</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \vec{N} )</td>
<td>0</td>
<td>1</td>
<td>( 2k_F )</td>
</tr>
<tr>
<td>( \vec{\Psi} )</td>
<td>2</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>( \theta^\dagger )</td>
<td>2</td>
<td>0</td>
<td>( 2k_F )</td>
</tr>
</tbody>
</table>

\( \theta \)-mode should appear as a sharp resonance in the TSC phase

Energy of the \( \theta \) mode softens at the first order transition between superconducting and antiferromagnetic phases
Conclusions

- New experimental tests of triplet pairing in Bechgaard salts:
  1) NMR for $T < 50\text{mK}$ and small fields. Expect strong suppression of $1/T_1$
  2) Possible spin flop transition for magnetic fields along the $b$ axis and field strength around 0.5 kG
  3) Microwave resonance in Bechgaard salts at $\omega/2\pi \sim 1 \text{GHz}$. (For Sr$_2$RuO$_4$ expect such resonance at $\omega/2\pi \sim 10 \text{GHz}$)

- SO(4) symmetry is generally present at the antiferromagnet to triplet superconductor transition in quasi-1d systems

- SO(4) symmetry helps to explain the phase diagram of (TMTSF)$_2$PF$_6$

- SO(4) symmetry implies the existence of a new collective mode, the $\theta$ resonance. The $\theta$ resonance should be observable using inelastic neutron scattering experiments (in the superconducting state)