Coexistence of Antiferromagnetism and Triplet Superconductivity

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The authors discuss the possibility of coexistence of antiferromagnetism and triplet superconductivity as a particular example of a broad class of systems where the interplay of magnetism and superconductivity is important. This paper focuses on the case of quasi-one-dimensional metals, where it is known experimentally that antiferromagnetism is in close proximity to triplet superconductivity in the temperature versus pressure phase diagram. Over a narrow range of pressures, the authors propose an intermediate non-uniform phase consisting of alternating insulating antiferromagnetic and triplet superconducting stripes.

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Figure 1: a) Phase diagram of \((\text{TMTSF})_2\text{PF}_6\) in a log-linear scale (from [1]), showing schematically the proposed AF-TS coexistence region (inset). b) Schematic drawing of the proposed stripe pattern for the AF-TS coexistence region.

\((\text{TMTSF})_2\text{PF}_6\) is a quasi-one dimensional organic material with a complex phase diagram involving antiferromagnetic (AF) insulating and triplet superconducting (TS) phases [1, 2, 3]. New experiments on this material in high magnetic fields have shown that TS phase is strongly affected by the proximity to AF phase characterized by a spin density wave (SDW) [2]. Motivated by these experiments and the known phase diagram of quasi-one-dimensional \((\text{TMTSF})_2\text{PF}_6\) we propose a new phase for quasi-one-dimensional systems where AF (SDW) and TS coexist. The coexistence of these phases implies that the new state is non-uniform, with alternating stripes of insulating AF and TS, due to the appearance of a negative interface energy between AF and TS regions. As indicated in the schematic phase diagram (Fig. 1), the inhomogeneous intermediate phase is expected to exist over a narrow range of pressures \(\Delta P = P_2(T) - P_1(T)\) around \(P_c\), where \(\Delta P \ll P_c\).

Effective Free Energy: The possibility of coexistence of SDW and TS in quasi-one-dimensional conductors transcends microscopic descriptions based on standard g-ology, where SDW and TS phase boundaries neighbor each other but do not coexist [4]. Inspired
by experiments \[3, 6\], we model \((\text{TMTSF})_2\text{PF}_6\) as a highly anisotropic orthorombic crystal, and we take the primary directions of the SDW vector order parameter to be the b-axis (y-direction), and the primary direction of the TS vector order parameter to be the c-axis (z-direction). Furthermore, we consider the spatial variation of the SDW or TS order parameter to be along the a-axis (x-direction), as a reflection of the quasi-one-dimensionality of the system. This simplifies the choices of the order parameters to be \(S(r) \rightarrow S_b(x)\), and \(D(r) \rightarrow D_c(x)\), and reduces the associated effective field theory to one spatial dimension.

Thus, the generalized Ginzburg-Landau free energy in real space can be written as

\[
\mathcal{F}_{\text{tot}} = \mathcal{F}_{\text{AF}} + \mathcal{F}_{\text{TS}} + \mathcal{F}_{\text{C}},
\]

where \(\mathcal{F}_{\text{AF}}, \mathcal{F}_{\text{TS}}, \mathcal{F}_{\text{C}}\) are the AF(SDW), TS and coupling contributions discussed below. The AF contribution is

\[
\mathcal{F}_{\text{AF}} = \int_{L_{\text{AF}}} dx \left[ U_{\text{AF}}(x) + V_{\text{AF}}(x) \right],
\]

where \(U_{\text{AF}}(x) = \alpha_{\text{AF}}|S_b(x)|^2 + \beta_{\text{AF}}|\partial_x S_b(x)|^2 + \gamma_{\text{AF}}|S_b(x)|^4\) represents a typical GL free energy density, and \(V_{\text{AF}} = \delta_{\text{AF}}|\partial_x S_b(x)|^4 + \theta_{\text{AF}}|S_b(x)|^2|\partial_x S_b(x)|^2\) represents the extra terms in the expansion, which are relevant close to \(P_1(T)\). The TS contribution is

\[
\mathcal{F}_{\text{TS}} = \int_{L_{\text{TS}}} dx \left[ U_{\text{TS}}(x) + V_{\text{TS}}(x) \right],
\]

where \(U_{\text{TS}}(x) = \alpha_{\text{TS}}|D_c(x)|^2 + \beta_{\text{TS}}|\partial_x D_c(x)|^2 + \gamma_{\text{TS}}|D_c(x)|^4\), and \(V_{\text{TS}} = \delta_{\text{TS}}|\partial_x D_c(x)|^4 + \theta_{\text{TS}}|D_c(x)|^2|\partial_x D_c(x)|^2\). To describe the coexistence region the two order parameters must couple. To conform with independent Parity invariance,

\[
\mathcal{F}_{\text{C}} = \sum_{\text{inter}} \int_0^{\ell_p} dx \lambda'_{bc}|S_b(x)|^2|D_c(x)|^2,
\]

where the sum is over all possible interfaces between AF and TS, the coupling constant \(\lambda'_{bc}\) is pressure and temperature dependent, and \(\ell_p\) is the length of proximity at which AF and TS order parameters coexist locally. Since the AF order is pair breaking to triplet electron pairs \[7, 8\], we estimate that \(\ell_p\) to be much smaller than the length of the AF
stripe $\ell_{AF}$, unless $P \to P_2(T)$, where $\ell_{AF}$ approaching zero. In this limiting case, the Josephson effect between two consecutive TS stripes becomes significant and the material will change from a 2D to a 3D superconductor. In the case where $\ell_p$ is small, both AF and TS order parameters inside the proximity region can be approximated by linear functions, thus

$$F_C = \sum_{\text{inter}} \lambda_{bc} |\partial_x S_b(x)|^2 |\partial_x D_c(x)|^2,$$

where $\lambda_{bc} = \lambda'_{bc} \int_{0}^{\ell_p} dx x^2 (\ell_p - x)^2$ is the new coupling constant.

**Saddle Point Equations:** To obtain the saddle point equations, we minimize $F_{\text{tot}}$ with respect to $S_b(x)$ and $D^*_c(x)$. Variation of $F_{\text{tot}}$ with respect to $S_b(x)$ lead to the differential equation

$$[2\alpha_{AF} + 4\gamma_{AF} S^2_b(x) - \beta_{AF} \partial_x^2] S_b(x) + \hat{M}_{AF} S_b(x) = 0,$$

with $\hat{M}_{AF} S_b(x) = -\delta_{AF} \partial_x [(\partial_x S_b(x))^2 + 2\theta_{AF} S_b(x)|\partial_x S_b(x)|^2]$. Variation of $F_{\text{tot}}$ with respect to $D^*_c(x)$ lead to a similar equation. Given that we are considering the possibility of coexistence of the two phases, the boundary conditions in the presence of AF-TS interfaces require that $S_b(x)|_{\text{inter}^+} = 0$ and $D_c(x)|_{\text{inter}^-} = 0$, where $\text{inter}^+$ and $\text{inter}^-$ denote the two boundaries of locally coexisting proximity $\ell_p$ at which $S_b(x)$ and $D_c(x)$ vanish respectively.

**Variational Free Energy:** We consider first the AF case and search for periodic solutions with period $\ell_{AF}$, with $S_b(x)|_{\text{inter}^+} = 0$ at the AF-TS interfaces. For a given volume of the AF region, controlled by $L_{AF}$, the Free energy associated with the AF phase becomes the sum of $N_{AF}$ identical terms, where $N_{AF} = L_{AF}/\ell_{AF}$ gives the number of AF stripes. Generally, each term in $F_{AF}$ corresponds to an insulating AF stripe characterized by the order parameter $S_b(x) = \sum_n A_n \sin(Q_n x)$, where $Q_n = 2\pi n/\ell_{AF}$. But here we take for simplicity the variational class where $S_b(x) = A_1 \sin(Q_1 x)$, which satisfies the appropriate boundary and merging conditions. To simplify notation, we use $A_1 \to A$ and $Q_1 \to Q$. In
this case
\[ \mathcal{F}_{AF} = L_{AF} \left[ C_2(Q)A^2 + C_4(Q)A^4 \right], \]
where \( C_2(Q) = (\alpha_{AF} + \beta_{AF}Q^2)/2 \) and \( C_4(Q) = (3\gamma_{AF} + \theta_{AF}Q^2 + 3\delta_{AF}Q^4)/8. \)

The same type of analysis applies to \( \mathcal{F}_{TS} \). In the absence of a magnetic field, we assume periodic solutions of the form \( D_c(x) = B \sin(Kx) \), Here \( B \) can be complex, but independent of position \( x \), making this choice consistent with a weak spin-orbit coupling interaction from a microscopic theory [9]. All the analysis discussed for the AF case applies with the following change of notation: \( L_{AF} \rightarrow L_{TS}, A \rightarrow B, Q \rightarrow K, \alpha_{AF} \rightarrow \alpha_{TS}, \beta_{AF} \rightarrow \beta_{TS}, \) etc.

And the coupling free energy is
\[ \mathcal{F}_C = N_{int} \Lambda(Q, K)A^2|B|^2, \]
where \( N_{int} = 2N \) is the total number of interfaces, \( \Lambda(Q, K)A^2|B|^2 = f_{int} \) is the free energy of one interface with \( \Lambda(Q, K) = \lambda_{bc}Q^2K^2. \)

\textit{Variational Solution:} Variations of \( \mathcal{F}_{tot} \) with respect to \( \phi_{AF} = A, \phi_{TS} = |B|, \) and \( q_{AF} = Q \) or \( q_{TS} = K \) lead to the non-trivial solutions
\[ \phi_i^2 = \frac{4\beta_i\theta_i - 24\alpha_i\delta_i}{36\gamma_i\delta_i - \theta_i^2}, \]
\[ q_i^2 = \frac{\alpha_i\theta_i - 6\beta_i\gamma_i}{\beta_i\theta_i - 6\alpha_i\delta_i}. \]

In addition, \( f_{int} = \lambda_{bc}\phi_{AF}^2\phi_{TS}^2q_{AF}^2q_{TS}^2. \) and the width of each stripe is given by
\[ \ell_i = 2\pi\sqrt{\frac{\beta_i\theta_i - 6\alpha_i\delta_i}{\alpha_i\theta_i - 6\beta_i\gamma_i}}, \]
where \( i = AF, TS. \) If \( \lambda_{bc}(P, T) > 0, \) the system phase separates, and there is no coexistence region, thus the line separating the AF phase from the TS phase indicates a discontinuous transition and \( (P_c, T_c) \) is bicritical. However, if \( \lambda_{bc}(P, T) < 0 \) then the formation of interfaces is preferred, and alternating stripes of AF and TS order appear in the system, creating a coexistence region dictated by the condition \( \lambda_{bc}(P, T) < 0. \) In this case, two
Figure 2: Free energies for the coexistence and the pure AF and TS phases. Solid line $\rightarrow F_{\text{tot}}$; stars $\rightarrow Lf_{\text{TS}}$; triangles $\rightarrow Lf_{\text{AF}}$; squares $\rightarrow F_C$. Exponents chosen are $\varepsilon_{\alpha_i} = 5.0$, $\varepsilon_{\beta_i} = 1.0$, $\varepsilon_{\theta_i} = 5.0$, $\varepsilon_{\lambda_i} = 1.0$ where $i = \text{AF, TS}$ and dimensionless parameters: $\tilde{\alpha}_1 = \tilde{\beta}_1 = 1.0$, $\tilde{\gamma}_1 = 0.05$, $\tilde{\delta}_1 = 0.005$, $\tilde{\theta}_1 = 0.001$; and $\tilde{\alpha}_2 = \tilde{\beta}_2 = 1.0$, $\tilde{\gamma}_2 = 0.07$, $\tilde{\delta}_2 = 0.006$, $\tilde{\theta}_2 = 0.002$, $\tilde{\lambda} = 0.004$.

additional transition lines emanate from $(P_c, T_c)$. This indicates that the point $(P_c, T_c)$ in the phase diagram illustrated in Fig. 1 can be bicritical, tricritical, or tetracritical and corresponds to the place where $\lambda_{bc}(P,T) = 0$.

**Phase Transitions:** Starting from the point $(P_c, T_c)$, two transition lines appear. The transition line $P_1(T)$ corresponds to the disappearance of the pure AF phase, and the transition line $P_2(T)$ corresponds to the appearance of the pure TS phase. (We estimate the Josephson effect region is small and look $P_2(T)$ and $P_3(T)$ as one single line.) For pressures between $P_1(T)$ and $P_2(T)$ there is coexistence between AF and TS order in the form of stripes. This implies that at $P_1(T)$ the TS stripe width $\ell_{\text{TS}} = 0$, while at $P_2(T)$ the AF stripe width $\ell_{\text{AF}} = 0$. Furthermore, for $P_1(T) < P < P_2(T)$, $\ell_{\text{TS}}$ increases from 0 to some finite value and $\ell_{\text{AF}}$ decreases from some other finite value to 0 with increasing pressure.

In order to meet these and the saddle point requirements, the parameters appearing in $F_{\text{tot}}$ must behave as follows. We define the reduced pressure changes $\Delta P_i = [P - P_i(T)]/P_c$, where $i = 1, 2$ to analyse the AF and TS parameters. For $P < P_2(T)$, the AF parameters have the form $\gamma_{\text{AF}} = \gamma_1 N(\epsilon_F)T_c^2 > 0$; $\delta_{\text{AF}} = \delta_1 N(\epsilon_F)T_c^2 > 0$; $\alpha_{\text{AF}} = \alpha_1 N(\epsilon_F)T_c^2 |\Delta P_2|^{\varepsilon_{\alpha_{\text{AF}}}}$. 
with $\alpha_1 < 0$; $\beta_{AF} = \beta_1 N(\epsilon_F)T_c^2|\Delta P_2|^{|\epsilon_{AF}|}$, with $\beta_1 < 0$; $\theta_{AF} = \theta_1 N(\epsilon_F)T_c^2|\Delta P_2|^{|\epsilon_{AF}|}$, with $\theta_1 < 0$; and $36\gamma_{AF}\delta_{AF} - \theta_{AF}^2 > 0$. For $P > P_1(T)$, the TS parameters have the form $\gamma_{TS} = \gamma_2 N(\epsilon_F)T_c^2 > 0$; $\delta_{TS} = \delta_2 N(\epsilon_F)T_c^2 > 0$; $\alpha_{TS} = \alpha_2 N(\epsilon_F)T_c^2|\Delta P_1|^{|\epsilon_{TS}|}$, with $\alpha_2 < 0$; $\beta_{TS} = \beta_2 N(\epsilon_F)T_c^2|\Delta P_1|^{|\epsilon_{TS}|}$, with $\beta_1 < 0$; $\theta_{TS} = \theta_2 N(\epsilon_F)T_c^2|\Delta P_1|^{|\epsilon_{TS}|}$, with $\theta_2 < 0$; and $36\gamma_{TS}\delta_{TS} - \theta_{TS}^2 > 0$. Consider now, the interface terms in the region $P_1(T) < P < P_2(T)$, which has the form $\lambda_{bc} = \lambda_0 N(\epsilon_F)T_c^2 \text{sgn}[(P - P_1)(P - P_2)]|\Delta P_1|^{|\epsilon_{AF}|}|\Delta P_2|^{|\epsilon_{TS}|}$, with $\lambda_0 > 0$. This form is required to make the interface energy negative between $P_1(T)$ and $P_2(T)$.

Next, we focus only on the analysis of $\ell_{TS}$ and $F_{tot}$ in the vicinity of $P_1(T)$. The requirement that $\ell_{TS} \to 0$ as $P \to P_1(T)$ forces a constraint $\varepsilon_{\alpha_{TS}} > \varepsilon_{\beta_{TS}}$. By considering $F_{tot}$ must less than the pure phase $F_{AF}(P_1)$, another condition $\varepsilon_{\alpha_{TS}} \geq 3\varepsilon_{\beta_{TS}} + 2\varepsilon_{\lambda_{TS}}$ is imposed. Furthermore, calculation of $\partial F_{tot}/\partial P$ shows the phase transition at $P_1$ is continuous if $\varepsilon_{\lambda_{TS}} + \varepsilon_{\beta_{TS}} > 1$ or discontinuous if $\varepsilon_{\lambda_{TS}} + \varepsilon_{\beta_{TS}} \leq 1$. In Fig. 2, we show the behavior of the various contributions to $F_{tot}$ for the case where the transitions are continuous at $P_1$ and $P_2$, and thus $(P_c, T_c)$ is tetracritical. Dimensionless parameters used are defined as $\tilde{\alpha}_i = \tilde{\beta}_i = \rho_i^{1/2}$, $\tilde{\gamma}_i = \gamma_i \sigma_i^{-1/2}$, $\tilde{\delta}_i = \delta_i \sigma_i^{3/2}$, $\tilde{\theta}_i = \theta_i \sigma_i^{1/2}$, and $\tilde{\lambda}_0 = \lambda_0 \sigma_1 \sigma_2$, where $\rho_i = \alpha_i \beta_i$, and $\sigma_i = \alpha_i / \beta_i$, with $i = 1, 2$. We note in passing that the analysis of $\ell_{AF}$ and $F_{tot}$ in the vicinity of $P_2(T)$ is non-trivial, since the Josephson effect between two consecutive TS stripes becomes important. An additional term $F_J$ should be added to the total free energy.

$$F_J = \sum_n \int_{\text{overlap}} dx |D_{c,(n+1)}(x) - D_{c,n}(x)|^2,$$  \hfill (11)

where the summation runs over all TS stripes. By adding this term, another line ($P_3$ in Fig. 1 inset) will emerge to denote a 2D $\to$ 3D superconductor crossover. Detailed calculations on refinement involving $F_J$ will be the topic of a future publication.

Summary: We have proposed the possibility of coexistence of antiferromagnetism and triplet superconductivity in the phase diagram of (TMTSF)$_2$PF$_6$. This intermediate phase is proposed to be inhomogeneous and to consist of alternating insulating AF and TS stripes. Two additional transition lines are present in a narrow range of pressures around $P_c$ sep-
arating the coexistence region from the pure AF and pure TS phases. We estimate the maximum pressure range to be \( \Delta P/P_c \approx 10\% \) at \( T = 0 \).

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