Coexistence of Spin Density Wave and Triplet Superconductivity

Wei Zhang and C. A. R. Sá de Melo
School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332

We discuss the possibility of coexistence of spin density wave (antiferromagnetism) and triplet superconductivity as a particular example of a broad class of systems where the interplay of magnetism and superconductivity is important. We focus 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, we propose an intermediate non-uniform phase consisting of alternating antiferromagnetic and triplet superconducting stripes. Within the non-uniform phase there are also changes between two and three dimensional behavior.

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The competition or coexistence of magnetic order and superconductivity is a very important problem in condensed matter physics. There is a broad class of systems that present magnetic order and superconductivity in close vicinity. One of the most important systems are the Copper Oxides, where singlet superconductivity is found next to antiferromagnetism \[1\]. In addition, striped phases, where coexistence of antiferromagnetic order and singlet d-wave superconductivity, were observed in Copper Oxides \[2\]. Another system where magnetism and superconductivity are intertwined is Strontium Ruthenate, where the proximity to ferromagnetism has been argued as being important to the existence of triplet superconductivity in these materials \[3\]. Furthermore the newly discovered ferromagnetic superconductors ZrZn\[2\] and UGe\[2\] have stimulated a debate on the coexistence of ferromagnetism and triplet or singlet superconductivity \[4\]. However, unlike any of these previous examples, we will discuss in this manuscript a system which may exhibit coexistence of antiferromagnetism (AF) and triplet superconductivity (TS).

New experiments on quasi-one-dimensional superconductors in high magnetic fields have shown that TS is strongly affected by the proximity to an AF phase characterized by insulating spin density wave (SDW) order \[5\]. From now on we will use interchangeably SDW and AF. Motivated by these experiments and the known phase diagram of quasi-one-dimensional (TMTSF)\[2\]PF\[6\] under pressure 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 SDW and TS, due to the appearance of a negative interface energy between SDW 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 \[6\]. Inspired by experiments \[7\], we model (TMTSF)\[2\]PF\[6\] as a highly anisotropic orthorhombic 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 choice of the order parameters to be \(S(x)\) and \(D(x)\), 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

\[ F_{\text{tot}} = F_{AF} + F_{TS} + F_C, \]

where \(F_{AF}, F_{TS}, \) and \(F_C\) are the AF, TS and coupling contributions discussed below. The AF contribution is

\[ F_{AF} = \int_{L_{AF}} dx \left[ U_{AF}(x) + V_{AF}(x) \right], \]

where \(U_{AF}(x) = \alpha_{AF}|S(x)|^2 + \beta_{AF}|\partial_x S(x)|^2 + \gamma_{AF}|S(x)|^4\) represents a typical GL Free energy density, and \(V_{AF} = \delta_{AF}|\partial_x S(x)|^4 + \theta_{AF}|S(x)|^2|\partial_x S(x)|^2\) represents the extra terms in the expansion, which are relevant close to \(P_1(T)\) (Fig. 1). The TS contribution is

\[ F_{TS} = \int_{L_{TS}} dx \left[ U_{TS}(x) + V_{TS}(x) \right], \]

where \(U_{TS}(x) = \alpha_{TS}|D(x)|^2 + \beta_{TS}|\partial_x D(x)|^2 + \gamma_{TS}|D(x)|^4\) represents a typical GL Free energy density, and \(V_{TS} = \delta_{TS}|\partial_x D(x)|^4 + \theta_{TS}|D(x)|^2|\partial_x D(x)|^2\) represents the extra terms in the expansion, which are relevant close to \(P_2(T)\) (Fig. 1). To describe the coexistence region the two order parameters must couple. To conform with independent Parity invariance,

\[ F_C = \sum_{\text{inter}} \int_{\ell_P} dx \chi_{bc}(x)|S_b(x)|^2|D_c(x)|^2, \]
where the sum is over all interfaces between AF and TS, the coupling constant $\lambda_{bc}$ is pressure and temperature dependent, and $\ell_p$ is the proximity length over which AF and TS order parameters coexist locally. This length can be written as $\ell_p = \ell_{p,AF} + \ell_{p,TS}$, where $\ell_{p,AF}$ is the AF proximity length into the TS region, and $\ell_{p,TS}$ is the TS proximity length into the AF region (See Fig. 2). If $\lambda_{bc} > 0$ it is more favorable for the AF and TS phases to phase-separate, however if $\lambda_{bc} < 0$ an inhomogeneous phase with a large number of interfaces is favored, and the coexistence of AF and TS is possible.

In non-triplet systems local AF order and local singlet superconductivity (SS) can in principle coexist since AF order favors singlet correlations, and the proximity lengths on SS/AF systems can be small or large depending on the SS and AF materials \cite{11,12}. However, we are interested in TS and not in SS. In this case, it is well known that AF order is pair breaking to triplet electron pairs \cite{13}, and it is expected that $\ell_{p,AF}$ and $\ell_{p,TS}$ are small in comparison to the lengths of $\ell_{TS}$ and $\ell_{AF}$ of the TS and AF stripes, respectively. Only when the pressure $P$ is close to the phase boundaries $P_1$ or $P_2$ (shown in Fig. 1) where $\ell_{TS}$ and $\ell_{AF}$ approach zero respectively, the proximity lengths $\ell_{p,TS}$ and $\ell_{p,AF}$ can be comparable to $\ell_{AF}$ and $\ell_{TS}$. Using WKB \cite{11} and the deGennes \cite{14} extrapolation methods the upper bound for $\ell_p$ is $\ell_p(P) \leq 0.1[\ell_{AF}(P) + \ell_{TS}(P)]$, and $\ell_{p,AF}(P) \leq 0.1\ell_{TS}(P_2)$ and $\ell_{p,TS}(P) \leq 0.1\ell_{AF}(P_1)$. Thus, extrapolating AF and TS order parameters in the proximity region by linear functions \textit{a la} deGennes \cite{14} leads to

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

where $\lambda_{bc} = \lambda_{bc} f_{bc}^p dx x^2 (\ell_p - x)^2$ is the new coupling constant. This coupling describes well the inhomogeneous phase where proximity effects between AF and TS stripes are weak, i.e., away but not too far from phase boundaries $P_1$ and $P_2$.

Proximity effects will be important close to either phase boundary ($P_1, P_2$) as they may lead to further coupling between like-stripes. The inter-TS-stripe coupling (Josephson-type)

$$F_{I,TS} = \sum_n \int_{\text{overlap}} dx \eta_{TS} |D_{c,n+1}(x) - D_{c,n}(x)|^2$$

is significant for $P \approx P_2$, where the system changes from 2D to 3D AF. The inter-AF-stripe coupling

$$F_{I,AF} = \sum_n \int_{\text{overlap}} dx \eta_{AF} |S_{b,n+1}(x) - S_{b,n}(x)|^2$$

is significant for $P \approx P_1$, where the system changes from 3D to 2D AF. The domain of integration for both cases above is the overlap region between two consecutive AF or TS stripes respectively.

\textit{Saddle Point Equations:} To obtain the saddle point equations, we consider $F_C$, $F_{I,AF}$ and $F_{I,TS}$ perturbatively and minimize $F_{tot}$ with respect to $S_b(x)$ and $D_c(x)$. Variations of $F_{tot}$ with respect to $S_b(x)$ lead to the differential equation

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

with $\tilde{M}_{AF} S_b(x) = -\delta_{AF} \partial_x [(\partial_x S_b(x))]^3 + 2\theta_{AF} S_b(x) |\partial_x S_b(x)|^2$. Variations of $F_{tot}$ with respect to $D_c(x)$ lead to a similar equation. In the case where $\lambda_{bc}(P, T) < 0$, the formation of an inhomogeneous phase of alternating AF and TS stripes is preferred, and two additional transition lines ($P_1, P_2$) emanate from ($P_1, T_c$). The presence of the inter-TS and inter-AF stripe Free energies indicates that $D_{n+1}(x) = D_{n}(x + x_0)$, and $S_{n+1}(x) = S_{n}(x + x_0)$ (in phase solutions), since $\eta_{AF}$ and $\eta_{TS}$ are both positive. For such inhomogeneous phase, the boundary conditions in the presence of AF-TS interfaces can be chosen as in deGennes method \cite{14} by requiring that $S_b(x)|_{\text{inter}^+} = 0$ and $D_c(x)|_{\text{inter}^-} = 0$, where $\text{inter}^+$ and $\text{inter}^-$ denote the two boundaries limiting the region of locally coexisting $S_b(x)$ (AF) and $D_c(x)$ (TS) (See Fig. 2).

\textit{Variational Free Energy:} We analyse $F_{tot}$ variationally. 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 $\mathcal{F}_{AF}$ corresponds to an insulating AF stripe characterized by the order parameter $S_0(x) = \sum_n A_n \sin(Q_n x)$, where $Q_n = 2\pi n/\ell_{AF}$. But here we take for simplicity the variational class where $S_0(x) = A_1 \sin(Q_1 x)$. To simplify notation, we will just 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 periodic solutions of the form $D_i(x) = \sum_n B_n \sin(K_n x)$. As in the AF case we confine ourselves to a single component variational form $D_i(x) = B_1 \sin(K_1 x)$, and use the simplifying notation $B_1 \to B$ and $K_1 \to K$. Here $B$ can be complex, but independent of position $x$. All the analysis discussed for the AF (SDW) case applies with the following change of notations: $L_{AF} \to L_{TS}$, $A \to B$, $Q \to K$, $\alpha_{AF} \to \alpha_{TS}$, $\beta_{AF} \to \beta_{TS}$, etc. Which in the TS case leads to:

$$\mathcal{F}_{TS} = L_{TS} \left[ D_2(K)|B|^2 + D_4(K)|B|^4 \right],$$

where $D_2(K) = (\alpha_{TS} + \beta_{TS} K^2)/2$ and $D_4(K) = (3\gamma_{TS} + \theta_{TS} K^2 + 3\delta_{TS} K^4)/8$. And the coupling Free energy is

$$\mathcal{F}_C = N_{int} \Lambda(Q, K, \ell_p)|A^2||B|^2,$$

where $N_{int} = 2N$ is the total number of interfaces, $f_{int} = \Lambda(Q, K, \ell_p)|A^2||B|^2$ is the Free energy of one interface with $\Lambda(Q, K, \ell_p) = \lambda_{BC} \int_{\ell_p} dx |\sin(Qx)\sin(K(x_0 + x))|^2$, where $x_0 = \ell_{TS} - \ell_p$.

Variational Solution: Variations of $\mathcal{F}_{tot}$ with respect to $\phi_{AF} = A$, $\phi_{TS} = |B|$, and $\phi_{AF} = Q$ or $q_{TS} = K$ lead to the non-trivial solutions

$$\phi_i^2 = \frac{4\beta_i \theta_i - 24\alpha_i\delta_i}{36\gamma_i\theta_i - \theta_i^3},$$

where $i = AF, TS$. In the case of $\lambda_{BC} < 0$, the transition line $P_1(T)$ corresponds to the disappearance of the pure AF (SDW) phase, and the transition line $P_2(T)$ corresponds to the appearance of the pure TS phase. This implies that at $P_1(T)$ the TS stripe width is $\ell_{TS} = 0$, while at $P_2(T)$ the AF stripe width is $\ell_{AF} = 0$. Furthermore, for $P_1(T) < P < P_2(T)$, $\ell_{TS} (\ell_{AF})$ increases (decreases) with increasing pressure. In order to meet these and the saddle point requirements, the parameters appearing in $\mathcal{F}_{tot}$ must behave as follows. We define the reduced pressure changes $\Delta P_{1c} = [P - P_{1c}(T)]/P_c$, where $m = 1,2$ and the density of states $N(E_F)$ at the Fermi energy $E_F$ to analyse the AF and TS parameters. For $P < P_2(T)$, the AF parameters have the form $\gamma_{AF} = \gamma_{1c} N(E_F) T_2^2 > 0$; $\delta_{AF} = \delta_{1c} N(E_F) T_2^2 > 0$; $\alpha_{AF} = \alpha_{1c} N(E_F) T_2^2|\Delta P_1^{\gamma_{AF}}$, with $\alpha_{1c} < 0$; $\beta_{AF} = \beta_{1c} N(E_F) T_2^2|\Delta P_2^{\gamma_{TS}}$, with $\beta_{1c} < 0$; $\theta_{AF} = \theta_{1c} N(E_F) T_2^2|\Delta P_2^{\gamma_{TS}}$, with $\theta_{1c} < 0$; and $3\gamma_{1c} - \beta_{1c}^2 > 0$. For $P > P_1(T)$, the TS parameters have the form $\gamma_{TS} = \gamma_{2c} N(E_F) T_2^2 > 0$; $\delta_{TS} = \delta_{2c} N(E_F) T_2^2 > 0$; $\eta_{TS} = \eta_{2c} N(E_F) T_2^2 > 0$; $\alpha_{TS} = \alpha_{2c} N(E_F) T_2^2|\Delta P_1^{\alpha_{TS}}$, with $\alpha_{2c} < 0$; $\beta_{TS} = \beta_{2c} N(E_F) T_2^2|\Delta P_1^{\beta_{TS}}$, with $\beta_{2c} < 0$; $\theta_{TS} = \theta_{2c} N(E_F) T_2^2|\Delta P_1^{\beta_{TS}}$, with $\theta_{2c} < 0$; and $3\gamma_{1c} + \beta_{1c}^2 > 0$. Consider now, the interface terms in the region $P_1(T) < P < P_2(T)$, which has the form $\lambda_{BC} = \lambda_{0c} N(E_F) T_2^2|\Delta P_1^{\gamma_{AF}}|\Delta P_2^{\gamma_{TS}}$, with $\lambda_{0c} > 0$. This form is required to make the interface energy negative between $P_1(T)$ and $P_2(T)$.

Phase Boundaries: Next, we focus only on the analysis of $\ell_{AF}$ and $\ell_{TS}$ in the vicinity of $P_2(T)$. We note in passing that the analysis of $\ell_{TS}$ and $\ell_{AF}$ in the vicinity of $P_1(T)$ is entirely analogous. Under these considerations, as $P \to P_2(T)$ the size of the AF stripes is given by $\ell_{AF} \approx W_1|\Delta P_2|^{(\epsilon_{AF} - \epsilon_{AF})/2}$, where $W_1 = 2\pi(\alpha_1\delta_1/\beta_1\gamma_1)^{1/2}$, when $\epsilon_{AF} + \epsilon_{AF} > \epsilon_{AF}$, and $\ell_{AF} + \epsilon_{AF} > \epsilon_{AF}$. The requirement that $\ell_{AF} \to 0$ as $P \to P_2(T)$ forces $\epsilon_{AF} > \epsilon_{AF}$. Since the number of AF and TS stripes are the same $N_{AF} = N_{TS} = N$, where $N = L/|\ell_{AF}(P) + \ell_{TS}(P) - \ell_{P}(P)|$, the number of interfaces is $N_{int} = 2N$. Therefore, the four contributions to $\mathcal{F}_{tot}$ in the coexistence region are $\mathcal{F}_{AF} = L_{AF}\ell_{AF}$, $\mathcal{F}_{TS} = L_{TS}\ell_{TS}$, $\mathcal{F}_{C} = 2N_{int}\ell_{P}$, $\mathcal{F}_{TS} = 2N_{int}\ell_{TS}$, with $L_{AF}(P) = N\ell_{AF}(P)$, $L_{TS} = N\ell_{TS}(P)$. As $P \to P_2$, the AF stripe length $\ell_{AF}(P) \to 0$, while the TS stripe length $\ell_{TS}(P) \to \ell_{TS}(P_2)$. Let us analyse the behavior of $\mathcal{F}_{tot}$ near $P_2(T)$ by term. The AF part $\mathcal{F}_{AF}$ is the product of $L_{AF}(P) \approx L\ell_{AF}(P)/\ell_{TS}(P_2)$, where $\ell_{AF}(P) = Const.|\Delta P_2|^{(\epsilon_{AF} - \epsilon_{AF})/2}$, and

$$q_i^2 = \frac{\alpha_i \theta_i - 6\beta_i \gamma_i}{36 \theta_i \gamma_i - \gamma_i^3},$$

The width of each stripe then 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 $i = AF, TS$. This expression is derived with the assumption that $\lambda_{BC} < 0$, and the transition line $P_1(T)$ corresponds to the disappearance of the pure AF (SDW) phase, and the transition line $P_2(T)$ corresponds to the appearance of the pure TS phase. This implies that at $P_1(T)$ the TS stripe width is $\ell_{TS} = 0$, while at $P_2(T)$ the AF stripe width is $\ell_{AF} = 0$. Furthermore, for $P_1(T) < P < P_2(T)$, the TS stripe width is $\ell_{TS} = 0$, and the AF stripe width is $\ell_{AF} = 0$. Furthermore, for $P_1(T) < P < P_2(T)$, the TS stripe width is $\ell_{TS} = 0$, and the AF stripe width is $\ell_{AF} = 0$.
This imposes the following requirement $\varepsilon_{\alpha AF} \geq 3\varepsilon_{\beta AF} + 2\varepsilon_{\lambda AF}$. If $\varepsilon_{\lambda AF} + \varepsilon_{\beta AF} > 1$ the phase transition at $P_2$ is continuous. If $\varepsilon_{\lambda AF} + \varepsilon_{\beta AF} \leq 1$ the phase transition at $P_2$ is discontinuous. Similar analysis close to $P_1$ leads to a continuous transition when $\varepsilon_{\lambda TS} + \varepsilon_{\beta TS} > 1$ and to a discontinuous transition when $\varepsilon_{\lambda TS} + \varepsilon_{\beta TS} \leq 1$. Thus, the point $(P_0, T_c)$ can be bicritical, tricritical or tetracritical. In Fig. 3, 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 $(P_c, T_c)$ is tetracritical. Dimensionless “volume” parameters are defined as $\tilde{\alpha}_i = \beta_i = \rho_i^2/2$, $\tilde{\gamma}_i = \gamma_i\sigma_i^{-1/2}$, $\tilde{\delta}_i = \delta_i\sigma_i^{3/2}$, $\tilde{\theta}_i = \theta_i\sigma_i^{1/2}$, “surface” ones are defined as $\tilde{\lambda}_0 = \lambda_0\sigma_i^{-1/4}\sigma_2^{-1/4}(\ell_p(P_i)\sigma_i^{1/2})^2$, $\tilde{\eta}_i = \eta_i\sigma_i^{-1/2}(\ell_p(P_i)\sigma_i^{1/2})^3$, where $\rho_i = \alpha_i\beta_i$, $\sigma_i = \alpha_i/\beta_i$, and $i = 1, 2$.

**Final Comments:** A more realistic description of the system should include variations of SDW and TS order parameters along the y and z (transverse) directions, and be highly anisotropic but truly three dimensional. This is important for a renormalization group (RG) analysis and the determination of critical exponents in the case of continuous transitions.

**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 appear in a narrow range of pressures around $P_c$ separating 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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[1] E. Dagotto, Rev. Mod. Phys. 66, 763-840 (1994)
[2] J. M. Tranquada, et. al., Phys. Rev. B 54, 7489 (1996)
[3] Y. Maeno, et. al., Nature 372, 532 (1994).
[4] C. Pfleiderer, et. al., Nature 412, 58 (2001).
[5] S. S. Saxena, et. al., Nature 406, 587 (2000).
[6] I. J. Lee, P. M. Chaikin, and M. J. Naughton, Phys. Rev. Lett. 88, 207002 (2002).
[7] D. Jérome, Mol. Cryst. Liq. Cryst. 79 155 (1982).
[8] J. Solyom, Adv. Phys. 28, 201 (1979).
[9] I. J. Lee, et. al., Phys. Rev. Lett. 88, 017004 (2002)
[10] K. Mortensen, Y. Tomkiewicz, and K. Beckgaard, Phys. Rev. B 25, 3319 (1982).
[11] I. Bozovic, et. al., Nature 422, 873 (2003).
[12] C. Bell, et. al., Phys. Rev. B 68, 144517 (2003)
[13] S. Nakajima, Prog. Theor. Phys. 50, 1101 (1973).
[14] P. G. de Gennes, *Superconductivity of metals and alloys*, W. A. Benjamin, INC., New York (1966).
[15] After we submitted this manuscript to Physical Review Letters on July 2nd 2004, a SO(4) theory suggesting coexistence of AF and TS in Beckgaard salts appeared. [Daniel Podolsky, et. al., Phys. Rev. Lett. 93, 246402 (2004)]. However, the coexisting phase pattern was not predicted within the framework of the SO(4) theory.