Mechanism for the coexistence of the antiferromagnetic phase and a triplet superconductivity in one-dimensional conductors

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The magnetic-anisotropy terms split the points of three-dimensional structural and antiferromagnetic transitions in quasi-one-dimensional conductors. In the problem of a single filament, fluctuations of the antiferromagnetic order and of the triplet pairing can coexist over broad ranges of the interaction constants.

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Compounds with the structural formula $(TMTSF)_2X$ become superconductors at low temperatures and various pressures.[1,3] The most surprising properties have been exhibited by the three compounds with $X = PF_6$, AsF_6, and SbF_6. At a pressure $P = 0$, these compounds exhibit the usual transition to a dielectric phase, but structural measurements[4] show convincingly that there are no so-called Kohn anomalies. Although no neutron measurements are available as of yet, experiments on the broadening of the NMR line,[5,6] experiments on the anisotropy of the magnetic susceptibility, and observation of a spin flip in moderate fields[7] indicate that the dielectric phase is antiferromagnetic.

In the one-dimensional model of a metal, the theory of Bychkov *et al.*[8] predicts the existence of structural fluctuations anmd Cooper pairing. Antiferromagnetism (accompanied by a structural instability!) can occur only in a half-filled band (Ref. 9; see also the review in Ref. 10). In the new materials of Ref. 1, aside from the slight dimerization of the conducting chain, the band is one-fourth filled. Consequently, the appearance of an antiferromagnetic phase demands explanation.

Our most natural suggestion is that spin—orbit interactions are important in these compounds. In the isostructural $(TMTTF)_2X$ compounds, in which the selenium atoms are replaced by sulfur atoms, the dielectric phase corresponds to a structural transition. In this connection let us examine how the theoretical conclusions of Refs. 8–11 are altered if the electron-electron interactions incorporate relativistic terms responsible for a magnetic anisotropy.

According to Ref. 11, the three-dimensional phase transition in an organic conductor results from either the three-dimensional nature of the forces (an interaction between electrons on different filaments) or a three-dimensional electron spectrum (tunneling from one filament to another). Ignoring the latter possibility (assuming a flat Fermi surface), we introduce some anisotropic increments in the amplitudes for electron-electron scattering:

$$\vec{\sigma}_{\alpha\gamma}\hat{g}^{ik}_{(1,2)}\vec{\sigma}_{\beta\delta}\,, \tag{1}$$

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where the spin-index pairs (α,γ) and (β,δ) refer to two electrons on filaments i and k, and the subscript on the magnetic anisotropy tensor $\hat{g}$ corresponds to scattering events involving either a large momentum transfer ($\pm 2p_F$, subscript 1) for a small momentum transfer (subscript 2). The increments in (1) have been used to rederive the so-called parquet equations for the effective electron-scattering amplitude[11]:

$$\Gamma^{iklm}_{\alpha\beta\gamma\delta} = (\gamma_1^{ik}\delta_{\alpha\gamma}\delta_{\beta\delta} + \vec{\sigma}_{\alpha\gamma}\hat{\gamma}_1\vec{\sigma}_{\beta\delta})\delta_{il}\delta_{km}$$

$$-(\gamma_2^{ik}\delta_{\alpha\delta}\delta_{\beta\gamma} + \vec{\sigma}_{\alpha\delta}\hat{\gamma}_2\hat{\sigma}_{\beta\gamma})\delta_{im}\delta_{kl}. \tag{2}$$

We will write out the result only in part; specifically, we will write in the equations those terms which are responsible for the three-dimensional effect:

$$(\gamma_1^{ik})' = \ldots - \sum_l \gamma_1^{il}\gamma_1^{lk}; \qquad (\hat{\gamma}_1^{ik})' = \ldots - \sum_l \hat{\gamma}_1^{il}\hat{\gamma}_1^{lk} \tag{3}$$

(the differentiation is with respect to $\xi = \ln\overline{E}/T$, where $\overline{E}$ is the cutoff energy). Transforming to the transverse Fourier components, $\gamma_1(\mathbf{p}_\perp)$ and $\hat{\gamma}_1(\mathbf{p}_\perp)$, of the two vertices in (3), we see [11] that Eqs. (3) allow singularities of the "moving-pole" type:

$$\gamma \propto A_1(\xi - \xi_0(\mathbf{p}_\perp))^{-1}. \tag{4}$$

[The functional dependence on the transverse momentum, $\xi_0(\mathbf{p}_\perp)$, makes all the fluctuations finite and makes the transition three-dimensional.[11]] The "moving pole" with $A = 1$ in the function γ_1 corresponds to a purely structural transition, while the pole in the tensor $\hat{\gamma}_1$ corresponds to antiferromagnetic ordering. The two singularities are independent, as assumed. In the case of a magnetic transition, we have the following condition for the tensor $\hat{\mathbf{A}}$:

$$\hat{\mathbf{A}} = \hat{\mathbf{A}}^2. \tag{4'}$$

If the tensor $\hat{\mathbf{A}}$ has an inverse matrix, then it follows from (4') that $\hat{\mathbf{A}} = \hat{1}$. Otherwise, (4') defines a projection operator. An easy axis along the vector 1 corresponds to $\hat{A}_{tp} = l_t l_p$ $(1^2 = 1)$.

The so-called "fast-parquet" equations[11] and Eqs. (3) of the present letter cannot be solved analytically, so we cannot state directly which type of transition occurs for given "seed" interaction constants. It is, however, interesting to follow the competition between the spin-orbit and ordinary interactions in the one-dimensional problem. In place of (3) we write a complete system of equations for a single chain (singling out the axis $1\|z$):

$$\gamma_1' = -\gamma_1^2 + (\gamma_1 - \gamma_{1z})\gamma_{2z}; \qquad \gamma_2' = -(1/2)(\gamma_1^2 + \gamma_{1z}^2); \tag{5}$$

$$\gamma_{1z}' = -\gamma_{1z}^2 - (\gamma_1 - \gamma_{1z})\gamma_{2z}; \qquad \gamma_{2z}' = -\gamma_1\gamma_{1z}.$$

We will again seek pole singularities of all quantities $\gamma_i \propto A(\xi - \xi_0)^{-1}$ (the quantity $\xi_0 = \ln\overline{E}/T_c$ determines the temperature scale, T_c, where the fluctuations are made large). Substituting this expression for γ_i in (5), we find three possible sets of residues:

$$\begin{array}{llll} A_1 & 1 & 1 & 0 \\ A_{1z} & 1 & 0 & 1 \\ A_2 & 1 & 1/2 & 1/2 \\ A_{2z} & 1 & 0 & 0 \end{array} \tag{6}$$

The residues in (6) have been used to study the behavior of the so-called response functions of the system near T_c to fluctuations of a charge or spin wave, or of a singlet or triplet superconducting order.[8,11] The first column provides no singularities in any of these quantities, and we will not consider it further. The second column corresponds to the solution of Ref. 8: the coexistence of structural and Cooper fluctuations. The last column in (6) corresponds to divergences of the type $(\xi - \xi_0)^{-1/2}$ only in the spin correlators (the wave vector $2p_F$, $s_z \neq 0$) and in triplet pairs (the spin projection of the pair is $s_z = 0$).

The coexistence of two new types of fluctuations in a one-dimensional conductor can occur over a broad range of the seed interactions $g_1 \sim g_2$, even if the magnetic interactions are weak. Let us transform to the functions $\gamma_{1\pm} = \gamma_1 \pm \gamma_{1z}$; $\gamma_{2\pm} = \gamma_2 \pm \gamma_{2z}$ in (5). After some straightforward calculations, imposing the boundary conditions at $\xi = 0$, we find

$$a + 2\gamma_{2-} = \sqrt{\Delta}\,\mathrm{ctg}\sqrt{\Delta}(\xi + g_1^{-1}) \tag{7}$$

[here $a = g_1 - 2g_2 + g_{1z}$, $\Delta = 4g_1(g_{1z} - g_{2z}) > 0$; in (7) and below, we can ignore the terms which are linear in g_z]. Yet another equation, $2\gamma_{2-}' = -\gamma_{1-}^2$, determines γ_{1-}:

$$\gamma_{1-} = \sqrt{\Delta}/\sin\sqrt{\Delta}(\xi + g_1^{-1}). \tag{8}$$

[In solution (7), (8) we have adopted the case $g_1 > 0$, i.e., the case opposite that of Ref. 8.] According to (6), we have the residue $A_{1-} = A_1 - A_{1z} = -1$. The pole is

$$\xi_0 = g_1^{-1}[(\pi/4)(g_1/g_{1z} - g_{2z})^{1/2} - 1]. \tag{9}$$

Solutions (7)–(9) determine a new temperature scale; the small value of the magnetic anisotropy enters in a nonlinear fashion, as a square root. We recall that the condition $g_1 - 2g_2 > 0$ denotes the attenuation of the one-dimensional Kohn anomaly with decreasing temperature.[10] These results correlate remarkably with the experimental results of Refs. 1–4, including the relatively low antiferromagnetic-ordering temperature[1] (12 K) at $P = 0$ and high sensitivity of the superconducting transition to defects[1)] (Ref. 12). With regard to three-dimensional effects, we might add that transverse tunneling of electrons[11] suppresses the spin-ordered phase.

A physical interpretation of the one-dimensional results runs as follows[8]: The growing spin (or structural) fluctuations represent an effective attraction mechanism for triplet (or singlet) Cooper pairs, and this attraction in turn amplifies the spin fluctuations. Three-dimensional effects do not rule out this attraction mechanism, simply restricting it. The role of this mechanism becomes important again as we ap-

proach the (pressure) stability boundary of the dielectric phase, as has been mentioned elsewhere in work on the theory of superconductors with the A15 structure.[15] The phonon attraction between electrons, for example, is intensified because of the soft mode over a significant part of the nearly flat Fermi surface.

Finally, in answer to the question of why the antiferromagnetic phase is observed in selenium compounds, while isostructural compounds containing sulfur undergo a Peierls transition, we will offer the following qualitative arguments: In addition to the Coulomb forces, with respect to which we have assumed $g_1 - 2g_2 > 0$, a phonon-induced attraction acts between electrons at low temperatures, $T < \omega_0$, where ω_0 is the characteristic phonon frequency. In relatively heavy compounds this interaction mechanism comes into play at a lower temperature than in relatively light compounds, while the spin–orbit interaction is slight in the relatively light compounds. For completeness, we note that the antiferromagnetic phase can be described by the three-dimensional model in Ref. 16, which, however, is based entirely on specific assumptions regarding the electron-dispersion law.

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[1)]Spin dependences in electron–electron interactions were formally introduced in Ref. 13 for the one-dimensional problem. Equations (5), in the form of equations for γ_f, are the same as the results of Ref. 14. There is no physical interpretation or discussion of the details of solutions (7)-(9) in Ref. 14.

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