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INSTABILITY OF METAL PHASE OF THE Q1D-CONDUCTOR IN MAGNETIC FIELD

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Abstract A Q1D-metal with a layered structure is unstable against the SDW pairing in the presence of a weak magnetic field near the boundary where the SDW is suppressed by pressure. The phase diagram of (TMTSF)₂X-compounds is discussed.

We suggest an explanation for the phase diagram of (TMTSF)2X-compounds in the (P,T,H)-space1,2 near the critical pressure, Pcr, where the SDW phase is inhibited and the material exhibits metallic properties. An applied magnetic field is known to restore the SDW--state in a series of metal-semimetal transitions3,4. The phenomenon occurs at low temperatures (T & 10 K), where the Fermi-liquid approach is expected to be adequate. Correspondingly, the Overhauser type diagram SDW susceptibility with a wave vector investigated and it is shown that this diagram always diverges at low temperatures in the presence of magnetic field, provided the electron spectrum possesses the 2D features, as is commonly accepted for the (TMTSF) X-family. Since it is known experimentally that the SDW state is a stable phase below the critical pressure, we believe that the SDW divergence is responsible for the restoration of the semimetallic magnetic phase. The so-called "threshold field" appears in this scheme due to finite 3D features of the electron spectrum 5.

The 2D anisotropic electron spectrum is assumed. The Fermi-surface consists of two open pieces positioned near the Fermi momentum $\pm K_F$ (across the main axis):

$$\mathcal{E}(P_{II},P_{\perp}) = \pm \sigma(P_{II} \mp \kappa_F) + t_{\perp}(P_{\perp}).$$

In the SDW pairing an electron from one side and a hole from the other side of the Fermi surface with equal $|E-E_p|$ are involved. At finite t_1 and given Q the nesting condition cannot be fulfilled for the arbitrary point on the Fermi surface (except for the case when the "perfect" nesting tight binding model6 is accepted). As a result, the common center-of-mass electron-hole wave function would contain the phase factor responsible for the independent motion of the two components of a pair in the perpendicular to the main axis direction. The magnetic field makes the relative phase of the electron and the hole finite over the whole Fermi surface This means that the motion of electrons and holes along the trajectories open (p_{fT}, p_T)-space corresponds to their collective motion along the longitudinal axis in the real space which is now restricted in the perpendicular direction Otherwise, the 2D electrons in magnetic field acquire the 1D properties and the SDW-channel is always unstable, if the tendency to the SDW pairing is known to present at lower pressure 5

The SDW state is established as the thermodynamic phase for a number of the $(TMTSF)_2X$ -compounds Therefore, while the SDW vector \underline{Q} is not determined yet by the direct neutron experiments, its transverse

component, Q_1 , is to be somehow fixed by some 3D mechanisms to prevent large fluctuations which would otherwise appear in the antiferromagnetic state. A conjecture is that Q_1 will not change, if low pressures or magnetic fields are applied to the material.

The plausible form of the 3D electron spectrum is

$$t_{\perp}(P_{\perp}) = 2t_{\beta} \cos \beta \delta^* + 2t_{c} \cos \beta c^* \qquad (1)$$

It has been argued ⁶ that this dispersion law by itself is able to provide the SDW pairing mechanism, since Eq (1) possesses the property of the "perfect" nesting with $\mathbf{Q} = (2\mathbf{K}_{\mathrm{F}}, \mathbf{TI}/\mathbf{C}^*, \mathbf{TI}/\mathbf{C}^*)$. This choice of \mathbf{Q} would contradict the recent experimental observations ^{3,4}, which have shown that the electron-hole pockets in the field induced magnetic phases are rather large Together with the above arguments concerning the role of the magnetic field, this leads us to the conclusion that

$$Q = (2K_F + K, 0, 0)$$
 (2)

The analysis of the metal phase stability $(t_c \ll t_b)$ gives the set of equations defining both the critical temperature and the K-value dependences on the magnetic field:

$$\ln \frac{t_{\theta}}{t_{\theta\alpha}} = \mathcal{I}_{n}^{2}(\lambda) \ln \frac{t \sigma n}{2 \pi T \chi_{H}}$$
 (3)

($\lambda = \frac{4ct_e}{veHe^*}$, $X_H = \frac{2ct}{eHe^*}$, $K = n\frac{eHe^*}{C}$). The bulk of the experimental results ^{3,4} is obtained in the low field region (at $t_b \sim 150$ K, H $\simeq 60$ KOe, $\lambda \sim 70$). According to Eq (3), the largest $J_n^2(\lambda)$ corresponds to $n \simeq \lambda$:

$$\ln \frac{t_{\theta}}{t_{\theta cr}} = \frac{2}{\Gamma(\frac{2}{3})^2 3^{\frac{2}{3}} \lambda^{\frac{2}{3}}} \ln \frac{t_{\theta cr}}{T}$$

and K is close to $K_{max} = 4t_b/V$. This nesting first gives the "pockets" with the "orbit area" $S = 8t_b\pi/\sqrt{\hbar v \ell^*}$. The structure vector displays small but fast oscillation with the field

$$\Delta \left[\frac{1}{H} \right] = \frac{2\pi e t}{c S} \tag{4}$$

(n is the integer part of λ , $\Delta[\lambda]$ = 1), which have been probably seen in the high field - high temperature behaviour of the magnetoresistance in (TMTSF)₂ ${\rm ClO}_4$. The fast variation of the Q-vector distinguishing different subphases found in Eq (4), hardly remains at lower temperature Instead, we expect at low temperature the SDW phases with a large enough order parameter whose structure vectors and other properties are changing with the magnetic field in a series of the first order phase transition. The qualitative (T,H)-phase diagram is summarized in Fig 1. Much more complicated analysis should be performed to find out the ground states of these subphases as a function of the magnetic field

In conclusion, our results point out unambiguously in favour of the SDW structure vector (2). Hence, the SDW pairing in the (TMTSF)₂X. family may be due to some one-dimensional mechanisms like that in the 1D Hubbard model

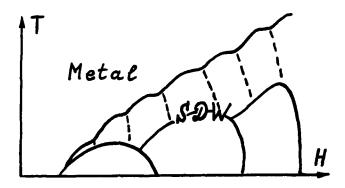


FIGURE 1 The (T,H)-phase diagram Dashed lines correspond to the fast variation (4) of the instability vector.

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