Anisotropy of an instability for a spin density wave induced by a magnetic field in a *Q1D* conductor

A. G. Lebed'

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR

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The threshold field for the formation of a spin density wave in $(TMTSF)_2X$ compounds is shown to have an oscillatory anisotropy in the plane perpendicular to the chains, **H**⊥**a**. This field is at a minimum for the direction making an angle $\varphi \approx 30°$ with the c^* axis.

An unusual phase diagram in a magnetic field was recently discovered[1,2] in layered $(TMTSF)_2X$ compounds. The effect in $(TMTSF)_2PF_6$, for example, can be summarized by saying that a strong field $H > H_0 \approx 6$ T restores the spin density wave which is destroyed by pressure (see the bibliography in Ref. 3). A simple mechanism was proposed in Ref. 4 to explain this phenomenon. Ordinarily, the appearance of a

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spin density wave in a $Q\,1D$ metal is associated with a congruence of two open regions of the Fermi surface. If this congruence is disrupted by an increase in the three-dimensionality of the electron spectrum (a pressure), the tendency toward a spin-density-wave pairing (i.e., a pairing of an electron and a hole with oppositely directed spins) is weakened, since the electron and the hole move off to infinity in real space when the $3D$ dispersion of the spectrum is taken into account. The explanation of Ref. 4 is based on an approximately layered nature of these compounds: In the $2D$ case, in the presence of a field, the semiclassical motion of the electrons along open Fermi surfaces corresponds in real space to a bounded periodic motion along the direction of **b**. The electrons and the holes thus "become one-dimensional," and if the interaction has the appropriate sign, they again form pairs, in this case in an arbitrarily weak magnetic field. Measurements are usually carried out in a magnetic field perpendicular to the plane of the layers $\mathbf{H}\|\mathbf{c}^*$. In this configuration, the motion along the field direction (a small but nonzero dispersion of the spectrum along the $\mathbf{c}^*$ axis) introduces three-dimensional features and gives rise to a threshold field H_0 for the spin-density-wave instability. Our purpose in the present letter is to point out a nontrivial anisotropy of the threshold field. This anisotropy arises because the motion of the electrons in real space, which is generally unbounded when three-dimensional effects are taken into account (the tunneling integral along the $\mathbf{c}^*$ axis), turns out to be periodic in this case and bounded for certain special orientations of the field with respect to the crystal axes.

The set of experimental data available[1,5] (see also the review in Ref. 6) in fact confirms that the electron spectrum of these $Q\,1D$ compounds corresponds to a Fermi surface in the form of two slightly corrugated planes, and, for simplicity, this spectrum can be described by

$$\epsilon_{1,2} = \pm\, v_F(p_x \mp k_F) + 2t_b\cos(p_y b\sin\gamma) + 2t_c\cos(p_z c^*). \qquad (1)$$

[We have chosen Cartesian coordinates **x**,**y**,**z** in the monoclinic $(TMTSF)_2X$ cell, so that the **y** axis is perpendicular to the $(\mathbf{a}, \mathbf{c}^*)$ plane, and we have $\mathbf{x}\|\mathbf{a}$, $\mathbf{z}\|\mathbf{c}^*$; here γ is the angle between the **a** and **b** axes.]

To explain this assertion, we consider the semiclassical equation of motion of electrons in a magnetic field:

$$\frac{d\mathbf{p}}{dt} = -\frac{e}{c}[\mathbf{v},\mathbf{H}]\,. \qquad (2)$$

Since we have $\mathbf{v} = \mathbf{v}_F\|\mathbf{a}$, we can write

$$p_y = \frac{e}{c}v_F H_z t, \qquad p_z = -\frac{e}{c}v_F H_y t.$$

Transforming to a motion in real space along the y and z axes in the customary manner, through the use of $\mathbf{v} = \partial\epsilon/\partial p$, and integrating the equations of motion, we find

$$y = \frac{2t_b c}{e v_F H_z}\cos(e v_F H_z b t\sin\gamma/c), \qquad z = -\frac{2t_c c}{e v_F H_y}\cos(e v_F H_y t c^*/c)\,. \qquad (3)$$

From (3) we already find that for "rational" directions of the magnetic field,

$$\tan\varphi = \frac{H_y}{H_z} = \frac{b\sin\gamma}{c^*}\frac{m}{n} \qquad (4)$$

(m and n are integers), the periods of the functions $y(t)$ and $z(t)$ are multiples; i.e., the motion in the plane perpendicular to the chains is again bounded and periodic. Consequently, for these directions we should again expect an exciton instability in an arbitrarily weak magnetic field at $T = 0$, according to Ref. 4.

Direct calculations completely analogous to those in Ref. 4 confirm these qualitative arguments. It turns out, for example, that the optimum orientation of the magnetic field for observing the field-induced instability with respect to spin-density-wave pairing is the orientation with $m = n = 1$ from (4):

$$\varphi = \arctan(b\sin\gamma/c^*) \approx 30^\circ . \qquad (5)$$

[The Lorentz force in (2) is directed strictly toward a corner of the reciprocal cell; here $b \approx 7.7$ A, $c^* \approx 13.3$ A, and $\gamma \approx 71°$]. It can be shown that even in the more general case this instability is not limited by three-dimensional effects as long as spectrum (1) has a form which allows separation of variables.

Actually, as in Ref. 4, we studied the generalized susceptibility of the system with respect to spin-density-wave pairing with a vector structure $\mathbf{Q} = (2k_F + k, 0,0)$; i.e., in accordance with Refs. 2 and 3, we assumed that an ideal superposition of Fermi surfaces does not occur in the case of a spin-density-wave transition. The result of the calculation can be written as a criterion of the Stoner type:

$$\ln\frac{t_b}{t_0} = \left[\sum_{p=-\infty}^{+\infty} J^2_{n_1+pm}\left(\frac{\lambda_b}{\cos\varphi}\right) J^2_{n_2+pn}\left(\frac{\lambda_c}{\sin\varphi}\right)\right]\ln\frac{t_b\cos\varphi}{T\lambda_b n} , \qquad (6)$$

where $J_n(x)$ are the Bessel functions of the first kind. Here t_0 is the stability boundary of the metallic state in the absence of a field; $\lambda_b \gg 1$ and $\lambda_c \gg 1$ are the parameters of the semiclassical nature of the motion of the electrons along the **y** and **z** axes, respectively, given by

$$\lambda_b = 4t_b c/ev_F bH\sin\gamma , \qquad \lambda_c = 4t_c c/ev_F c^* H ;$$

and the integers n_1 and n_2 are related to the additional vector of the spin-density-wave structure,

$$k = 4(t_b n_1 \cos\varphi/\lambda_b - t_c n_2 \sin\varphi/\lambda_c)/v_F . \qquad (7)$$

Analysis of (6) shows that the maximum temperature of the instability corresponds to $k \approx 4t_b/v_F$.

We wish to point out that in (6) we are dealing with a logarithmic divergence in the limit $T \to 0$, i.e., with an absolute instability of this system with respect to spin-density-wave pairing in an arbitrary weak field. At $T = 0$, this instability is limited either by the terms in the spectrum, which do not allow a separation of the variables p_y and p_z (the latter, however, are obviously extremely small), or by defects. The coefficient of the logarithm in (6) falls off rapidly with increasing n and m; its maximum value corresponds to the choice of direction in (5), for which we find

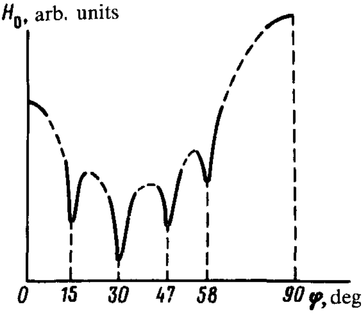

FIG. 1. Schematic angular dependence of the threshold field at low temperatures. Several of the principal minima, corresponding to small values of m and n in (4), are shown.

$$T_c \approx (t_b/\lambda_b)\exp[-2.4\lambda_b^{2/3}\ln(t_b/t_0)]. \quad (8)$$

We have thus demonstrated the oscillatory and sharply anisotropic behavior of the threshold field for a given temperature as a function of the orientation of the magnetic field in the plane perpendicular to the chains. Figure 1 shows the expected shape of the $H_0(\varphi)$ curve. It appears that these results warrant an experimental test, since we know of only a few measurements which have been carried out for a geometry with $\varphi \neq 0$ (Refs. 7–10). A maximum was found in the resistance of $(TMTSF)_2ClO_4$ in Refs. 7 and 8 as a function of the magnetic field direction at the angle $\varphi \approx 30°$, close to the optimum value in (5), at fields $H > 4$ T. It appears to us that this anomaly in the resistance, the first indication of the existence of the predicted effect, stems from the appearance of a spin density wave, seen for the first time, for field direction (5). In $(TMTSF)_2PF_6$ under pressure, we also observe an additional maximum in the resistance at the value[9] $\varphi \approx 14°$, which corresponds well to the second optimum direction, with $m = 1$ and $n = 2$, from (4) (Fig. 1). Furthermore, oscillations with an unusual period were observed at $H > 5$ T for the geometry in (5) in Ref. 10, but, to the best of our knowledge, no one has made an experimental study of how the excitonic subphases reorganize, depending on the magnetic field direction. We note in conclusion that measurements of the dependence $H_0(\varphi)$ will also make it possible to finally resolve the value of the structural vector of the spin-density-wave phase, since this phenomenon would be less apparent in the case of an ideal superposition of Fermi surfaces.

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[1]M. Ribault, D. Jerome, J. Tuchendler, *et al.*, J. Phys. Lett. **44**, 953 (1983).
[2]P. M. Chaikin, Choi Mu-Yong, J. F. Kwak, *et al.*, Phys. Rev. Lett. **51**, 2333 (1983).
[3]L. P. Gor'kov, Usp. Fiz. Nauk **144**, 381 [Sov. Phys. Usp. **27**, 809 (1984)].
[4]L. P. Gor'kov and A. G. Lebed', J. Phys. Lett. **45**, 433 (1984).
[5]P. M. Grant, J. Phys. (Paris) Coll. **44**, C3-847 (1983).
[6]D. Jerome and H. J. Schulz, Adv. Phys. **31**, 299 (1982).
[7]R. Brusetti, K. Bechgaard, G. G. Lonzarich, *et al.*, J. Phys. (Paris) Coll. **44**, C3-1055 (1983).
[8]K. Murata, H. Bando, K. Kajimura, *et al.*, Mol. Cryst. Liq. Cryst. **119**, 131 (1985).
[9]J. F. Kwak, J. E. Schirber, R. L. Greene, *et al.*, Mol. Cryst. Liq. Cryst. **79**, 111 (1982).
[10]K. Kajimura, H. Tokumoto, M. Tokumoto, *et al.*, J. Phys. (Paris) Coll. **44**, C3-1059 (1983).

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