Rapid Communications

Destruction of the spin-density-wave phase by magnetic field in a quasi-one-dimensional conductor

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It is known that, in a pure one-dimensional case, the charge-density-wave phase is destroyed by a magnetic field, whereas the spin-density-wave (SDW) phase does not "feel" the field. In reality, the SDW phase is often observed in quasi-one-dimensional (Q1D) conductors due to the so-called "nesting" property of their electron spectra. We show that, in the latter case, a high magnetic field generates some "antinesting" term in a Q1D electron spectrum, which destroys the SDW phase. We suggest performing the corresponding experiments in SDW phases of the real Q1D organic conductors with chemical formula $(TMTSF)_2X$ ($X = PF_6$, ClO_4, etc.).

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We recall that a pure one-dimensional (1D) metal is unstable with respect to the so-called Peierls transition into some density-wave (DW) state [1,2]. The DW state can be characterized by either a spatial modulation of a charge [i.e., charge-density-wave (CDW) phase] or spatial modulation of a spin [i.e., spin-density-wave (SDW) one] [2–4]. Let us discuss in briefly the above-mentioned phenomenon [1,2]. Indeed, near two plane Fermi surfaces (FS), it is possible to linearize a 1D spectrum,

$$\epsilon(p_x) = -2t_a \cos(p_x a^*), \tag{1}$$

in the following way:

$$\epsilon^{\pm}(p_x) = \pm v_F(p_x \mp p_F), \tag{2}$$

where v_F and p_F are the Fermi velocity and momentum, correspondingly, and a^* is a lattice constant. (Note that here and everywhere below we make use for an actual electron spectrum its tight-binding model, since we apply our results to organic conductors [3,4], where this model is known to work well [3]).

It is important that the electron spectrum (2) possesses the following special (i.e., "nesting") property of electron-hole pairing,

$$\epsilon^{+}(\Delta p_x) + \epsilon^{-}(\Delta p_x) = 0, \tag{3}$$

which makes some DW with wave vector $2p_F$ to be a ground state at low enough temperatures [1,2]. In an external magnetic field, the electron spectra (1) and (2) split into two branches due to the Pauli spin-splitting effect:

$$\epsilon^{\pm}_{\sigma}(p_x) = \pm v_F(p_x \mp p_F) - \sigma \mu_B H, \tag{4}$$

where $\sigma = \pm 1$ for spin up (down) and μ_B is the Bohr magneton. From Eq. (4), it directly follows that the condition (3) for electron-hole pairing in a magnetic field is not changed for the SDW phase and changed for the CDW one. Therefore, we can make the well-known conclusion that the SDW phase is stable in the presence of the Pauli spin-splitting effects in a magnetic field [4,5], whereas the CDW one is destroyed by the field [6].

Let us consider a quasi-one-dimensional (Q1D) conductor with the following electron spectrum [3]:

$$\epsilon(\mathbf{p}) = -2t_a \cos(p_x a^*/2) - 2t_b \cos(p_y b^*) - 2t_c \cos(p_z c^*), \tag{5}$$

where $t_a \gg t_b \gg t_c$. Near two open sheets of the FS, it can be linearized as

$$\epsilon^{\pm}(\mathbf{p}) = \pm v_F(p_x \mp p_F) - 2t_b \cos(p_y b^*) - 2t_c \cos(p_z c^*). \tag{6}$$

It is important that electron spectrum (6) still possesses the above discussed nesting electron-hole symmetry, since for Eq. (6) the following equation is valid:

$$\epsilon^{+}(\Delta p_x, p_y, p_z) + \epsilon^{-}(\Delta p_x, p_y + \pi/b^*, p_z + \pi/c^*) = 0. \tag{7}$$

It is possible to make sure [7] that the nesting property (7) corresponds to a stability of some DW with the wave vector:

$$Q^0 = (2p_x, \pi/b^*, \pi/c^*). \tag{8}$$

As also suggested in Ref. [7], the nesting property (7) is responsible for the appearance of SDW in the real Q1D conductors from chemical family $(TMTSF)_2X$, where $X = PF_6$, ClO_4, etc. [3,4].

In Refs. [5,7], a more realistic electron spectrum is considered:

$$\epsilon^{\pm}(\mathbf{p}) = \pm v_F(p_x \mp p_F) - 2t_b \cos(p_y b^*) - 2t_b' \cos(2p_y b^*) - 2t_c \cos(p_z c^*), \tag{9}$$

where it includes also the next-neighbor electron jumping in the tight-binding model, $t_b' \ll t_b$. The electron spectrum (9) contains the so-called "antinesting" term, $2t_b' \cos(2p_y b^*)$. This term destroys the ideal nesting condition (7) and thus, at large enough values of the parameter t_b', restores a metallic phase. For the theory of experimentally observed in the Q1D conductors $(TMTSF)_2X$ the field-induced spin-density-wave (FISDW) phases [8,9], where the antinesting term in Eq. (9) plays a central role, see Refs. [5,10]. For further development,

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it is important that electron spectra (6),(9) still show the same properties in a parallel to the conducting chains magnetic field, where the orbital effect [5] is negligible. More specifically, the SDW phase still does not fill the Pauli spin-splitting effects, whereas the CDW one is destroyed by them.

The goal of our Rapid Communication is to consider an unexpected effect—a destruction of SDW phase in Q1D conductors with nesting properties (7) by the Pauli spin-splitting effect. Here, we restrict our calculations to the case of a parallel magnetic field to avoid complications due to possible appearance of the FISDW phases as a result of orbital electron quantization [5,8–10]. Note that below we consider a model, which can be solved analytically, and suggest performing the corresponding experiments in the Q1D organic conductors $(TMTSF)_2X$. The physical meaning of the suggested phenomenon is as follows. We show that, due to the nonzero Q_y^0 component of the SDW wave vector (8) and due to nonlinearity of the electron spectrum along the conducting chains, the Pauli spin-splitting effect generates a special antinesting term. This term increases with a growing magnetic field and eventually destroys the SDW phase. We stress that the above mentioned statement is against a common belief that the Pauli spin-splitting effect does not influence the SDW phase.

Below, we consider the following 2D model of the Q1D spectrum in the $(TMTSF)_2X$ conductors in a parallel magnetic field:

$$\epsilon_\sigma(\mathbf{p}) = -2t_a\cos(p_x a^*/2) - 2t_b\cos(p_y b^*) - 2t_b'\cos(2p_y b^*) - \mu_B\sigma H. \quad (10)$$

[Note that, as is well known [3,4,5,7,10], the 2D model (10) well describes the SDW and FISDW phases in these conductors, since $t_b \gg t_c$ in Eq. (5)]. In contrast to all existing works, we do not linearize the electron spectrum along the conducting $\mathbf{a}^*$ axis near two sheets of the FS, but also take into account the next quadratic term:

$$\epsilon^+(p_x) = v_F(p_x - p_F) + \alpha(p_x - p_F)^2,$$
$$\epsilon^-(p_x) = -v_F(p_x + p_F) + \alpha(p_x + p_F)^2, \quad (11)$$

where

$$v_F = \frac{t_a a^*}{\sqrt{2}}, \quad \alpha = \frac{t_a (a^*)^2}{4\sqrt{2}}. \quad (12)$$

[In Eqs. (10)–(12), we take into account that $p_F = \pi/2a^*$ in the $(TMTSF)_2X$ conductors.]

Let us derive electron energy spectra in a parallel magnetic field near two sheets of the FS by means of Eqs. (10)–(12). To this end, first let us rewrite Eq. (10) in the following way:

$$\epsilon_\sigma^+(\mathbf{p}) = v_F(p_x - p_F) + \alpha(p_x - p_F)^2 - 2t_b\cos(p_y b^*) - 2t_b'\cos(2p_y b^*) - \mu_B\sigma H \quad (13)$$

and

$$\epsilon_\sigma^-(\mathbf{p}) = -v_F(p_x + p_F) + \alpha(p_x + p_F)^2 - 2t_b\cos(p_y b^*) - 2t_b'\cos(2p_y b^*) - \mu_B\sigma H. \quad (14)$$

Then, we define the shapes of two sheets of the FS for the value of small parameter $\alpha = 0$ in Eqs. (13) and (14) (i.e., in the linear approximation):

$$(p_x - p_F) = \frac{2t_b\cos(p_y b^*) + 2t_b'\cos(2p_y b^*) + \mu_B\sigma H}{v_F} \quad (15)$$

and

$$(p_x + p_F) = -\frac{2t_b\cos(p_y b^*) + 2t_b'\cos(2p_y b^*) + \mu_B\sigma H}{v_F}. \quad (16)$$

Now, let us put the obtained values of $p_x - p_F$ and $p_x + p_F$, given by Eqs. (15) and (16), only in terms which contain the small parameter, $\alpha \neq 0$, in Eqs. (13) and (14). As a result, for $t_b, \mu_B H \gg t_b'$, we obtain the following electron spectra near two sheets of the FS in the quadratic approximation:

$$\epsilon_\sigma^+(\mathbf{p}) = v_F(p_x - p_F) + t_b^+(p_y,\sigma) - \mu_B\sigma H + \Delta\epsilon,$$
$$t_b^+(p_y,\sigma) = -2t_b\cos(p_y b^*) + 2\tilde{t}_b'\cos(2p_y b^*) + 2t_H\sigma\cos(p_y b^*) \quad (17)$$

and

$$\epsilon_\sigma^-(\mathbf{p}) = -v_F(p_x + p_F) + t_b^-(p_y,\sigma) - \mu_B\sigma H + \Delta\epsilon,$$
$$t_b^-(p_y,\sigma) = -2t_b\cos(p_y b^*) + 2\tilde{t}_b'\cos(2p_y b^*) + 2t_H\sigma\cos(p_y b^*), \quad (18)$$

where $t_H = \mu_B H t_b/(\sqrt{2}t_a)$, $\tilde{t}_b' = -t_b' + t_b^2/(2\sqrt{2}t_a)$, and $\Delta\epsilon = \mu_B^2 H^2/(2\sqrt{2}t_a)$. Note that Eqs. (17) and (18) contain the magnetic field dependent term, $t_H \sim H$, which, for SDW pairing, breaks the electron-hole pairing condition (7) and thus destroys the SDW phase at high magnetic fields. In contrast, terms $-\mu_B H$ and $\Delta\epsilon$ in Eqs. (17) and (18) do not destroy SDW pairing. Indeed, term $-\mu_B H$ disappears for SDW pairing, whereas term $\Delta\epsilon$ just shifts the wave vector of the SDW phase.

Our goal is to describe quantitatively the destruction of SDW by a magnetic field due to the antinesting term in Eqs. (17) and (18), which contains magnetic field dependent parameter t_H. Let us calculate the linear response of our system to the following external field, corresponding to SDW pairing:

$$\hat{h}(\mathbf{Q}) = (\hat{\sigma}_x)_{\alpha\beta}\exp(i\mathbf{Qr}). \quad (19)$$

We do this in a similar way as it is done in Ref. [5] for different Q1D spectrum without the above mentioned magnetic field dependent term. In mean field approximation, we obtain for susceptibility the so-called Stoner's equation:

$$\chi(\mathbf{Q}) = \frac{\chi_0(\mathbf{Q})}{[1 - g\chi_0(\mathbf{Q})]}. \quad (20)$$

Here g is the effective electron coupling constant and $\chi_0(\mathbf{Q})$ is susceptibility of noninteracting electrons:

$$\chi_0(\mathbf{Q}) = T\sum_{\omega_m}\sum_\sigma\int\frac{dp_y}{2\pi}\int dx_1 g^{++}(i\omega_n, p_y; x, x_1; \sigma) \times g^{--}(i\omega_n, p_y - Q_y; x_1, x; -\sigma), \quad (21)$$

where ω_n is the so-called Matsubara's frequency [11].

In Eq. (21), slow varying parts of the electron Green's functions near two sheets of Q1D FS are related to the electron Green's functions by the following equation:

$$G^{++}(i\omega_n,p_y;x,x_1;\sigma)=e^{ip_F(x-x_1)}g^{++}(i\omega_n,p_y;x,x_1;\sigma), \tag{22}$$

$$G^{--}(i\omega_n,p_y;x,x_1;\sigma)=e^{-ip_F(x-x_1)}g^{--}(i\omega_n,p_y;x,x_1;\sigma). \tag{23}$$

Slow varying parts of Green's functions of noninteracting electrons are possible to determine by using the method similar to that suggested in Ref. [5]. As a result, we obtain the following equations:

$$\left[i\omega_n+iv_F\frac{d}{dx}-t_b^+(p_y,\sigma)+\mu_B\sigma H-\Delta\epsilon\right]\times g^{++}(i\omega_n,p_y;x,x_1;\sigma)=\delta(x-x_1), \tag{24}$$

$$\left[i\omega_n-iv_F\frac{d}{dx}-t_b^-(p_y,\sigma)+\mu_B\sigma H-\Delta\epsilon\right]\times g^{--}(i\omega_n,p_y;x,x_1;\sigma)=\delta(x-x_1), \tag{25}$$

where $\delta(x-x_1)$ is the Dirac's delta function. It is important that Eqs. (24) and (25) can be exactly solved:

$$g^{++}(i\omega_n,p_y;x,x_1;\sigma)=\frac{\mathrm{sgn}(\omega_n)}{iv_F}\exp\left[-\frac{\omega_n(x-x_1)}{v_F}-\frac{i}{v_F}t_b^+(p_y,\sigma)(x-x_1)+\frac{i}{v_F}\mu_B\sigma H(x-x_1)-\frac{i}{v_F}\Delta\epsilon(x-x_1)\right],\quad \omega_n(x-x_1)>0, \tag{26}$$

$$g^{--}(i\omega_n,p_y;x,x_1;\sigma)=\frac{\mathrm{sgn}(\omega_n)}{iv_F}\exp\left[\frac{\omega_n(x-x_1)}{v_F}+\frac{i}{v_F}t_b^-(p_y,\sigma)(x-x_1)-\frac{i}{v_F}\mu_B\sigma H(x-x_1)+\frac{i}{v_F}\Delta\epsilon(x-x_1)\right],\quad \omega_n(x-x_1)<0. \tag{27}$$

Now, let us substitute the known Green's functions [i.e., Eqs. (26) and (27)] into Eqs. (20) and (21). After straightforward but rather lengthy calculations, we obtain the following equation, which determines a stability region of the SDW phase:

$$\frac{1}{g}=\max_{\tilde{k},\Delta t}\int_d^\infty\frac{2\pi T_c dz}{v_F\sinh\left(\frac{2\pi T_c z}{v_F}\right)}\left\langle\cos\left[\frac{4\Delta t}{v_F}\sin(p_yb^*)\,z-\frac{4\tilde{t}_b'}{v_F}\cos(2p_yb^*)\,z+\tilde{k}z\right]\cos\left[\frac{4t_H}{v_F}\cos(p_yb^*)\,z\right]\right\rangle_{p_y}, \tag{28}$$

where $Q_y=\pi/b^*+q$ $(qb^*\ll 1)$, $\Delta t=t_bqb^*/2$, $\tilde{k}=k-2\Delta\epsilon/v_F$, and d is a cutoff distance; $\langle\ldots\rangle_{p_y}$ stands for averaging procedure over variable p_y. Note that, in Eq. (28), we maximize the SDW transition temperature, T_c, with respect to longitudinal, k, and transverse, Q_y, wave vectors under the condition that $t_b\gg t_b'$.

As follows from Eq. (28), the last term with t_H will eventually destroy the SDW phase at high magnetic fields. In this Rapid Communication, we do not intend to investigate Eq. (28) for all possible cases and all possible values of the parameters t_b, T_c, and $\tilde{t}_b'$. Our goal is to demonstrate that high enough magnetic field indeed destroys SDW phase even at $T_c=0$ and estimate the corresponding critical field. To this end, we consider the case of very high magnetic fields, where $t_H\gg\tilde{t}_b'$ at $T_c=0$. As we show below, this case can be analytically solved. Indeed, at $t_H\gg\tilde{t}_b'$ and $T_c=0$, we have from Eq. (28)

$$\frac{1}{g}=\max_{\tilde{k},\Delta t}\int_d^\infty\frac{dz}{z}\left\langle\cos\left[\frac{4\Delta t}{v_F}\sin(p_yb^*)\,z+\tilde{k}z\right]\times\cos\left[\frac{4t_H}{v_F}\cos(p_yb^*)\,z\right]\right\rangle_{p_y}. \tag{29}$$

For $\tilde{t}_b'=0$ and $H=0$, from Eq. (28), we can obtain another simple equation, which connects the electron coupling constant, g, with the SDW transition temperature at $H=0$, T_{c0}:

$$\frac{1}{g}=\int_{\frac{2\pi T_{c0}d}{v_F}}^\infty\frac{dz}{\sinh(z)}. \tag{30}$$

Our current problem is to find the maximum of the integral (29) over longitudinal and transverse momenta. This maximum defines the critical field, H_0, which can be expressed through T_{c0}, using Eq. (30).

So, let us first consider Eq. (29). By means of simple but rather lengthy calculations, it is possible to demonstrate that it is equivalent to the following simpler equation:

$$\frac{1}{g}=\max_{\tilde{k},\Delta t}\int_d^\infty\frac{dz}{z}\,J_0\left[\sqrt{\left(\frac{4\Delta t}{v_F}\right)^2+\left(\frac{4t_H}{v_F}\right)^2}\,z\right]\cos(\tilde{k}z), \tag{31}$$

where we use the following formula for the zeroth-order Bessel function [12]:

$$J_0(z)=\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\exp(iz\,\sin\phi). \tag{32}$$

From Eq. (31), it directly follows that the integral (31) takes its maximum at $\Delta t=0$ (i.e., for transverse component of the SDW wave vector $Q_y=\pi/b^*$). Therefore, Eq. (31) can be simplified as

$$\frac{1}{g}=\max_{\tilde{k}_1}\int_{\frac{4t_Hd}{v_F}}^\infty\frac{dz}{z}\,J_0(z)\cos(\tilde{k}_1z),\quad \tilde{k}_1=\frac{v_F\tilde{k}}{4t_H}. \tag{33}$$

Here, we express the inverse electron coupling constant through the SDW transition temperature in the absence of $\tilde{t}_b'$ and magnetic field, $H=0$, and cutoff distance, d, using Eq. (30). Exact integration of integral (30) over variable z

gives us the following relationship in the so-called logarithmic approximation:

$$\frac{1}{g} = \ln\left(\frac{v_F}{\pi T_{c0} d}\right). \tag{34}$$

Our task now is to find the maximum of Eq. (33) with respect to variable $\tilde{k}_1$ and express the critical magnetic field for destruction of SDW, H_0, as a function of T_{c0} by means of Eq. (34). It is easy to rewrite Eq. (33) for small values of the cutoff parameter, d, in the following way:

$$\frac{1}{g} = \max_{\tilde{k}_1}\left\{\int_0^\infty \frac{dz}{z} J_0(z)\,[\cos(\tilde{k}_1 z) - 1] + \int_0^\infty \frac{dz}{z}\,[J_0(z) - \cos(\tilde{k}_1 z)] + \int_{d\tilde{k}}^\infty \frac{dz}{z}\cos(z)\right\}. \tag{35}$$

To simplify (35), we use the following mathematical formulas [12]:

$$\int_0^\infty \frac{dz}{z}\,[J_0(z) - \cos(\alpha z)] = \ln(2\alpha), \quad \alpha > 0, \tag{36}$$

$$\int_0^\infty \frac{dz}{z}\,[1 - \cos(\alpha z)] J_0(\beta z) = \operatorname{arccosh}\left(\frac{\alpha}{\beta}\right), \quad 0 < \beta < \alpha, \tag{37}$$

$$\int_0^\infty \frac{dz}{z}\,[1 - \cos(\alpha z)] J_0(\beta z) = 0, \quad 0 < \alpha < \beta, \tag{38}$$

$$-\int_x^\infty \frac{\cos(z)}{z} dz = C + \ln(x) + \int_0^x \frac{\cos(z) - 1}{z} dz, \tag{39}$$

where $C = \ln(\gamma)$ is the so-called Euler constant. As directly follows from Eqs. (36)–(39), the integral (35) has maximal value at $|\tilde{k}| < 4t_H/v_F$, which is equal to

$$\frac{1}{g} = \ln\left(\frac{v_F}{2\gamma t_H d}\right), \tag{40}$$

where $\gamma \approx 1.78$. Comparison of Eqs. (34) and (40) results in the following value of magnetic field, H_0, which destroys the SDW phase at $T = 0$:

$$t_{H_0} = \frac{\pi T_{c0}}{2\gamma}, \quad H_0 = \frac{1}{\mu_B}\left(\frac{\pi T_{c0}}{2\gamma}\right)\left(\frac{\sqrt{2}t_a}{t_b}\right). \tag{41}$$

To summarize, in the Rapid Communication, we have shown that magnetic field generates some antinesting term in Q1D conductors due to the Pauli spin-splitting effect. This term destroys SDW phases, which exist in some Q1D conductors due to the "nesting" condition. We suggest performing the corresponding experiments in the organic conductors $(TMTSF)_2X$. Let us estimate the critical magnetic field, which destroys the SDW phase. From Eq. (41), it follows that at ambient pressure, where $T_{c0} = 12$ K in $(TMTSF)_2PF_6$, the critical magnetic field is $H_0 = 185$ T. Although such high magnetic field is experimentally available (see, for example, Refs. [13,14]), we recommend applying pressure to decrease the value of H_0. Indeed, at pressure $P = 5$ kbar, the SDW transition temperature in the $(TMTSF)_2PF_6$ conductor becomes $T_{c0} = 5$ K [15] and thus the critical magnetic field can be estimated as $H_0 = 77$ T. Here, let us discuss briefly the validity of the above suggested estimations by Eq. (41) of the critical magnetic fields to destroy the SDW phase in the real Q1D compound $(TMTSF)_2PF_6$. Note that, in Eq. (41), we don't explicitly take into account the first antinesting term, containing unknown parameter $\tilde{t}_b'$ [see Eqs. (13)–(18)]. Our application of Eq. (41) to the real compound $(TMTSF)_2PF_6$ is based on the suggestion that both antinesting terms independently decrease the SDW transition temperature. This suggestion is based on the fact that the two antinesting terms have different momentum dependence and thus cannot, for example, cancel each other. Of course, this is just a reasonable suggestion and, therefore, the above mentioned calculations of the values of the critical magnetic fields in $(TMTSF)_2PF_6$ at ambient pressure and $P = 5$ kbar are just some reasonable estimations.

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