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Theory of magnetic field-Induced charge-density-wave phases

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We elaborate an analytical theory of a cascade of magnetic field-induced charge-density-wave (FICDW) phases. It is shown that the following features distinguish it from the well-known spin-density-wave cascade: 1) the FICDW phases exist at temperatures much lower than the characteristic CDW transition temperature at $H = 0$; 2) the cascade of the FICDW phases dramatically changes at certain directions of a magnetic field due to an interplay of Zeeman spin-splitting and an electron motion along open Fermi surfaces. Theoretical results are compared with the recent experimental attempts to reveal the FICDW phases in organic conductors α-$(ET)_2MHg(SCN)_4$ (M = K, Tl, Rb, etc.).

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A cascade of the magnetic field-induced spin-density-wave (FISDW) phases has been intensively studied since its experimental discovery in $(TMTSF)_2X$ and $(DMET\text{-}TSeF)_2X$ organic compounds [1, 2] (for the first theories of this phenomenon, see Refs. [3, 4, 1, 2]; for the recent theoretical analysis, see Ref. [5]; for the recent experiments, see Ref. [6]). A possibility that a similar phenomenon, a cascade of the magnetic field-induced charge-density-wave (FICDW) phases, may exist in some solids was discussed in Ref. [3] and was numerically proved in Ref. [7]. Indeed, if a charge-density-wave (CDW) state is destroyed by pressure in a quasi-one-dimensional (Q1D) conductor, it can be restored in a magnetic field which increases 1D Peierls instability for both SDW and CDW phases due to "one-dimensionalization" of electron's motion, as shown in Ref. [3 – 5, 7]. Nevertheless, the existence of the FICDW phases in real materials has not been firmly established and an analytical theory of the FICDW states has not been elaborated so far. The major problem to observe the FICDW phenomenon is high enough CDW transition temperatures, $T_{\rm CDW} \simeq 100\,\rm K$, in traditional Q1D conductors. Due to high $T_{\rm CDW}$, the CDW states normally demonstrate very low responses to the experimental magnetic fields, $H \simeq 10 - 30\,\rm T$, and experimental pressures, $P \leq 10\,\rm kbar$.

Very recently, the first experimental indications [8 – 10] that the FICDW phases perhaps exist in layered organic conductors α-$(ET)_2MHg(SCN)_4$ (M = K, Tl, Rb, etc.) with low enough DW transition temperatures at $H = 0$ and $P = 1\,\rm bar$, $T_{\rm CDW} \simeq 8 - 10\,\rm K$, have appeared. To be more specific, the unexpected changes in slope of the low temperature magnetoresistence at $T \ll T_{\rm CDW}$ accompanied by hysteresis [8] (observed under pressure $P \geq 3\,\rm kbar$, which destroys the CDW state at $H = 0$) were interpreted [8] in terms of the FICDW phase transitions. Moreover, the recent low-temperature measurements in a tilted magnetic field [9, 10] in α-$(ET)_2MHg(SCN)_4$ conductors were suggested [9] to reflect an interplay of Zeeman spin-splitting and the orbital effects of electron's motion along open Fermi surfaces (FS). Note that the most popular description of the ground states in α-$(ET)_2MHg(SCN)_4$ compounds at $T \leq 8 - 10\,\rm K$ is based on an idea [11] about a formation of some density-wave (DW) phase. Although a physical nature of this DW phase is still controversial (see, for example, discussions in Refs. [7, 8 – 10, 12 – 14]), the experimental confirmation [8] of the theory [7] at low enough magnetic fields and the interpretation of the experiment [9] seem to be strong arguments in favor of the CDW-scenario.

Our goals are: 1) To elaborate an analytical theory of a cascade of the FICDW phase transitions in a magnetic field perpendicular to the conducting layers (i.e., $[\mathbf{x}(\mathbf{a}), \mathbf{z}(\mathbf{c})]$-plane); 2) To suggest a theory of the above mentioned cascade at some "commensurate directions" of a magnetic field. (We note that a possibility that some special directions of a magnetic field may exist due to interplay of the Zeeman spin-splitting and the orbital electron motion along open orbits was discussed in Refs. [15, 7]. Nevertheless, no theoretical description of this phenomenon in the FICDW phases has been proposed yet.) Below, we reveal some peculiar features of the FICDW phase diagram which distinguish it from the FISDW one [3 – 5, 1, 2] and present an additional argument in favor of the CDW-FICDW scenario for the ground states in α-$(ET)_2MHg(SCN)_4$ compounds.

Let us consider the FICDW phases in a tilted magnetic field perpendicular to the conducting chains [i.e., $\mathbf{x}(\mathbf{a})$-axis],

$$\mathbf{H} = (0, \cos\theta, \sin\theta)H, \quad \mathbf{A} = (0, \sin\theta, -\cos\theta)Hx, \quad (1)$$

in a layered conductor with a Q1D FS [11, 1 – 4, 7, 8, 16]:

$$\begin{gathered} \epsilon^{\pm}(\mathbf{p}) = \pm v_F\ (p_x \mp p_F) - t_{\perp}(p_y, p_z), \\ t_{\perp}(p_y, p_z) = 2t_c \cos(p_z c^*) + \\ +2t'_c \cos(2p_z c^*) + 2t_b \cos(p_y b^*), \end{gathered} \quad (2)$$

where θ is the angle between the field direction and the normal to the conducting plane, $+(-)$ stands for the right (left) sheet of the FS; v_F and p_F are the Fermi velocity and Fermi momentum; $t_c \gg t_b \sim t'_c$ are the overlapping integrals of the electron wave functions [11, 7, 1 – 5].

As in Refs. [1-5,7,8], we suppose that under external pressure the "antinesting term" t'_c is bigger than its critical value, $t'_c > t^*_c$, which corresponds to a destruction of the CDW phase [3, 4, 7, 8, 1, 2]. Let us find a metal-FICDW phase transitions temperature, $T_{\mathrm{FICDW}}(H)$, where the FICDW phases exist at high enough magnetic fields and low enough temperatures. They correspond to the following order parameters:

$$\begin{gathered} \Delta_{FICDW}(\mathbf{r}) = \Delta\ \exp(i\mathbf{Q}\mathbf{r}), \\ \mathbf{Q} = (2p_F + K,\ \pi/b^*,\ \pi/c^*). \end{gathered} \quad (3)$$

Using Green's functions method [17, 3 – 5, 1, 7], we can find that the Green functions in the mixed representation [3, 4], $G^{\pm}_{\sigma}(i\omega_m; p_y, p_z; x, x_1)$, where

$$\begin{gathered} G^{\pm}_{\sigma}(i\omega_m; p_y, p_z; x, x_1) = \\ = \exp[\pm i p_F(x - x_1)]\ g^{\pm}_{\sigma}(i\omega_m; p_y, p_z; x, x_1), \end{gathered} \quad (4)$$

obey the following equations:

$$\begin{gathered} \Bigg[i\omega_m \pm i v_F \frac{d}{dx} - \\ - t_{\perp}\left(p_y - \frac{eH\sin\theta x}{c},\ p_z + \frac{eH\cos\theta x}{c}\right) - \mu_B H\sigma \Bigg] \times \\ \times\, g^{\pm}_{\sigma}(i\omega_m; p_y, p_z; x, x_1) = \delta(x - x_1). \end{gathered} \quad (5)$$

Here $i\omega_m$ is the so-called Matsubara frequency [17], $\sigma = +(-)$ stands for electron with spin up (down); μ_B is the Borh magneton, c is the velocity of light; the Planck constant $h = 1$.

Note that the main difference between Eqs. (4), (5) and the equations determining the Green functions in the FISDW case [3 – 5, 1] is the appearance of the Zeeman spin-splitting term, $\mu_B H$, in Eq. (5). Let us solve Eqs. (4), (5) using a procedure described in Refs. [3, 4]. Then, let us use the Gor'kov-type equations [17, 3 – 5, 1] to determine the metal-FICDW phase transition temperature, $T_{\mathrm{FICDW}}(H)$. As a result, we find that, in contrast to the well known case of the metal-FISDW phase transitions [3 – 5, 1], the equation

$$\begin{gathered} \frac{1}{g} = \int\limits_{d}^{\infty} \frac{2\pi T_{\mathrm{FICDW}}\, dZ}{v_F \sinh\left(\dfrac{2\pi T_{\mathrm{FICDW}} Z}{v_F}\right)} \times \\ \times J_0\left[\frac{4t'_c}{\omega_c\cos\theta} \sin\left(\frac{\omega_c Z\cos\theta}{v_F}\right)\right] \times \\ \times \cos\left(\frac{2\mu_B H Z}{v_F}\right) \cos(KZ), \end{gathered} \quad (6)$$

determining the metal-FICDW phase transition temperature, $T_{\mathrm{FICDW}}(H)$, contains the Zeeman spin-splitting term, $2\mu_B H$. (Here, g is a bare coupling constant for the CDW instability, $J_0[...]$ is the Bessel function, $\omega_c(H) = eHc^* v_F/c$ is a frequency of an electron motion along the open sheets of the FS (2).)

To describe a cascade of the FICDW phases analytically, we suppose that the magnetic field is strong enough to satisfy a condition of the so-called "quantum limit", $\pi T_{\mathrm{FICDW}}(H) \ll \omega_c(H)$ (for discussions, see Ref. [5]). In this case, we find with a logarithmic accuracy the following expression for the metal-FICDW phases transition temperature from Eq. (6):

$$\begin{gathered} T_{\mathrm{FICDW}}(H) \simeq\ \omega_c(H)\ \exp\left[-\frac{1}{g_{\mathrm{eff}}(H)}\right]; \\ \omega_c(H) = e v_F H c^*/c, \end{gathered} \quad (7)$$

$$\begin{gathered} g_{\mathrm{eff}}(H) = \frac{1}{2\ln(t'_c/t^*_c)} \times \\ MAX\left(\left\langle J_0\left[\frac{4t'_c}{\omega_c(H)\cos\theta} \sin\left(\frac{\omega_c(H)Z\cos\theta}{v_F}\right)\right] \times \right.\right. \\ \times \left(\cos\left[\frac{(Kv_F - 2\mu_B H)Z}{v_F}\right] + \right. \\ \left.\left.\left. + \cos\left[\frac{(Kv_F + 2\mu_B H)Z}{v_F}\right]\right)\right\rangle_Z\right)_K, \end{gathered} \quad (8)$$

where t^*_c is a critical value of the "antinesting term" t'_c, which destroys the CDW phase at $H = 0$; $< ... >_Z$ means an averaging over the coordinate Z, $MAX(...)_K$ stands for the maximum value of a function with respect to the variable K.

As it follows from Eq. (8), the FICDW effective interaction constant $g_{\mathrm{eff}}(H)$ is non-zero only for the FICDW phases (3) with the "quantized" longitudinal component of the wave vector,

$$K_1(H, L_1) = +\frac{2\mu_B H}{v_F} + 2L_1 \frac{\omega_c(H)\cos\theta}{v_F}, \quad (9)$$

$$K_2(H,L_2) = -\frac{2\mu_B H}{v_F} + 2L_2\frac{\omega_c(H)\cos\theta}{v_F}, \qquad (10)$$

where L_1 and L_2 are integers. It is possible to rewrite Eq. (8) as follows:

$$g_{\rm eff}(H) = \frac{1}{2\ln(t_c^{'}/t_c^*)} J_N^2\left[\frac{2t_c^{'}}{\omega_c(H)\cos\theta}\right],$$

$$J_N^2\left[\frac{2t_c^{'}}{\omega_c(H)\cos\theta}\right] = MAX\left(J_L^2\left[\frac{2t_c^{'}}{\omega_c(H)\cos\theta}\right]\right)_L, \qquad (11)$$

where the effective FICDW coupling constant (11) defines the metal-FICDW phase transition line for the FICDW order parameters (3) with

$$K_{1,2,3,4}(H) = \pm\frac{2\mu_B H}{v_F} \pm 2N\frac{\omega_c(H)\cos\theta}{v_F}, \qquad (12)$$

where N and L are integers. Note that the order parameters (3) with four possible wave-vectors (12) correspond to the same value of the metal-FISDW transition temperature (see Eqs. (7), (11)). In other words, the layered Q1D metal (2) is unstable in a magnetic field (1) with respect to the formations of four FICDW phases with the "quantized" wave vectors (12). Our theoretical results (7)–(12) are summarized on Fig. 1 where the cascade of the FICDW phase transitions (calculated for $\theta = 0$) is compared with the FISDW cascade [4, 5, 1, 2, 18 – 20].

In contrast to the FISDW case [1 – 5, 18 – 20], the quantization rules (12) for the FICDW wave vector (3) contain the Zeeman spin-splitting term. This leads to significant differences between physical properties of the FICDW and FISDW phases. Indeed, as it follows from Eq. (11), the effective interaction constant for the formation of the FICDW phases is two times smaller than the corresponding constant for the formation of the FISDW phases [2 – 4, 1, 18 – 20] (see Fig.1). Therefore, unlike the FISDW phases, the FICDW ones can appear only at temperatures much lower than the CDW characteristic temperature at $H = 0$ and $P = 1$ bar:

$$T_{FICDW}(H) \ll T_{CDW}(H=0, P=1\text{ bar}). \qquad (13)$$

Note that this result is in agreement with the experiment [8] and, thus, supports the hypothesis [7 – 12] about the CDW ground states in α-$(ET)_2KHg(SCN)_4$ compound at $H = 0$ and $P = 1$ bar.

As it follows from Eqs. (7)–(10), the second distinctive feature of the FICDW phases is that the effective FICDW coupling constant changes at "commensurate directions" of a magnetic field,

$$\cos\theta = (1/M)\ [2\mu_B H/\omega_c(H)], \qquad (14)$$

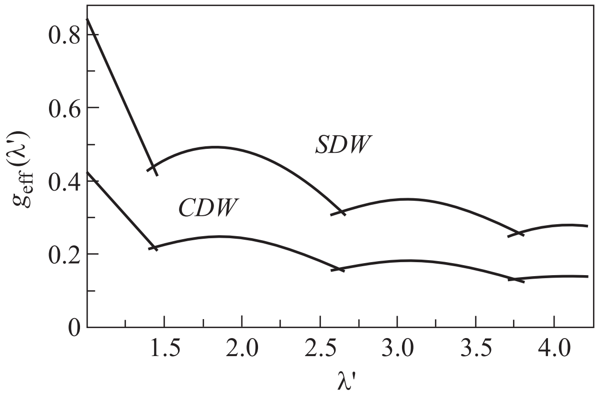

Fig.1. Upper curve: phase transitions between the FISDW phases [3 – 5] with $K = 2N\omega_c(H)/v_F$; lower curve: the phase transitions between the FICDW phases with $K = 2\mu_B H/v_F + 2N\omega_c(H)/v_F$ [see Eqs. (3), (12)] calculated in the paper for $\theta = 0$ [see Eqs. (7), (11)], where N is an integer. The following notations and values of the parameters are used: $\lambda' = 2t_c^{'}/\omega_c(H) \sim 1/H$; $\ln(t_c^{'}/t_c^*) = 1.4$. Note that the FICDW phase transition temperatures are much lower than the FISDW phase ones

where $M \neq 0$ is an integer, $2\mu_B H/\omega_c(H) = 1/\sqrt{2}$: $\cos\theta = 1/\sqrt{2}$ $(\theta = \pi/4)$, $\cos\theta = \frac{1}{2}\frac{1}{\sqrt{2}}, \ldots$

Starting from Eq. (8), it is possible to show that the effective coupling constant for the "commensurate directions" of a magnetic field (14) is equal to

$$g_{\rm eff}^M(H) = \frac{1}{2\ln(t_c^{'}/t_c^*)} \times$$
$$MAX\left(J_L^2\left[\frac{2t_c^{'}}{\omega_c(H)\cos\theta}\right] + J_{L+M}^2\left[\frac{2t_c^{'}}{\omega_c(H)\cos\theta}\right]\right)_L, \qquad (15)$$
$$T_{\rm FICDW}(H) = \exp\left[-\frac{1}{g_{\rm eff}^M(H)}\right],$$

where L and N are integers. Thus, the cascades of the FICDW phase transitions at the "commensurate directions" of a magnetic field (14) are qualitatively different from the cascade at $\theta = 0$ (see Fig.2). As it is seen from Eq. (15) and Fig.2, the FICDW transition temperatures at "commensurate directions" of a magnetic field can be significantly higher than the FICDW transition temperatures for standard experimental geometry where magnetic field is perpendicular to the conducting layers (i.e., at $\theta = 0$). This provides a method to detect the FICDW phases in other Q1D compounds. We speculate that the experimental results [9], where some novel phases were observed only at angles higher than $\theta \geq \pi/4$, may be related to the main "commensurate angles" (14) (see Fig.2).

Below, we discuss an applicability of the analytical theory of the cascades of the FICDW phase tran-

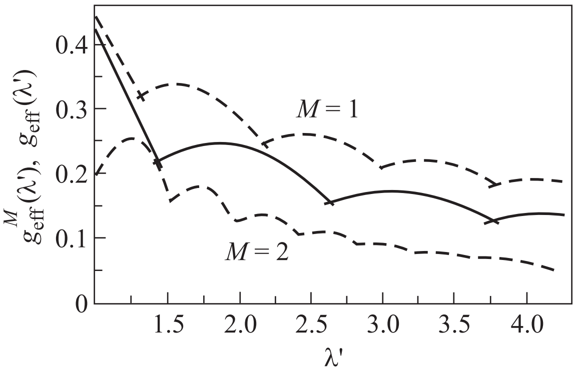

Fig.2. Phase transitions between the metallic and the FICDW phases are calculated for $\theta = 0$ (solid line) [see Eqs. (3), (7), (11), (12)] and for two "commensurate directions" of a magnetic field [see Eq. (14)]. Upper dashed line corresponds to $\theta = \pi/4$ (i.e., $M = 1$), whereas the lower dashed line corresponds to $M = 2$ [see Eqs. (14), (15)]; $\ln(t_c^{'}/t_c^{*}) = 1.4$, $2\mu_B H/\omega_c(H) = 1/\sqrt{2}$; $\lambda^{'} = 2t_c^{'}/\omega_c(H) \sim 1/H$. Note that $T_{\rm FICDW}(H, \theta = \pi/4)$ is higher than $T_{\rm FICDW}(H, \theta = 0)$

sitions suggested in the paper to real experiments. We stress that in the paper we have extended the so-called "Quantized Nesting" (QN) model [1–4, 18–20] to describe the cascade of the FICDW phase transitions. As it is shown in Ref. [5], the analytical QN model in the case of the FISDW phase transitions is an approximation which is qualitatively correct in the quantum limit where $\omega_c(H) \geq \pi T_{\rm FISDW}(H)$. Therefore, we expect that the analytical theory suggested by us is qualitatively correct at least if $\omega_c(H) \geq \pi T_{\rm FICDW}(H)$. In contrast to the FISDW case, an application of the present theory is restricted by the second condition, $\omega_c(H) \leq 2t_c^{'}$, since Eqs. (7)–(15) are valid only with a logarithmic accuracy. Using the typical values of the parameters [8], $\omega_c(H) \simeq 1\,{\rm K/T}$, $T_{\rm FICDW}(H) \simeq 1\,{\rm K}$, and $t_c \simeq 10\,{\rm K}$, we can conclude that the analytical theory suggested in the paper is an appropriate description of the FICDW phases in a broad region of magnetic fields, $3\,T \leq H \leq 20\,{\rm T}$.

To summarize, an analytical theory of a cascade of the FICDW phase transitions in a magnetic field perpendicular to the conducting chains in layered Q1D metals (predicted by L. P. Gor'kov and the author in Ref. [3] and numerically proved in Ref. [7]) is elaborated. As a result, we come to a conclusion that, in contrast to the FISDW phases, the FICDW ones can exist only at low enough temperatures (13). This is an agreement with the experimental data [8] and is an extra argument in favor of the CDW/FICDW nature of the ground states existing at low temperatures in organic conductor α-$(ET)_2KHg(SCN)_4$. We have suggested a theory of the FICDW phases in an inclined magnetic field and calculated the FICDW phase diagram for some "commensurate directions" [15, 7] of a magnetic field (see Eq. (14), (15) and Fig.2). It is shown that the FICDW transition temperatures can be higher for some "commensurate directions" of a magnetic field than for the field perpendicular to the conducting plane (see Eqs. (11), (14), (15) and Fig.2). This provides an experimental method to detect the FICDW phases in other Q1D compounds and may be related to the experiment [9] where some novel phases are observed only in inclined magnetic fields.

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16. In this paper, we study the generic features of the FICDW phases using, as usually, a model Q1D spectrum (2). Note that the real organic compounds α-$(ET)_2MHg(SCN)_4$, in addition to the Q1D sheets of the FS, have also Q2D parts of the FS. An influence of the Q2D electron orbits on the physical properties of the FICDW phases will be studied elsewere. As shown in Ref. [7], from phenomenological point of view, the FICDW phase is mixed with the component of the FISDW state characterizing by zero projection of the total spin on the magnetic field direction. Nevertheless, the CDW-FICDW scenario (see Refs. [8, 9, 12]) considered in this paper is based on the suggestion that the SDW instability is the secondary phenomenon comparable with the CDW one. In other words, we assume that a bare coupling constant for the CDW instability is significantly bigger than a bare coupling constant for the SDW instability (see for discussions Refs. [8, 9, 12]).
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