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DOES THE "QUANTIZED NESTING MODEL" PROPERLY DESCRIBE THE MAGNETIC-FIELD-INDUCED SPIN-DENSITY-WAVE TRANSITIONS?

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Theoretical reinvestigation of a so-called field-induced spin-density-wave (FISDW) phase diagram in a magnetic field in quasi-one-dimensional compounds $(TMTSF)_2X$ ($X=PF_6$, ClO_4, AsF_6, etc.) has revealed some novel qualitative features. Among them, are: 1) the FISDW wave vector is never strictly quantized; 2) the FISDW phase diagram consists of two regions: a) "Quantum FISDW", where there exist jumps of the FISDW wave vectors between different FISDW-subphases, b) "Quasiclassical FISDW", where the jumps disappear above some critical points and only one FISDW phase (characterizing by a wave vector oscillating with a magnetic field) exists. Both these features are due to taking account of a breaking of an electron-hole symmetry. They contradict to the previous text-book theoretical results (including the calculations of the "Three Dimensional Quantum Hall Effect") performed by means of the "Quantized Nesting Model" which explicitly assumes the existence of the electron-hole symmetry. We stress that some effects related to the phenomena described above were experimentally observed but were not properly interpreted.

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Quasi-one-dimensional (Q1D) organic compounds $(TMTSF)_2X$ ($X = PF_6$, ClO_4, AsF_6, etc.) demonstrate a unique and complicated phase diagram in a magnetic field. The primary distinct feature of the phase diagram is a cascade of transitions between different field-induced spin-density-wave (FISDW) subphases [1, 2] (for the reviews, see Refs.[3 – 6]). There is a related "three dimensional quantum Hall effect" (3D QHE) [7, 8, 3 – 5]. According to Refs. [9, 10], the explanation of the metal-SDW phase transition [1 – 8] lies in a "one-dimensionalization" of a Q1D electron spectrum in a magnetic field and the appearance of an instability in the "Peierls channels". So far, the different FISDW subphases (which appear in a magnetic field) have been described within a so-called "quantized nesting (QN) model" [11 – 14] (for the recent developments of the QN model, see, for example, Refs. [15, 16, 3, 4]). The QN model describes the FISDW-subphases by the "quantized SDW order parameter" $\Delta(\mathbf{r})$ which has a form of a plane wave with a quantized value of a longitudinal wave vector:

$$\Delta(\mathbf{r}) = \Delta_N \exp(2ip_F x)\exp(ip_x x)\exp(i\frac{\pi}{b^*}y)\exp(i\frac{\pi}{c^*}z), \tag{1}$$

$$p_x = 2N(\omega_c/v_F), \tag{2}$$

where N is an integer; $\omega_c = eHv_F b^*/c$ is a cyclotronic frequency of the electron's motion along open orbits of a Q1D electron spectrum,

$$\epsilon^{\pm}(\mathbf{p}) = \pm v_F\ (p_x \mp p_F) - 2t_b\cos(p_y b^*) - 2t_b'\cos(2p_y b^*) - 2t_c\cos(p_z c^*), \tag{3}$$

in a transverse magnetic field $\mathbf{H} \parallel \mathbf{z} \parallel \mathbf{c}^*$ [Here $+(-)$ stands for the right (left) sheet of the FS; $v_F \simeq 10^7$ cm/sec and p_F are the Fermi velocity and Fermi momentum, respectively; $t_b \simeq 200\,\mathrm{K}$, $t'_b \simeq 10\,\mathrm{K}$, and $t_c \simeq 5\,\mathrm{K}$ are the tunneling integrals of the wave functions across the chains [3 – 6]; c is the velocity of light, $\hbar \equiv 1$.

According to the QN model [11 – 16, 3 – 5], each "quantized FISDW phase" (see Eqs. (1),(2)) at a given magnetic field H is characterized by its metal-SDW transition temperature $T_N(H)$ [11, 15, 16, 3, 4] and its free energy $F_N(H,T)$ [12 – 14, 3 – 5] which is lower than the energy of a metallic phase. Thus, to determine the FISDW phase diagram in a framework of the QN model, it is necessary to find the biggest value of $T_N(H)$ and the lowest value of $F_N(H,T)$ with respect to an integer parameter N. As a result, one finds a cascade of the first order phase transitions between the different FISDW subphases [11 – 16, 3 – 5] with wave vectors being quantized in accordance with Eqs. (1),(2). Note that the existing calculations of the 3D QHE in the FISDW subphases [17, 3, 4] of $(TMTSF)_2X$ conductors are based on Eqs.(1),(2).

The goals of our Letter are:

1) To show that, due to the electron-hole asymmetry, the QN model is a limiting case (corresponding to $T_N(H)/\omega_c \to 0$) of a more common approach. This means that the basic equations of the QN model (i.e., the quantization of the FISDW wave vector (1),(2)) are valid only approximately in the case $T_N(H)/\omega_c \ll 1$ (see Fig.1). They may be qualitatively used for the determination of the FISDW phase diagram of $(TMTSF)_2ClO_4$ compound, where $T_N(H)/\omega_c$ is a small value.

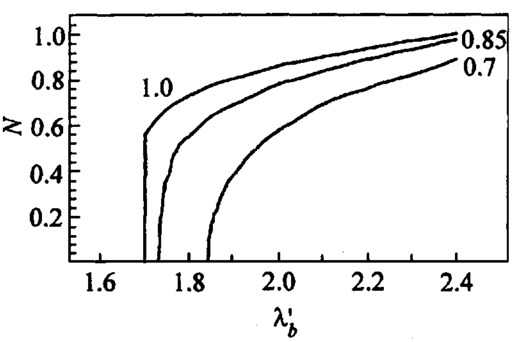

Fig.1. Three calculated magnetic field dependencies of the parameter N (see Eqs.(1), (2)) ($\lambda'_b \sim 1/H$). At $h \equiv H/2\pi T = 1$, there is a jump of the FISDW wave vector which corresponds to the first order phase transition (i.e., "quantum FISDW" region). At $h = 0.7$, the parameter N and thus the wave vector changes without jump (i.e., "quasi-classical FISDW" region). The value $h = 0.85$ corresponds to an isolated point of the first order transition (see Fig.2 and the text).

2) To demonstrate that our calculations (which account of the electron-hole asymmetry) lead to a theoretical FISDW diagram of $(TMTSF)_2PF_6$ conductor which is not even in a qualitative agreement with the results of the QN model calculations (see Figs.1,2). We recall that $(TMTSF)_2PF_6$ conductor is the basic material for the observation of the FISDW phase diagram [3, 4] and the related 3D QHE [7, 8, 15, 16] and that experiments [7, 8] performed in $(TMTSF)_2PF_6$ are usually claimed [7, 8, 3, 4] as one of the most reliable confirmations of an applicability of the QN model (i.e., Eqs.(1), (2)) to the FISDW phase diagram. We argue that the real FISDW phase diagram consists of two regions: a) "quantum low-temperature region", where there exist jumps of the FISDW wave vectors (i.e., the first order transitions) between different FISDW-subphases. Unlike the results of the QN model [11 – 16, 18, 3 – 5], we show that each such subphase is characterized by a non-integer parameter N in Eqs.(1), (2) and thus the jumps of the wave vectors (1),(2) between different FISDW subphases are also non-integers; b) "quasiclassical moderate-temperature region", where the jumps and the first order transitions

disappear above some critical points and the FISDW phase is characterized by a wave vector oscillating with a magnetic field (see Fig.2).

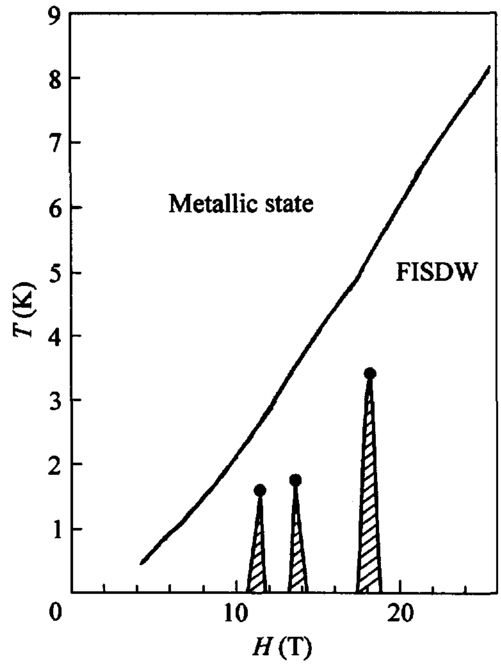

Fig.2. The FISDW phase diagram suggested in this Letter. A solid line stands for the metal-FISDW phase transition; shaded areas corresponds to the first order transitions between different FISDW subphases; full circles corresponds to the isolated points of the first order transitions above which only one FISDW phase is stable with a wave vector being an oscillating function of a magnetic field (see Fig.1 and the text)

3) To point out that the existing methods to calculate the 3D QHE [15 −17,3,4] has to be reinvestigated since they are based on the condition that the parameter N is an exact integer in Eqs. (1),(2) which is not the case as shown in this Letter.

We recall that the Gor'kov-like equation to determine the transition temperatures, $T_N(H)$, of the FISDW subphases (1),(2) in a transverse magnetic field ($\mathbf{H} \parallel \mathbf{z} \parallel \mathbf{c}^*$) [9, 11, 15, 16, 18] contains the following matrix elements:

$$\exp[i\frac{(\epsilon_1+\epsilon_2)x}{v_F}]\exp[i\lambda_b'\sin(p_b b^* - \frac{\omega_c x}{v_F})]\exp[2iN(\frac{\omega_c}{v_F})x]\Delta_N, \tag{4}$$

where ϵ_1 and ϵ_2 are energies of the pairing quasiparticles ($\epsilon_1+\epsilon_2 \simeq T$), $\lambda_b' = 2t_b'/\omega_c$, and x is a coordinate which changes on the scale $l_T = v_F/2\pi T$. So far, the analytical and numerical calculations of $T_N(H)$ have been performed at $T=0$ or at negligible ratios of the parameter $T_N(H)/\omega_c$. In this case, one can put $\epsilon_1 = \epsilon_2$ in Eq. (4) and the scale $l_T \to \infty$. Since it is necessary to integrate Eq. (4) over the coordinate x, it was made a conclusion that the parameter N in Eq. (4) is always integer. Note that an integer N corresponds to a logarithmic divergence of the Peierls-type diagram at $T \to 0$ [11 − 14, 3, 4]. In the consequent works (see, for example, Refs. [3, 4, 16 −18]) the parameter N was considered to be an integer even at finite temperatures, $T_N(H)$, and the so-called QN model [11−14] (i.e., Eqs. (1) and (2)) have been intensively applying to different phenomena [3, 4, 16−18]. Our current analysis shows that, due to the breaking of the electron-hole symmetry in phases with $N \neq 0$, the parameter N in Eqs. (1), (2) is never integer at finite temperatures.

Below, we calculate the FISDW phase transitions from a metallic phase to the phases with $N \simeq 1$ and $N = 0$. For these purpose, it is convenient to use Eq. (13) from Ref. [19],

$$\ln(\frac{T_0}{T_N}) = \sum_{L=-\infty}^{+\infty} J_L^2(\frac{2t'_b}{\omega_c}) \sum_{M=0}^{+\infty} (\frac{1}{2M+1} - \frac{1}{2M+1+i\delta_N} + \text{c.c}), \tag{5}$$

$$\delta_N = \frac{\omega_c}{2\pi T_N(H)} (L-N) \ , \tag{6}$$

where T_0 is a temperature of a phase transition to the last FISDW phase characterizing by $N = 0$.

Numerical solutions of Eqs. (5),(6) for the values of the band parameters of $(TMTSF)_2PF_6$ (see their values above) are summarized in Fig.1 and in a caption to Fig.1. It is shown that there are two regions of the FISDW phase diagram: a) "quantum FISDW": a cascade of the first order transitions with the non-integer jumps of the wave vectors; b) "quasiclassical FISDW" which is characterized by the oscillation of a wave vector in a magnetic field and which exists above critical points of the first order transitions (see Figs.1,2 and the figure captions).

Summarizing our results, we claim that the text-book QN model [3 −5, 11 −14, 16, 18] is a limiting case of a more general physical scheme and that an applicability of the QN model to the real FISDW transitions gives the results which are qualitatively inconsistent with the exact numerical calculations. In particular, the existing calculations of the 3D QHE has to be completely reinvestigated. At the end of the paper, we would like to point out that a number of experimentally observed features of the FISDW phase diagram in $(TMTSF)_2PF_6$ could not be interpreted in terms of the QN model. Indeed, the authors of Ref.[7] were not able to find the phase boundaries between different FISDW subphases at $T \geq 2$ K and the authors of Ref.[8] could not detect the hysteresis (which is an evidence of the cascade of the first order FISDW transitions) above $T \simeq 3$ K. Note that in both cases the metal-FISDW transition temperatures were significantly bigger than 3 K. From Fig.2, it is seen that these features are in accordance with the FISDW phase diagram suggested in the Letter. To prove more firmly the FISDW phase diagram suggested by us, A.Kornilov et al. have recently studied the behavior of the hysteresis inside the FISDW diagram[1)]. Their preliminary results are in a qualitative agreement with our calculations.

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