Soliton Wall Superlattice in Quasi-One-Dimensional Conductor

$(\text{Per})_2\text{Pt(mnt)}_2$

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Abstract

We suggest a model to explain the appearance of a high resistance high magnetic field charge-density-wave (CDW) phase, discovered by D. Graf et al. [Phys. Rev. Lett. 93, 076406 (2004)] in $(\text{Per})_2\text{Pt(mnt)}_2$. In particular, we show that the Pauli spin-splitting effects improve the nesting properties of a realistic quasi-one-dimensional electron spectrum and, therefore, a high resistance Peierls CDW phase is stabilized in high magnetic fields. In low and very high magnetic fields, a periodic soliton wall superlattice (SWS) phase is found to be a ground state. We suggest experimental studies of the predicted phase transitions between the Peierls and SWS CDW phases in $(\text{Per})_2\text{Pt(mnt)}_2$ to discover a unique SWS phase.

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It is well known that the charge-density-wave (CDW) phases are destroyed by the Pauli spin-splitting effects in a magnetic field [1-6], whereas the spin-density-wave (SDW) phases are not sensitive to them [2,7-12]. Moreover, it is demonstrated both theoretically [2,7-9,12] and experimentally [10-12] that the SDW phases can be generated by the orbitals effects in a magnetic field due to the so-called field induced dimensional crossovers (FIDC) [2,12]. An idea about the FIDC has been applied to the CDW phases [3,4], where they can also be restored by the orbital effects in a magnetic field at very low temperatures [4]. Therefore, the recent remarkable discovery of the high resistive high magnetic field CDW phases in (Per)$_2$X(mnt)$_2$ ($X = Pt$ and $Au$) quasi-one-dimensional (Q1D) conductors by Graf et al. [13] has been tentatively prescribed [13-15] to the FIDC effects [2-4,12]. This explanation may be adequate to some degree only in the case of $X = Au$, where the high resistance CDW phase occurs only for a magnetic field, perpendicular to the conducting chains, $H \parallel c$ and $H \parallel a$ (see discussion in the end of the Letter).

On the other hand, the high resistance high magnetic field CDW phase in (Per)$_2$Pt(mnt)$_2$ conductor is shown [13,14] to appear at any direction of a magnetic field. In particular, this phase exists for a magnetic field, parallel to the conducting chains, $H \parallel b$, where the orbital effects are absent and, thus, the FIDC effects [2-4,12] do not occur. Independence of the main features of the CDW phase diagram in (Per)$_2$Pt(mnt)$_2$ conductor on a magnetic field direction indicates that the high resistance CDW phase in this compound is unique and cannot be described by the previous theories [1-4,7-9,12].

The main goals of our Letter are as follows. Firstly, we suggest a theoretical approach, based on a realistic model for a Q1D electron spectrum, to describe the main properties of the CDW phase diagram in (Per)$_2$Pt(mnt)$_2$. In particular, we demonstrate that the Pauli spin-splitting effects in a magnetic field improve the nesting properties of the Q1D electron spectrum. This stabilizes a textbook high resistance Peierls phase in high arbitrary directed magnetic fields, in contrast to the previous theories. [Below, we call this phenomenon spin improved nesting (SINe)].

Secondly, we show that, in low and very high magnetic fields, a unique CDW phase - a soliton wall superlattice (SWS) state - has to appear. This semiconducting phase with two energy gaps is characterized by a periodically arranged soliton and anti-soliton walls with distance between them and values of the energy gaps being functions of a magnetic field. We predict that phase transitions occur between the conventional Peierls and unconventional SWS phases and suggest to study them to discover a unique SWS phase in (Per)$_2$Pt(mnt)$_2$. It is important that the existing experimental data on an activated behavior of resistivity [13] are in agreement with the Peierls-SWS phase transitions scenario, suggested in the Letter.

Let us discuss the SINe phenomenon, which results in a stabilization of the Peierls CDW phase in high magnetic fields, using qualitative arguments. Below, we accept a simplified
Q1D electron spectrum of \((\text{Per})_2\text{Pt(mnt)}_2\) conductor with four plane sheets of the Fermi surface (FS) [16],

\[ \varepsilon_{\alpha}^{\pm}(p) = \pm v_F [p_x \mp p_F \pm (\Delta p/2)(-1)^\alpha], \]  

(1)

where +(-) stands for right (left) part of the FS; \(p_F\) and \(v_F\) are the average Fermi momentum and the Fermi velocity, \(\alpha = 1(2)\) stands for the first (second) perylene conducting chain [16], \(\Delta p\) is a difference between the values of the Fermi momenta on two conducting chains. (We note that such kind of an electron spectrum with four slightly corrugated sheets of the FS has been suggested on a basis of the band calculations [17], experimentally observed quantum interference oscillations [18], and Landau levels quantization [19]).

In a magnetic field, the electron spectrum (1) is split into eight plane sheets of the FS,

\[ \varepsilon_{\alpha\sigma}^{\pm}(p) = \pm v_F [p_x \mp p_F \pm (\Delta p/2)(-1)^\alpha] - \sigma \mu_B H, \]  

(2)

where \(\sigma = +1(-1)\) stands for spin up (down), \(\mu_B\) is the Bohr magneton (see Fig.1). As seen from Fig.1, there exist four competing nesting vectors, \(Q_{1,+1}\), \(Q_{1,-1}\), \(Q_{2,+1}\), and \(Q_{2,-1}\), for the CDW instability, which pair electrons near \(+p_F\) with spin up (down) and holes near \(-p_F\) with spin up (down).

It is natural that four nesting vectors,

\[ Q_{\alpha\sigma} = 2p_F + q_{\alpha\sigma}, \quad q_{\alpha\sigma} = (-1)^\alpha \Delta p - 2\sigma \mu_B H/v_F, \]  

(3)

may correspond to several energy gaps in an electron spectrum at high values of the parameters \(\Delta p\) and \(2\mu_B H/v_F\). As we show below, this results in the appearance of the SWS phase with two energy gaps [20] (see Fig.2), which is in a qualitative agreement with a general theory of solitons and soliton superstructures [21-24].

Nevertheless, as seen from Eq.(3) and Fig.1, at some critical magnetic field,

\[ H^* = \Delta p v_F/2\mu_B, \]  

(4)

two nesting vectors coincide, \(Q_{1,-1} = Q_{2,+1} = 2p_F\). Therefore, in the vicinity of this critical field, \(H \approx H^*_p\), the Peierls CDW phase with \(Q = 2p_F\) and one gap in an electron spectrum becomes more stable than the SWS one (see Figs.2,3). In other words, at \(H \approx H^*_p\), the Pauli spin-splitting effects improve nesting properties of the electron spectrum (2), which stabilizes a textbook Peierls phase with the nesting vector,

\[ Q = (2p_F, 0, 0). \]  

(5)

We suggest that this SINe phenomenon is responsible for the experimental stabilization of the high resistance high magnetic field phase in \((\text{Per})_2\text{Pt(mnt)}_2\) [13-15].
Let us consider a formation of the CDW phase, corresponding to the nesting vector,

\[ \mathbf{Q} = (2p_F + q, 0, 0), \]  

where the CDW order parameter is

\[ \Delta_{CDW}(x) = \Delta_q e^{i(2p_F+q)x} + \Delta_q^* e^{-i(2p_F+q)x}, \]

using Green functions methods [25]. In this case, a mean field Hamiltonian of the electrons interacting with the crystalline lattice can be written as,

\[
\hat{H} = \sum_{\alpha=1,2} \sum_{\sigma=\pm1} \sum_{\xi} \left\{ a_{\alpha\sigma}^\dagger(\xi) a_{\alpha\sigma}(\xi) \left[ \epsilon_{\alpha\sigma}(\xi) - \mu \right] + b_{\alpha\sigma}^\dagger(\xi) b_{\alpha\sigma}(\xi) \left[ \epsilon_{\alpha\sigma}^-(\xi) - \mu \right] \right\} \\
+ \sum_{\alpha=1,2} \sum_{\sigma=\pm1} \sum_{\xi} \left\{ a_{\alpha\sigma}^\dagger(\xi) b_{\alpha\sigma}(\xi-q) \Delta_q + b_{\alpha\sigma}^\dagger(\xi) a_{\alpha\sigma}(\xi+q) \Delta_q^* \right\},
\]

where

\[ \Psi_{\alpha\sigma}(x) = \exp(-ip_F x) \sum_{\xi} e^{i\xi x} b_{\alpha\sigma}(\xi) + \exp(ip_F x) \sum_{\xi} e^{i\xi x} a_{\alpha\sigma}(\xi) \]

is a field operator, \( a_{\alpha\sigma}(\xi) \) and \( b_{\alpha\sigma}(\xi) \) are electron annihilation operators near right and left sheets of the Q1D FS (1), correspondingly.

Using standard definitions of the normal and anomalous (Gor’kov) Green functions,

\[
G_{\alpha\sigma}^{++}(\xi,i\omega) = \frac{-\langle T_\tau a_{\alpha\sigma}(\xi,\tau) a_{\alpha\sigma}^\dagger(\xi,0) \rangle}{\omega + \epsilon_{\alpha\sigma}(\xi) - \mu}, \\
G_{\alpha\sigma}^{--}(\xi,i\omega) = \frac{-\langle T_\tau b_{\alpha\sigma}(\xi-q,\tau) a_{\alpha\sigma}^\dagger(\xi,0) \rangle}{\omega + \epsilon_{\alpha\sigma}^-(\xi-q) - \mu},
\]

we find that the Green functions obey the following equations,

\[
\left( i\omega_n - [\epsilon_{\alpha\sigma}^+(\xi) - \mu] \right) G_{\alpha\sigma}^{++}(\xi,i\omega_n) - \Delta_q G_{\alpha\sigma}^{--}(\xi,i\omega_n) = 1,
\]

\[
\left( i\omega_n - [\epsilon_{\alpha\sigma}^-(\xi-q) - \mu] \right) G_{\alpha\sigma}^{--}(\xi,i\omega_n) - \Delta_q^* G_{\alpha\sigma}^{++}(\xi,i\omega_n) = 0,
\]

where the self-consistent gap equation is

\[
\Delta_q^* = -g^2 \sum_{\alpha=1,2} \sum_{\sigma=\pm1} \sum_\xi T \sum_{\omega_n} G_{\alpha\sigma}^{--}(\xi,i\omega_n),
\]

with \( \omega_n = 2\pi T(n + \frac{1}{2}) \) being the Matsubara frequency.

Below, we are interested in a phase transition line between the metallic and CDW phases, therefore, we need to solve the linearized Eqs.(11)-(13). As a result, we find the following expression,

\[
\ln \left( \frac{T_c}{T_{\text{eq}}} \right) = \frac{1}{4} \sum_{\alpha=1,2} \sum_{\sigma=\pm1} \sum_{n=0}^{\infty} \frac{v_F^2 (q - q_{\alpha\sigma})^2 / (4\pi T_c)^2}{(n + \frac{1}{2})^2 + v_F^2 (q - q_{\alpha\sigma})^2 / (4\pi T_c)^2},
\]
where $q_{\alpha\sigma}$ is given by Eq. (3). Eq.(14) may be rewritten using a so-called $\psi$-function [26],

$$\ln \left( \frac{T_c}{T_c} \right) = \frac{1}{4} \sum_{\alpha=1,2} \sum_{\sigma=\pm 1} \left( \frac{1}{2} \psi \left[ \frac{1}{2} + i \frac{v_F (q - q_{\alpha\sigma})}{4 \pi T_c} \right] + \frac{1}{2} \psi \left[ \frac{1}{2} - i \frac{v_F (q - q_{\alpha\sigma})}{4 \pi T_c} \right] - \psi \left[ \frac{1}{2} \right] \right).$$ (15)

[Note that Eqs.(14),(15) are the main analytical results of the Letter. They connect a transition temperature of the CDW phase, $T_c$, in the presence of a magnetic field, $H \neq 0$, with a transition temperature, $T_{c0}$, corresponding to $H = 0$ and $\Delta p = 0$. As it directly seen from Eqs.(14),(15), there exist a competition between four nesting vectors, $Q_{\alpha\sigma} = 2p_F + q_{\alpha\sigma}$, from Eq.(3) (see Fig.1)].

In Fig.3, we present the results of our numerical solutions of Eq.(14), which demonstrate a stabilization of the Peierls phase with $Q = 2p_F$ at high enough magnetic fields, $29T < H < 49T$. At very high magnetic fields, $H > 49T$, and low magnetic fields, $H < 29T$, a unique SWS phase is shown to be a ground state (see Fig.2). Note that, in the vicinity of the metal-CDW phases transition line, the SWS phase is characterized by the following order parameter,

$$\Delta_{SWS} (x) = \cos(qx) \cos(2p_Fx),$$ (16)

which corresponds to mixing of two order parameters (7) with $+q$ and $-q$, where $q \neq 0$ [27]. It is important that the SWS phase is characterized by periodically arranged soliton and anti-soliton walls, where the distance between them is $x_H = \pi/q$ [21]. In our case, $x_H$ demonstrate a non-trivial dependence on a magnetic field. As it seen from Fig.3, the calculated phase diagram is in good qualitative and quantitative agreements with the measured ones [13-15]. [Note that for the numerical calculations we have used $T_c(H = 0) = 7K$ [13] and $\Delta pv_F = 60K$. The latter parameter is in a qualitative agreement with Refs.[17-19] (see discussions in Ref. [29])].

To summarize, our theory suggests an explanation of the existence of the high resistance high magnetic SDW phase in (Per)$_2$Pt(mnt)$_2$ conductor [13-15] in terms of the SINe effects. It also predicts the existence of phase transitions between the high resistance Peierls phase with large activation gap, $\Delta_p$, and a unique SWS phase with two equal magnetic field dependent energy gaps, $\Delta_{SWS}$. The SWS phase is also characterized by an activation behavior of a resistivity with the activation gap being $\Delta_{SWS} \ll \Delta_p$ (see Fig.2). It is important that these results are in agreement with the existing measurements of the activation gaps in (Per)$_2$Pt(mnt)$_2$ [13]. In our notations, the measured gaps are: $\Delta_p = 40K \gg \Delta_{SWS} \simeq 6-15K$, which are in accordance with the theory. We suggest more detailed measurements of the activation behavior of resistivity in the vicinities of the Peierls-SWS phase transitions to establish the existence of the SWS phase. We also think that ac infrared measurements may be useful to detect the existence of two gaps in an electron spectrum of the SWS phase.
We stress that a restoration of the high resistance phase in a sister compound \((\text{Per})_2\text{Au(mnt)}_2\) occurs only in a magnetic field, perpendicular to the conducting chains, where the FIDC effects are expected \([2,4]\). On the other hand, its transition temperature is too high to be explained only by the FIDC effects, which are expected in the CDW phases only at very low temperatures \([4]\). Therefore, for explanation of the phase diagram in \((\text{Per})_2\text{Au(mnt)}_2\) a combination of the FIDC and SINe effects has to be considered \([28,30]\). In particular, at very high magnetic fields, we expect the appearance of the SWS phase in this compound \([28]\).

In conclusion, we point out that a possibility of the SWS phases to exist in quasi-low-dimensional conductors was earlier discussed in Refs. \([24,31]\) for very different physical situations. To the best of our knowledge, the SWS phase has never been experimentally observed yet and, as we hope, it is discovered in Q1D \((\text{Per})_2\text{Pt(mnt)}_2\) conductor. In particular, the SWS phase does not exist in other CDW systems - \(\alpha-(\text{ET})_2\text{M(SCN)}_4\) materials \([5,6]\) - where corrugations of the Q1D FS are large and an activation behavior of resistivity is not observed.

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In fact, there exist eight almost plane sheets of the FS in (Per)$_2$M(mnt)$_2$ conductors, but the first four of them are almost identical to the other four (see Ref.[17]) and, thus, we do not distinguish between them.

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[16] We stress that our model is equivalent to that in Ref.[21] in two limiting cases: at zero magnetic field, $\mu_B H/\Delta_{pvF} \rightarrow 0$, and at high magnetic fields, $\mu_B H/\Delta_{pvF} \rightarrow \infty$. Therefore, at high enough and low enough magnetic fields, the SWS phase is characterized by two energy gaps at any temperatures in accordance with Ref.[21] (see Fig.2). As shown in the Letter, the SWS phase is characterized by two energy gaps in the vicinity of the metal-SWS phase transition line for the values of the parameters, $T_c(H = 0) = 7 \, K$ and $\Delta_{pvF} = 60 \, K$. Note that, for higher value of the parameter $\Delta_{pvF}$, the SWS phase may be characterized by four gaps in its electron spectrum.

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To demonstrate that the periodic SWS phase is a ground state, we prove that: (1) two degenerate solutions with \( Q_{1,2} = 2p_F \pm q \) \((q \neq 0)\) correspond to a maximum of the transition temperature in Eq.(14), (2) the fourth order terms in the Landau theory of the second order phase transitions, in our case, result in mixing of the above mentioned two order parameters. As a result, the order parameter (16) is a ground state in the vicinity of the metallic-CDW phases transition line, which is known to be a corresponding limiting case for the periodic SWS [21,24]. A detailed consideration of the fourth order terms in the Landau theory will be published elsewhere [28].

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From band structure calculations [17], it follows that \( \Delta p_F \approx 35 - 70 \) K, an analysis of the quantum interference oscillations in \((\text{Per})_2\text{Au(mnt)}_2\) under pressure gives \( \Delta p_F \approx 70 \) K, whereas the Landau levels quantization analysis in \((\text{Per})_2\text{Au(mnt)}_2\) gives \( \Delta p_F \approx 50 \) K.

According to our point of view, a sister compound \((\text{Per})_2\text{Au(mnt)}_2\) is characterized by a high value of warping of its Q1D electron spectrum. This makes the orbital FIDC effects [2,4] to be as important as the SINe ones. Therefore, a combination of the FIDC and SINe effects restores the Peierls CDW phase only for favorite directions of a magnetic field.

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FIG. 1: Electron spectrum of a two chains Q1D conductor [16] in a magnetic field is split into eight sheets of the Fermi surface [see Eq.(2)]. Therefore, there exist a competition between the CDW phases, characterized by four different nesting vectors, $Q_{1,+1}$, $Q_{1,-1}$, $Q_{2,+1}$, and $Q_{2,-1}$ [see Eqs.(3),(6) and the text]. At magnetic field $H^* = \Delta p v_F / 2 \mu_B$, two nesting vectors coincide, $Q_{1,-1} = Q_{2,+1} = 2p_F$, which results in a restoration of the Peierls CDW phase with $Q = 2p_F$ at high magnetic fields [see Eqs.(5),(14) and Figs.2,3].
FIG. 2: Electron spectrum of the SWS phase with two energy gaps (right) is qualitatively different from that in the Peierls phase with one energy gap (left) [20] [see Eqs.(5),(16)].

\[ T_c (K) \]

FIG. 3: Solid line: phase transition line between the metallic and CDW Peierls and SWS phases is calculated by means of Eq.(14). Dotted lines: phase transitions between the Peierls and SWS phases [see Eq.(16)]. In our case, \( H^* \approx 40 \ T \) [see Eq.(4)].