Pis'ma v ZhETF, vol. 86, iss. 2, pp. 144 – 147

Soliton wall superlattice charge-density-wave phase in a magnetic field

A. G. Lebed[+*], *S. Wu*[+]

[+]*Department of Physics, University of Arizona, 1118 E. Tucson, AZ 85721, USA*

[*]*Landau Institute for Theoretical Physics RAS, 117334 Moscow, Russia*

Submitted 6 June 2007

We suggest a model, where phase transitions between the Peierls and periodic soliton wall superlattice (SWS) charge-density-wave phases occur in a magnetic field. The model accounts for peculiarities of an electron spectrum in a quasi-one-dimensional conductor $(Per)_2Pt(mnt)_2$. We discuss possible experimental investigations of the theoretically predicted phase transitions in $(Per)_2Pt(mnt)_2$ to discover a unique SWS phase.

PACS: 71.45.Lr, 74.70.Kn

Since a discovery of the magnetic field-induced spin-density-wave (FISDW) phase diagrams [1, 2] and their explanations in terms of the field-induced dimensional crossovers (FIDC) [3 – 6] high magnetic field phase diagrams of quasi-one-dimensional (Q1D) conductors have been intensively studied [7 – 10]. In particular, it has been shown [8, 3] that, in the absence of the Landau levels quantization, other quantum effects – the Bragg reflections of electrons moving in the extended Brillouin zone – result in a momentum quantization law [8] and the $3D \to 2D$ FIDC [3, 8] in a magnetic field. The above mentioned decrease of an effective dimensionality of electron wave functions is shown [3 – 8] to lead to the Peierls instability and, as a result, to the formation of the FISDW phases. In case of the FISDW phase diagrams, the paramagnetic spin-splitting effects do not play an important role [3 – 10] and, therefore, the FISDW phases are observed in very high magnetic fields in $(TMTSF)_2X$ ($X=PF_6$, ClO_4, etc.) organic conductors [1, 2, 9] and some other materials [8].

On the other hand, it is well known [11 – 13] that the paramagnetic spin-splitting effects in a magnetic field destroy the charge-density-wave (CDW) phases. This is a reason why a density-wave (DW) phase, destroyed by high magnetic fields in α-$(ET)_2M(CNS)_4$ (M = K, Tl, Rb) organic compounds [14, 15], is interpreted as a CDW [12 – 15]. Unusual states, observed in these compounds at rather low temperatures and high magnetic fields [14, 15], are correspondingly interpreted as the field-induced charge-density-wave (FICDW) phases [13]. As theoretically shown in Ref. [13], the FICDW phases may appear in high magnetic fields due to the $3D \to 2D$ FIDC [3, 8] only at rather low temperatures.

Therefore, a recent discovery [16] of high magnetic field CDW phases in a Q1D organic conductor $(Per)_2Pt(mnt)_2$ at relatively high temperatures is very surprising. Their existences are not expected in any of the previous theories [3 – 13], which excludes the suggested interpretation [16] in terms of FICDW [12, 13] phases.

There are two main goals of our Letter. Firstly, we suggest a simple realistic model of a Q1D electron spectrum of $(Per)_2Pt(mnt)_2$ conductor. We show that the nesting properties of this model electron spectrum are improved in a magnetic field due to the paramagnetic spin-splitting effects, in contrast to the results of the previous theories [12, 13]. We call the above mentioned phenomenon spin improved nesting (SINe). The SINe effects allow us to explain the appearance of the high temperature CDW phase in $(Per)_2Pt(mnt)_2$ in high magnetic fields at any direction of a magnetic field. Secondly, we predict the existence of the phase transitions between the high temperature and high magnetic field Peierls CDW phase and a unique periodic soliton wall superlattice (SWS) phase. We also suggest experimental investigations of the above mentioned phase transitions to discover the SWS phase, which, to the best of our knowledge, has never been observed in solids.

At first, we consider the SINe phenomenon, which results in a stabilization of the Peierls CDW phase in high magnetic fields, using qualitative arguments. In this Letter, we accept a simplified Q1D electron spectrum of $(Per)_2Pt(mnt)_2$ conductor with four plane sheets of the Fermi surface (FS), suggested in Ref. [17] on a basis of the band calculations,

$$\varepsilon_i^{\pm}(\mathbf{p}) = \pm v_F \left[p_y \mp p_F \pm (\Delta p/2)(-1)^i\right], \qquad (1)$$

where $+(-)$ stands for right (left) part of the FS; p_F and v_F are the average Fermi momentum and the Fermi velocity, $i = 1(2)$ stands for the first (second) perylene conducting chain [17], Δp is a difference between the values of the Fermi momenta on two conducting chains (see Fig.1).

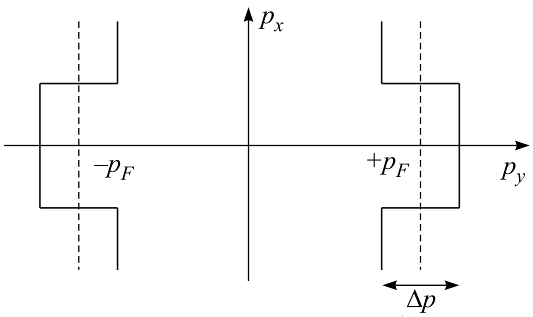

Fig.1. Q1D electron spectrum of $(Per)_2Pt(mnt)_2$ conductor is shown for a simplified two perylene chains model (see Eq. (1)). For details, see Ref. [17]

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

$$\varepsilon^{\pm}_{i,\sigma}(\mathbf{p}) = \pm v_F \left[p_y \mp p_F \pm (\Delta p/2)(-1)^i\right] - \sigma \mu_B H, \quad (2)$$

where $\sigma = +1(-1)$ stands for spin up (down), μ_B is the Bohr magneton. As seen from Fig.2, there exist four competing nesting vectors for the CDW instability,

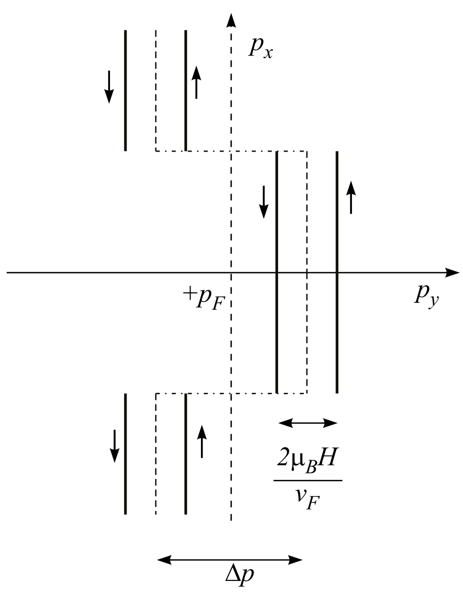

Fig.2. Electron spectrum of a two chains Q1D conductor in a magnetic field is shown in the vicinity of $p_y \simeq p_F$ (see Eq. (2))

which pair electrons near $+p_F$ with spin up (down) and holes near $-p_F$ with spin up (down).

It is important that these four nesting vectors,

$$Q_{i,\sigma} = 2p_F + k_{i,\sigma}, \quad k_{i,\sigma} = (-1)^i \Delta p - 2\sigma \mu_B H / v_F, \quad (3)$$

may correspond to several energy gaps in an electron spectrum. As we show below, in our case, this results in the appearance of the SWS phase with two energy gaps (see Fig.3). This result is in a qualitative agreement

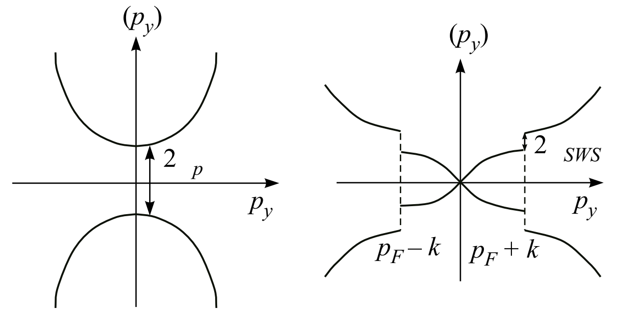

Fig.3. Peierls phase is characterized by a single gap in an electron spectrum, whereas the SWS phase is characterized by two energy gaps

with a general theory of solitons and soliton superstructures [18–20].

As it follows from Eq.(3) and Fig.2, at some critical magnetic field,

$$H^* = \Delta p v_F / 2\mu_B, \quad (4)$$

two nesting vectors coincide. Therefore, in the vicinity of this critical field, $H \approx H^*$, the Peierls CDW phase with $Q = 2p_F$ (i.e., $k = 0$) and one gap in an electron spectrum becomes more stable than the SWS phase (see Fig.4). In other words, at $H \approx H^*$, the Pauli spin-splitting effects improve nesting properties of the electron spectrum (2), which stabilizes a textbook Peierls phase with the nesting vector,

$$\mathbf{Q} = (2p_F, 0, 0). \quad (5)$$

We suggest that this SINe phenomenon is responsible for the experimental stabilization of the high resistance high magnetic field phase in $(Per)_2Pt(mnt)_2$ [16].

Let us consider a formation of the CDW phase with the order parameter,

$$\Delta_{CDW}(x) = \Delta_k e^{i(2p_F + k)x} + \Delta^*_k e^{-i(2p_F + k)x}, \quad (6)$$

corresponding to the following nesting vector,

$$\mathbf{Q} = (2p_F + k, 0, 0). \quad (7)$$

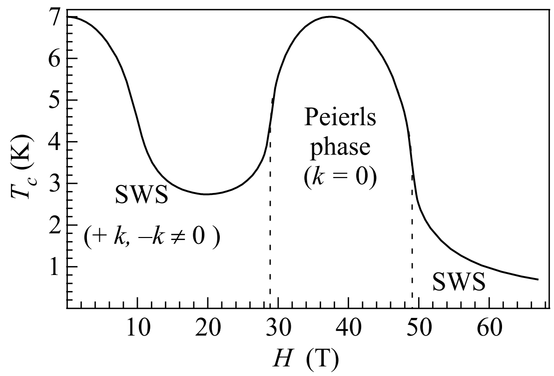

Fig.4. Metal-CDW phase transition temperature, calculated by means of Eq.(10). Peierls phase is stabilized at high enough magnetic fields, $30\ T \geq H \leq 50\ T$, whereas SWS phase is stabilized at low, $H \leq 30\ T$, and ultra-high, $H \geq 50\ T$, magnetic fields

In this case, a mean field Hamiltonian of the electrons interacting with the CDW potential (6) can be written as,

$$\hat{H} = \sum_{i=1,2} \sum_{\sigma=\pm 1} \sum_{\xi} \Big\{ a^{\dagger}_{i,\sigma}(\xi) a_{i,\sigma}(\xi) \left[\varepsilon^{+}_{i,\sigma}(\xi) - \mu \right] + + b^{\dagger}_{i,\sigma}(\xi) b_{i,\sigma}(\xi) \left[\varepsilon^{-}_{i,\sigma}(\xi) - \mu \right] \Big\} + + \sum_{i=1,2} \sum_{\sigma=\pm 1} \sum_{\xi} \Big\{ a^{\dagger}_{i,\sigma}(\xi) b_{i,\sigma}(\xi - k) \Delta_k + + b^{\dagger}_{i,\sigma}(\xi) a_{i,\sigma}(\xi + k) \Delta^{*}_{k} \Big\}, \tag{8}$$

where

$$\Psi_{i,\sigma}(x) = \exp(-ip_F x) \sum_{\xi} e^{i\xi x} b_{i,\sigma}(\xi) + + \exp(ip_F x) \sum_{\xi} e^{i\xi x} a_{i,\sigma}(\xi) \tag{9}$$

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

Using calculations of a generalized susceptibility in the presence of a mean field electron-phonon interactions (8) similar to calculations, performed in Ref. [20], we obtain the following expression for the metal-CDW phase transition temperature,

$$\ln\left(\frac{T_{c0}}{T_c}\right) = \tag{10}$$

$$\frac{1}{4} \sum_{i=1,2} \sum_{\sigma=\pm 1} \sum_{n=0}^{\infty} \frac{v_F^2 (q - k_{i,\sigma})^2 / (4\pi T_c)^2}{(n+\frac{1}{2}) \left[(n+\frac{1}{2})^2 + v_F^2 (q - k_{i,\sigma})^2 / (4\pi T_c)^2 \right]},$$

where $k_{i,\sigma}$ is given by Eq. (3).

Eq.(10) is the main analytical result of the Letter. It connects 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 Eq.(10), there exist a competition between four nesting vectors, $Q_{i,\sigma} = 2p_F + k_{i,\sigma}$, from Eq.(3) (see Fig.2).

In Fig.4, we present the results of our numerical solutions of Eq.(10), which demonstrate a stabilization of the Peierls phase with $Q = 2p_F$ at high enough magnetic fields, $29\ T \leq H \leq 49\ T$. At very high magnetic fields, $H \geq 49\ T$, and low magnetic fields, $H \leq 29\ T$, a unique SWS phase is shown to be a ground state (see also Fig.3). Note that, in the vicinity of the metal-CDW phase transition line, the SWS phase is characterized by the following order parameter,

$$\Delta_{SWS}(x) = \cos(kx) \cos(2p_F x), \tag{11}$$

which corresponds to mixing of two order parameters (7) with $+k$ and $-k$, where $k \neq 0$ [18-20]. [Note that the SWS phase is characterized by periodically arranged soliton and anti-soliton walls, where the distance between them is $x_H = \pi/q$. As seen from Fig.4, the calculated phase diagram is in good qualitative agreement with the measured one [16].

To summarize, our theory suggests an explanation of the existence of the high resistance high magnetic field SDW phase in $(Per)_2Pt(mnt)_2$ conductor [16] in terms of the SINe effects. It also predicts the existence of phase transitions between the high resistance Peierls phase with large activation gap, Δ_p, and a unique SWS phase with two equal magnetic field dependent energy gaps, Δ_{SWS}. It is important that the SWS phase is characterized by an activation behavior of a resistivity with the activation gap being $\Delta_{SWS} \ll \Delta_p$ (see Fig.3). We suggest 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.

The author is thankful to N.N. Bagmet, J.S. Brooks, and P.M. Chaikin for useful discussions.

1. P. M. Chaikin, Mu-Yong Choi, J.F. Kwak et al., Phys. Rev. Lett. **51**, 2333 (1983).
2. M. Ribault, D. Jerome, J. Techendler et al., J. Phys. (Paris) Lett. **44**, L-953 (1983).
3. L. P. Gor'kov and A. G. Lebed, J. Phys. (Paris) Lett. **45**, L-433 (1984).
4. M. Heritier, G. Montambaux, and P. Lederer, J. Phys. (Paris) Lett. **45**, L-943 (1984).

5. A. G. Lebed, Zh. Eksp. Teor. Fiz. **89**, 1034 (1985) [Sov. Phys. JETP **62**, 595 (1985)].
6. A. Virosztek, L. Chen, and K. Maki, Phys. Rev. B **34**, 3371 (1986).
7. A. G. Lebed, Phys. Rev. Lett. **88**, 177001 (2002).
8. See reviews by A. G. Lebed and M. Heritier in *The Physics of Organic Superconductors and Conductors*, Ed. A. G. Lebed, Springer-Verlag, Berlin-Heidelberg, in preparation.
9. A. V. Kornilov, V. M. Pudalov, Y. Kitaoka et al., Phys. Rev. B **65**, 060404R (2002).
10. T. Ishiguro, K. Yamaji, and G. Saito, *Organic Superconductors*, 2nd edn, Springer, Berlin-Heidelberg, 1998.
11. W. Dieterich and P. Fulde, Z. Phys. **265**, 239 (1973).
12. D. Zanchi, A. Bjelis, and G. Montambaux, Phys. Rev. B **53**, 1240 (1996).
13. A. G. Lebed, Pis'ma v Zh. Eksp. Teor. Fiz. **78**, 170 (2003) [JETP Lett. **78**, 138 (2003)].
14. J. S. Qualls, L. Balicas, J. S. Brooks et al., Phys. Rev. B **62**, 10008 (2000).
15. D. Andres, M. V. Kartsovnik, P. D. Grigoriev et al., Phys. Rev. B **68**, 201101(R) (2003).
16. D. Graf, E. S. Choi, J. S. Brooks et al., Phys. Rev. Lett. **93**, 076406 (2004).
17. E. Canadell, M. Almeida, and J. S. Brooks, Eur. Phys. J. B **42**, R453 (2004).
18. S. A. Brazovskii, I. E. Dzyaloshinskii, and N. N. Kirova, Zh. Eksp. Teor. Fiz. **81**, 2279 (1981) [Sov. Phys. JETP **54**, 1209 (1981)]; M. Fujita, K. Machida, and H. Nakanishi, J. Phys. Soc. Jpn. **54**, 3820 (1985).
19. S. A. Brazovskii, S. A. Gordyunin, and N. N. Kirova, Pis'ma v Zh. Eksp. Teor. Fiz. **31**, 486 (1980) [JETP Lett. **31**, 456 (1980)].
20. S. A. Brazovskii, L. P. Gor'kov, and A. G. Lebed, Zh. Eksp. Teor. Fiz. **83**, 1198 (1982) [Sov. Phys. JETP **56**, 683 (1982)].