SOME PROPERTIES OF THE QUASI-1D CONDUCTORS IN A MAGNETIC FIELD

G. Montambaux

Laboratoire de Physique des Solides, Université Paris XI, 91405 Orsay, France

ABSTRACT

A short review is given of the successes and of the failures of the Quantized Nesting model, at the light of recent experiments in the Bechgaard salts (TMTSF)$_2$ClO$_4$ and (TMTSF)$_2$PF$_6$. A preliminary work gives a complete description of the spectrum of the Field Induced Spin Density Wave phases. It is compared to the well known Hofstadter spectrum.

1 QUANTIZED NESTING IN BECHGAARD SALTS

The Quantized Nesting (QN)[1] model has been successful to describe the magnetic Field Induced Spin Density Wave (FISDW) phases of the Bechgaard salts (TMTSF)$_2$ClO$_4$ and (TMTSF)$_2$PF$_6$. The two essential ingredients of this mean field theory are the nesting of the Fermi surface and the quantization of electronic orbits in a field[1,2,3,4,5,6]. As a result of this duality, the metallic is unstable and the spectrum of the ordered phase exhibits a series of gaps which open at quantized values of the wave vector. This structure leads to very interesting magnetothermodynamic and magnetotransport properties. Many features of the experimental data are well described by this theory[7]: cascade of first order transitions, structure of the phase diagram, frequency of the transitions, evolution of the phase diagram with pressure, threshold field, magnetization and specific heat data, quantization of the Hall effect.

However, finer or more recent data in (TMTSF)$_2$ClO$_4$, the most studied of these compounds, are not understood in the simplest version of this model: negative magnetization[8], reentrances of the metallic phase in low field[9], irregularities in the sequence of the transitions[7], destruction of the SDW ordering in high field with reentrance of the metallic phase[10], arborescent phase diagram at low temperature[11], changes in sign in the Hall effect[12], fast oscillations in the magnetic field dependence of thermodynamic and transport data[7], etc...

Some of these unexplained data have been described coherently with a simple thermodynamic analysis[13]. It has been shown under very general conditions that the ground state magnetization $M$ is simply related to the variation with the field of the metal-SDW transition line $T_c(H)$: $M(H) = 0.236 \gamma d T_c^2 / dH$. In this framework, the reentrances of the metallic phase where shown to be related to the negative excursions of the magnetization. The large diamagnetic variation in high field has been proven to be a direct consequence of the destruction of the SDW ordering[13]. To explain this metallic phase reentrance in high field, non mean-field theories have been proposed[14,15]. We have recently stressed that, since magnetization in high field depends on the cooling rate, the reentrance is sensitive to anion ordering[13]. Preliminary results seem to confirm this sensitivity[16]. This indicates that the anion ordering is an essential ingredient to understand the reentrant and should be taken into account in a complete theory.

On the other hand, recent magnetotransport data in (TMTSF)$_2$PF$_6$ under pressure agree very well with the predictions of the QN model[17,18]. Hall effect data show a series of seven phases with plateaus in each phase. The phases are characterized by successive numbers 6 to 0. The transition fields obey the rule $H_n = H_f / (n + \gamma)$ where $H_f \sim 60T$ is the fundamental field related to the deviation from perfect nesting and $\gamma$ is of order 3. as it was predicted quantitatively from the QN model[19]. The origin of this number is the variation with the field of the electron density above the SDW gap.

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The QN model also predicted the occurrence of the $n = 0$ insulating phase at a field $H_0 = H_f/\gamma$ [1,19]. This phase has been discovered exactly at the right place[17,18]. There is at the moment no evidence of reentrance but it cannot be ruled out above 30 T. But an important difference with (TMTSF)$_2$ClO$_4$ is the existence of the $n = 0$ phase.

Although Hall effect exhibits plateaus in both compounds, the magnetoresistance never vanishes in the subphases as expected and is very sample dependent. This is not surprising considering that the sample may not be SDW ordered everywhere. A extremely elementary model with association of metallic and "quantized Hall" regions show that it is very easy to get quantization of Hall effect and non zero magneto resistance [20].

The physics seems to be simpler in (TMTSF)$_2$PF$_6$ than in (TMTSF)$_2$ClO$_4$, probably because of the crucial role of the anion ordering. However, common features are still puzzling. The origin of the fast oscillations and their disappearance at low temperature are quite unusual and not understood. The change in sign of the Hall effect has been attributed to the complex hierarchy of subphases appearing at low T[15,21,22]. But in (TMTSF)$_2$PF$_6$, this change in sign is not always observed even at very low temperature[17].

2 ELECTRONIC SPECTRUM OF QUASI-1D CONDUCTORS IN A FIELD

Recent thermodynamic data in (TMTSF)$_2$ClO$_4$ have shown that new phases may occur at low temperature with an arborescent phase diagram[11]. These results suggest the existence of a finer structure in the electronic spectrum of the FISDW. In all the theoretical treatments up to now, the dispersion relation along the direction of the chains has been linearized around the Fermi level. This trick leads to simple analytical results but it misses the lattice periodicity along the chains. It has been proposed that this periodicity leads to a more complex structure of the spectrum with a new possible set of nesting vectors[15,21]. This prediction has been based on a perturbative calculation. We found it interesting to use a non perturbative approach although not self-consistent. We present here preliminary results. We fix the amplitude of the order parameter and derive the structure of the spectrum with such an order parameter.

It has often been suggested that the complexity of the Hofstadter spectrum[23] has something to do with the spectrum of the FISDW phases[11,15,21,24]. Here, we show that these spectra differ significantly and that the spectrum of the FISDW has much less complex structure. The Hofstadter spectrum is recalled on fig.1. It is the spectrum of isotropic tight binding electrons in a field. Gaps open at wave vectors $2k = t2\pi/a + seHb/h$ (which correspond to band fillings $\nu = t + se\phi$ where $\phi$ is the flux inside one plaquette of the lattice). $t$ and $s$ are integer numbers and $a$, $b$ are interatomic distances. Here, we describe an highly anisotropic system with an anisotropy ratio $t_a/t_b$ of order 10. The number of gaps is unchanged but most of them are exponentially small. This is shown on fig.2. Only gaps with $s=0$ and $s=1$ are visible.

Now we add an external potential of the form $\Delta \cos(Qx)$ with $Q = \pi/a$(which is not the real situation in Bechgaard salts since the band is 3/4 filled). This potential opens new gaps at $2k = t2\pi/a + seHb/h + jQ$. The case $s = 0$ corresponds to the usual SDW gap. Other gaps separate the Landau bands described by the QN model. The structure is shown on fig.3. The subphases with a field dependent wave vector $Q = \pi/a + neHb/h$ are shown on fig.4. For this set of wave vectors, the FISDW spectrum do not have the complexity of the Hofstadter spectrum (one should also remember that the experimental accessible region corresponds to $r = \phi/\phi_0 < 10^{-2}$).

In the future, we want to investigate this spectrum with a 2D nesting vector $\vec{Q} = (Q_x, Q_y)$, with a fractional set of nesting vectors as proposed by M. Héritier[15,21], and also with non commensurate wave vectors $Q(H = 0) \neq \pi/a$. We hope it will lead to a complete description of the possible phase diagrams for the quasi-1D conductors in a field.
Fig. 1: Spectrum $E(\phi)$ of isotropic tight binding electrons [21]. $e = E/4t$ and $r = \phi/\phi_0$.

Fig. 2: Spectrum $E(\phi)$ of anisotropic tight binding electrons ($t_a/t_b = 10$). Only values of $r = p/q$ with $q < 50$ wave been calculated. This is the reason for the white vertical spaces.
Fig. 3: Spectrum $E(\phi)$ of anisotropic tight binding electrons with a modulation at wave vector $Q = (\pi/a, 0)$.

Fig. 4: Spectrum $E(\phi)$ of anisotropic tight binding electrons with a modulation at wave vector $Q = (\pi/a + neHb/h, 0). a)n = 1; b)n = 2.$
3 CONCLUSION

The QN model describes fairly well many features of the FISDW transitions in Bechgaard salts. The better agreement in (TMTSF)$_2$PF$_6$ than in (TMTSF)$_2$ClO$_4$ shows that the anion ordering is probably an essential ingredient to understand the puzzling data in (TMTSF)$_2$ClO$_4$ such as the reentrance in high field. A complete description of the spectrum of the FISDW is in progress.

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