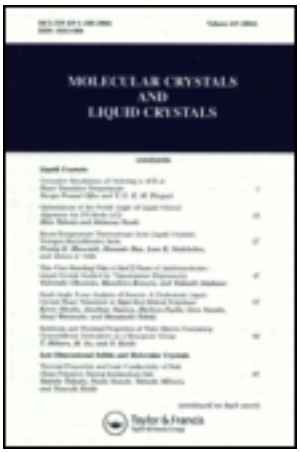

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STABILITY OF SPIN DENSITY WAVES IN QUASI 1D CONDUCTORS : APPLICATION TO $(TMTSF)_2CLO_4$.

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Abstract - We study the stability of the SDW phases in quasi-1D conductors. Magnetic field effects on renormalized interactions as well as on nesting properties are explored. The latter are shown to explain the data in $(TMTSF)_2ClO_4$: anion ordering effects, field induced SDW, quantized Hall conductance.

Depending on the cooling rate through the anion ordering temperature, $(TMTSF)_2ClO_4$ can be obtained in different states, with different stabilities of the SDW phase.[1] In rapidly quenched samples the SDW phase is stable at ambient pressure up to 4 K. In relaxed crystals, the stable phase at ambient pressure and low temperature is superconducting ($T_c \simeq 0.8$ kG in the c*-direction).[2] However the SDW phase can be restored by applying a large enough magnetic field in the c*-direction. At a threshold field which depends on temperature ($\sim$ 40 kG) a continuous transition from the normal metallic phase to a semimetallic phase is observed.[3-5] In a field larger than 40 kG and below 0.7 K, steps and plateaux of the Hall resistance have been observed.[5]

The purpose of this paper is to show that anion ordering and magnetic field effects on SDW stability are closely related and can be consistently interpreted within the same picture. Given the strongly anisotropic band structure, the stability of a SDW long range order depends, in principle, on two different factors : 1) the electron coupling renormalized by large 1D fluctuations down to the 1D $\rightarrow$ 3D crossover temperature, 2) the details of 3D anisotropic Fermi surfaces nesting. We have explored these two possible interpretations.

First, we have studied the g-ology model of the 1D electron

gas under field, with a two cut-off renormalization group study ; the two energy scales are the bandwith and the Zeeman energy.[6] The main effect of the field is to freeze the backward scattering processes between electrons of opposite spins, $g_{1\perp}$. As a result, when the bandwith parameter is of order of the Zeeman energy, $g_{1\perp}$ becomes irrelevant and the renormalization of $g_{1//}$ is stopped. Thus, one obtains field dependent exponents for the response functions, and a field dependent phase diagram.[6] In the low coupling region ($g_{1//} > |g_{1\perp}|$) which is relevant to the $(TMTSF)_2X$ family,[7] it can be shown that dominant singularities are not affected but that SDW as second singularity is favoured by the field. Then, this SDW stabilization is recovered in the more realistic situation of a quasi-1D conductor where 1D chains are weakly coupled by electron transfer $t_\perp$. Below the 3D → 1D crossover temperature T_{co}, transverse coupling between 1D chains decouples the Cooper and zero-sound channels allowing a 3D long range order.[8] Here, diamagnetism is taken into account only in as much as it suppresses superconductivity ($H > H_{c_2}$). Above H_{c_2}, we found an increase of the metal-SDW transition temperature, due to the field effect on the 1D fluctuations. This effect occurs only when $H > T_{co}$. If there is no SDW in zero field, such a phase appears at a threshold field H_T. From this treatment, a (T,P,H) phase diagram has been obtained.[6]

This picture faces two problems. 1) We must explain the moderate value of the transition field (40-60 kG). In $(TMTSF)_2ClO_4$, $t_b \sim 300$ K. $T_{co} \overset{\sim}{\sim} t_b/\pi$ is larger by a factor 20 than the observed value. Bourbonnais argued that this one-electron value t_b/π is reduced to 6-8 K by many-body effects.[9] The field effect on the deviation from Korringa's law recently observed above 10 K in $(TMTSF)_2ClO_4$ could be due to such a field effect.[9] 2) The observed anisotropy of the SDW stability is a more serious difficulty : one cannot understand that $T_{SDW}(H)$ does not seem to depend on the field component along b".[4,5] Although the field effect on the

interactions must be considered in a system with very small $t_\perp$ and can even influence some properties of the $(TMTSF)_2X$ family, it is thus clear that orbital effects and nesting properties must be taken into account. Their importance is clearly demonstrated by the anisotropy of the field effects and by the importance of the anion ordering on the electronic properties.

Therefore we have explored a second approach in which the SDW stability is determined by nesting properties of the Fermi surface.[10] First we propose to explain why a SDW is stable at ambient pressure and low T in the quenched state, while this is not the case in the relaxed state. The essence of our interpretation is to describe anion ordering by an additional Bragg reflection in the transverse direction and to neglect the anion potential when they are disordered. The phase stability is discussed in the mean-field approximation assumed to describe correctly the phase diagram in the 3D regime. Stoner's criterion gives us the condition for SDW formation : $1 - \lambda\chi^\circ(\vec{Q},T) < 0$, where λ is the molecular field constant and $\chi^\circ(\vec{Q},T)$ is the magnetic susceptibility of non interacting electrons, at wave vectors $\vec{Q}$ and temperature T. In the quenched state, departure from perfect nesting (which would be obtained with linear electron dispersion in the longitudinal direction and a tight binding one with transfer integral $t_\perp$ in the transverse direction) is weak. We modelize it by an effective next nearest neighbour transfer integral $t'_\perp$, which in fact originates from the curvature of the longitudinal dispersion relation. The SDW wave vector $\vec{Q}$ is that joining the two inflexion points of the Fermi surface, very close to $(2k_F,\pi/b'',\pi/c'')$, which corresponds to a quasi-1D Kohn singularity in $\chi^\circ(\vec{Q})$. In the relaxed state, the modulation of wave vector $(0,\pi/b'',0)$ doubles the unit cell, inducing new Bragg reflections [11] and opening a gap Δ. Now, the Kohn singularity is quasi-2D and, thus, much weaker, because the Fermi surface curvature radii at the contact point cannot be equal but differ by a term proportional to $(\Delta t'_\perp / t_\perp^2)$: the relaxed

state is much more easily metallic.

Now, we investigate the SDW stability in the relaxed state in the presence of an applied magnetic field H in the c^*-direction. The basic idea is due to Gorkov and Lebed [12]: orbital effects on χ° can improve the nesting and restore the SDW, because the field makes the electron motion more one dimensional. In the following, we show that, by allowing the SDW wave vector to adapt to the field, we obtain a phase diagram accounting more satisfactorily for the experimental data. Assuming a wave vector independent molecular field constant, we look for the best SDW wave vector in the presence of the field, $\vec{Q}(H) = (2k_F + q_x, \pi/b^* + q_y, \pi/c^* + q_z)$. Extending ref. 12 to a general wave vector, we determine $\vec{Q}(H)$ by the condition that χ° is maximum. Using standard notations, we set:

$$\nu = q_x/eHb^* = S(q_x)/S_o \qquad (\hbar = 1) \tag{1}$$

ν is the ratio of the area $S(q_x)$ enclosed between the Fermi surface and itself translated by $\vec{Q}$ to the quantum of momentum space area in the presence of H. χ° is convergent even in the limit $T \to 0$ for any value of ν, except if ν is an integer. In the latter case, the Stoner criterion defines a critical temperature T_n for SDW formation for each integer value of ν. At a given n, q_y is determined by the condition that T_n is maximum. For not too small fields, this corresponds to :

$$\frac{4t_\perp}{v_F} \sin q_y \frac{b^*}{2} \simeq q_x \tag{2}$$

where v_F is the Fermi velocity. The SDW leaves a pocket of unpaired charge carriers. In the presence of H, the section in the (k_x, k_y) plane of this pocket has a quantized area. The condition $\nu = n$ tells us that the pocket involves an integer number of completely filled Landau levels.[10,13] Condition (2) tells us that the best nesting is obtained (approximately for small values of n) when the Fermi surface and itself translated by $\vec{Q}$ are tangent. With increasing H, the degeneracy of the Landau levels increase linearly, and so does $S(q_x)$. q_x and q_y vary while the quantized orbits inflate.

At smaller field, equation (2) is no longer valid. q_x and q_y depend on $t_\perp$, $t'_\perp$ and Δ. The stable value of n, determined by the highest value of $T_n(H)$ depends on H. As H is varied, transitions from a given value of n to a different one are obtained in field ranges in which Δ, $t'_\perp$ and $t_\perp$ are important. Accurate values of the translation fields H_n could be obtained only numerically. The order of magnitude when $\Delta < t'_\perp$ is given by $H_A \sim \frac{4t'_\perp}{ev_F b^{::}} \times \frac{1}{n}$.

Qualitatively, the phase diagram is as follows : at a given H, a 2^{nd} order transition from semimetallic SDW phase to metal is predicted. At a given T, as H increases, we obtain, first, a 2^{nd} order transition from metal to SDW, then a cascade of 1^{st} order transition between different SDW phases. Although the theory is strictly valid for the metal-SDW transition line only, the existence of this cascade is infered from a Landau-Ginzburg expansion, following which, within each phase, the wave vector varies continuously so that the number of unpaired charge carriers is proportional to the field, but is discontinuous at the transition. The description of the low T part of the phase diagram requires a theory of the ordered phases. $\nu = n$ is a quantized relationship valid along the metal-SDW transition line. Although the theory of the low T Hall conductance requires that of the ordered phase this quantization suggests the explanation for the observed Hall conductance plateaux : within a phase, it is quantized according to the values $\sigma_H = (e^2/h)gn$, where g is a degeneracy factor. $\vec{Q}(H)$ can adapt itself to the field variation so that the nesting quantization is preserved. The electron-hole paired states act as a reservoir to fill in completely the Landau levels. Energetically, the diamagnetic energy is minimum when the Landau levels are filled, at the expense of a pairing energy per electron $\sim k_B T_n$ smaller than the diamagnetic energy decrease. Since this mechanism lowers the electron-hole condensation energy and, therefore, T_n, when $\vec{Q}(H)$ departs too much from the best zero-field nesting wave

vector $\vec{Q}_o$, one jumps to a different value of n. Thus, as H is varied, $\vec{Q}(H)$ oscillates around $\vec{Q}_o$. Although the pocket size (and thus the oscillation of $\vec{Q}$ is very small, its quantization is meaningful, even in the presence of disorder, provided the width of the Landau levels is larger than their separation . Given the high Hall mobilities ($\sim 5\ 10^4 cm^2/V.s$)[5], this is realized for fields larger than $\sim$ 5 kG.

Our model also exhibits the possibility of a succession of positive and negative quantized plateaux ; the reason is that in the relaxed state, nesting may produce either electron or hole pocket, depending on the location of the nesting point with respect to the Fermi surface inflexion point provided the samples are very well ordered. [5]

A different SDW wave vector $\vec{Q} \simeq (2k_F + \varepsilon, 0, 0)$ has been proposed.[12] Such a choice leads to a number of electron per unit cell in the SDW state $\sim t_\perp/t_{//}$, where $t_{//}$ is the longitudinal transfer integral, much larger than in our model ($\sim (t_\perp/t_{//})^2$). Contrary to our case, a strong decrease at low T is necessary to account for the experimental number of carriers ($\sim 4\ 10^{-3}$).[5] Moreover, for such a wave vector, the effect of anion ordering on SDW stability [1] and on Hall effect [5] are not simple to understand. On the other hand, we are not able, at present time, to explain in our picture the "Shubnikov-de Haas" like structures observed in the magnetoresistance at higher temperature.[4,14] These might be due to fluctuation effects.

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