Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

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Version of record first published: 17 Oct 2011.

Mol. Cryst. Liq. Cryst. 1985, Vol. 119, pp. 11-18
0026-8941/85/1194-0011/$15.00/0

Printed in the United States of America

THE DIMENSIONALITY CROSSOVER IN QUASI-1D CONDUCTORS

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ABSTRACT A fermion path integral formalism is used for the study of one-dimensional (1D) gapless of Tomanaga-Luttinger (T-L) like electron gas models with interchain hopping. Scaling arguments and exact T-L1D results show that the one-particle crossover temperature T_x is smaller than its free-electron gas value. Renormalized properties at T_x and applications to $(TMTSF)_2X$ compounds are discussed.

I- INTRODUCTION

A problem of interest in the study of interchain coupling[1] in quasi 1D conductors is the calculation of the dimensionality crossover temperature T_x for the electronic correlations. When applied to real organic conductors, this is of major importance whenever we are tempted to interpreted the observed properties in terms of 1D effects. In this paper, we propose a description of the influence of single electron interchain hopping on intrachain collective effect and finally we correlate the results with observed properties of organic compounds.

For the 1D problem, we will focus our attention on a repulsive backward scattering between electrons namely $g_1 \geq 0$, a forward scattering g_2 with arbitrary sign, and a weak umklapp scattering g_3 ($g_1 - 2g_2 > 1$). Multiplicative renormalization group arguments[2] (MRG) tell us that this model scales into the 1D Tomonaga-Luttinger (T-L) problem for which an exact treatment is available[3]. The T-L like models have been of particular interest for application to $(TMTSF)_2X$ compounds[4], since they do not show any gaps in the charge or spin degrees of freedom[5]. As it is well known, this is a direct consequence of the interference between the electron hole (zero-sound) and pairing (Cooper) channels both divergent in 1D[2]. This property contrast with the 3D case (isotropic) where only the Cooper channel is logarithmically divergent and where a negative value of $g_2 \pm g_1$ gives a pole in the ladder summation. Collective effects exist however in 1D and can induce power law singularities in the correlation functions of both channels. The one-particle density of state at the Fermi level has a power law decay with a non-

Invited paper of the International Conference on the Physics and Chemistry of Low-dimensional Synthetic Metals, (ICSM) Abano Terme Italy (1984).

universal exponent α (pseudo-gap)[3,6]. Consequently, when we include the effect of small interchain transfer of single electron, the transverse coherent motion which tends to decouple the two channels of correlations will be less effective. This leads to a decrease of T_x compared to its value in the non-interacting case. In this work, we analyse the renormalization of the electronic spectrum and couplings by making use of standard crossover arguments[7] and exact 1D results for the T-L model. We find the expression for T_x in terms of its symmetry breaking field $t_\perp$ ($T_x \sim t_\perp^{1/\phi}$) through the crossover exponent $\phi = 1 - \alpha$. The non-universality features of ϕ, the value of renormalized lengths scale, energies and couplings at T_x are analyzed and compared to the observed properties $(TMTSF)_2X$ compounds.

II- PARTITION FUNCTION

The Hamiltonian of a linear array of T-L metallic chains with interchain hopping is given by:

$$H = \sum_{K q_\perp} \sum_{\rho\sigma} \left[v_F \rho K - 2 t_\perp(q_\perp) \right] a^+_{\rho\sigma}(K, q_\perp)\, a_{\rho\sigma}(K, q_\perp) + \frac{g_2}{L} \sum_{\{K, q_\perp, \sigma\}_\rho} \delta_{1+2=3+4}\, a^+_{\rho\sigma_1}(K_1, q_{\perp 1})\, a^+_{-\rho\sigma_2}(2)\, a_{\rho\sigma_1}(3)\, a_{-\rho\sigma_2}(4), \quad (1)$$

where $a^{(+)}_{\rho\sigma}$ is the annihilation (creation) operator for electrons around the Fermi wave vector $\pm K_F(\rho = \pm)$. K is the longitudinal wave vector measured from K_F in the linear approximation. σ is the spin index and $E_F = v_F K_F$ is Fermi energy. $t(q_\perp)$ stands for the Fourier transform of the band structure in the transverse direction. In the tight binding approach, $t_\perp(q_\perp) = t_\perp \cos q_\perp d_\perp$ with $d_\perp$ as the interchain distance and $q_\perp$ for the perpendicular wave vector. g_2 is the forward scattering in the g-ology formulation of the T-L model. The partition function $Z = Tr\{e^{-\beta H}\}$ can be put in a fermion functional integral form[8]:

$$Z = \int\int \mathcal{D}\psi^* \mathcal{D}\psi\, e^{S[\psi^*, \psi]}, \quad (2)$$

where the integral is made over Grassman field variables ψ with anti-commuting properties $\{\psi^*, \psi\} = \{\psi^{(*)}, \psi^{(*)}\} = 0$, $\psi^2 = 0$. S is the action functional taken in the Euclidian space. Its Fourier transform is given by:

$$S[\psi^*, \psi] = \sum_{\tilde{q}, \rho\sigma} \mathcal{G}^{(0)-1}_{\rho\sigma}(\tilde{q})\, \psi^*_{\rho\sigma}(\tilde{q})\, \psi_{\rho\sigma}(\tilde{q}) + \frac{T g_2 \Gamma_\perp^0}{N_\perp L} \sum_{\{\tilde{q}, \sigma\}_\rho} \delta_{1+2=3+4}\, \psi^*_{\rho\sigma_1}(\tilde{q}_1)\, \psi^*_{-\rho\sigma_2}(\tilde{q}_2)\, \psi_{\rho\sigma_1}(\tilde{q}_3)\, \psi_{\rho\sigma_2}(\tilde{q}_4), \quad (3)$$

where $\tilde{q} = (\omega_m, K, q_\perp)$, $\mathcal{G}^{(0)} = \left[\mathcal{G}^{(0)-1}_{\rho\sigma,1D} + 2 t_\perp(q_\perp)\right]^{-1}$ and $\mathcal{G}^{(0)}_{\rho\sigma,1D} = (i\omega_m - v_F \rho K)^{-1}$

are the 2D and the 1D bare propagators of the system. The $\omega_m = (2m+1)\pi T$ are the Matsubara frequencies for fermions. Here, quasi-one-dimensionality is characterized by the anisotropy ratio $t_\perp/E_F \ll 1$ between transverse and longitudinal band energy. Therefore $t_\perp$ can be treated as a perturbation. The two quantities g^0 and the forward scattering vertex Γ_2 or the coupling g_2 ($\Gamma_2^0 = 1$) parametrize the action S in the same way classical field functional do for standard theory of critical phenomena[9,7]. However, here the fields ψ reflect fermion degrees of freedom which are quite relevant for correlations whenever the system has no strong coupling regime or gaps. Perturbation theory of vertex, single-particle and pair correlation functions of the ψ's is the same as for the original Hamiltonian representation and presents the logarithmic divergencies in both channels of correlations[2]. This indicates scaling features for the partition function.

III- KADANOFF HYPOTHESIS

The presence of logarithms in the 1D perturbation theory indicates clearly that fluctuations at different energy (or length scale smaller than ξ) give the same contribution and can therefore be simply connected by a change of scale[9]. According to the Kadanoff hypothesis,[10] this means that the integration of small length or high energy scale fluctuations of the ψ field will not change the form of S except for a possible renormalization of various couplings and for an additive constant which can be ignored for the present discussion. As usual, this renormalization procedure can be put as a partial trace of Z [9,10].

$$Z = \int\int [\mathcal{D}\psi^* \mathcal{D}\psi]' \int\int [\mathcal{D}\psi^* \mathcal{D}\psi]'' e^{S} = \int\int [\mathcal{D}\psi^* \mathcal{D}\psi]' e^{S'} \quad (4)$$

$[\mathcal{D}\psi^* \mathcal{D}\psi]'' = \prod_{E' < E \leq W_{\parallel}} d\psi^* d\psi$ gives the energy range for the integration of the ψ degrees of freedom whereas $[\mathcal{D}\psi^* \mathcal{D}\psi]'$ is the remaining part ($E \leq E'$) . Here $W_{\parallel} = 4t_{\parallel}$ is the longitudinal bandwidth cut-off which makes the theory free from ultraviolet divergences. Its physical meaning in real space corresponds to the shortest distance $\Lambda_0 = \frac{2\pi V_F}{W_{\parallel}}$ for electrons-electrons and electrons-holes correlations. One must note that in the quasi-1D problem at hand, there is also another natural cut-off given by the transverse bandwidth $W_\perp = 4t_\perp$ which gives the characteristic energy for transverse coherent hopping. S' is the effective action functional with renormalized values of $g^{(0)}$ and Γ_2 (or g_2) and scaled cut-off energy[9,10] E'.

For the first renormalization where $E' \leq]W_\perp, W_{\parallel}]$, we decrease the magnification of fermions correlations for both channels in the parallel direction. In this range, $|V_F K| > |2t_\perp(q_\perp)|$ and

the scaling hypothesis for anisotropic systems tells us that $t_\perp$ can be neglected[7]. Consequently the renormalization of S to S'[9,10] must have a purely 1D character:

$$g_{\rho\sigma}^{(a)-1} \longrightarrow g_{\rho\sigma}^{(a)-1)} = Z_1 g_{\rho\sigma 1D}^{(a)-1} + 2t_\perp(q_\perp) \tag{5.a}$$

$$\Gamma_2 \longrightarrow \Gamma_2' = Z_2 \Gamma_2 \tag{5.b}$$

$$g_2 \longrightarrow g_2' = (Z_2 Z_1^{-2}) g_2 \,. \tag{5.c}$$

According to the standard theory of renormalization[9], the Z_i factors do not depend on $\tilde{q}$ but only on the integrated degrees of freedom ratio $E'/W_\parallel$ and the coupling g_2. It is worth mentioning that for $t_\perp = 0$, this result is equivalent to the Menyhard and Solyom HRG approach of the 1D electron gas model[2]. However, from (4) Z_1 is considered here as invariant under the Kadanoff transformation whereas in the Menyhard and Solyom approach, it is the Dyson equation which is taken as scale invariant[2]. From (5.a) anisotropy is increased in the 1D regime since $Z_1 > 1$. The explicit form of Z_1 can be extracted from the exact T-L solution[3,6]:

$$Z_1 = C\left(E'/W_\parallel\right)^{-\alpha}, \tag{6}$$

with $\alpha = \frac{1}{2}\left\{\left[\frac{2\pi v_F + g_2}{2\pi v_F - g_2}\right]^{1/2} + \left[\frac{2\pi v_F - g_2}{2\pi v_F + g_2}\right]^{1/2} - 2\right\}$ and C is a constant. $\left(E'/W_\parallel\right)^{\alpha}$ is of the order of the decrease of the density of states at the Fermi level at $T = E'$ due to 1D collective **effects**[6]. This lowers the number of quasi-particles which can participate to the transverse notion. Hence, one dimensionality is effectively increased.

In the quasi-1D range of the RG where $E' \leq]T_x, W_\perp]$, the corrections to S are still 1D but interchain single electron transfer becomes relevant in addition to the one in the parallel direction. Therefore, correlations in the transverse direction have also to be integrated. But as long as the scale energy E' is greater than T_x, we get the same transformations (5) for $S \rightarrow S'$. However, due to the transverse coarse graining, the transverse cut-off wave vector $q_\perp^0 = \pi/d_\perp$ scales to $q_\perp^{0\prime} = \pi/d_\perp'$ where $d_\perp'$ is the effective interchain distance or the transverse Kadanoff block size:

$$d_\perp' = d_\perp\left[\frac{2}{\pi}\,\mathrm{ARC\,Cos}\left(-\frac{E'}{W_\perp}\right) - 1\right]^{-1},$$
$$d_\perp' \simeq \frac{W_\perp}{E'} d_\perp + \ldots\ldots \quad (E'/W_\perp \ll 1). \tag{7}$$

T_x is determined by the renormalized condition for crossover which reads[7]:

$$2Z_1 MAX(\varepsilon_{//}(K)) \approx - MAX(2t_\perp(q_\perp)), \tag{8}$$

where $MAX(\varepsilon_{//}(K)) = v_F K_{MAX}$ and $MAX(2t_\perp(q_\perp)) = -2t_\perp \cos q_{\perp MAX} d'_\perp = 2t_\perp$. $K_{MAX} = \frac{\pi}{\xi_{//}}$ and $q_{\perp MAX} = \frac{\pi}{\xi_\perp}$ with $\xi_{//} \sim \frac{v_F}{T_x}$ and $\xi_\perp = d'_\perp$ as the longitudinal and tranverse coherence lengths at T_x for fermions field ψ. With the aid of the exact T-L result (6) for Z_1 and eq. (8) we get for T_x:

$$T_x \approx T_x^0 \left(\frac{t_\perp}{E_F} \right)^{\frac{\alpha}{1-\alpha}} \tag{9}$$

where $T_x^0 = t_\perp/\pi$ is the crossover temperature for a free quasi-1D electron gas[4,11]. The symmetry breaking field ($t_\perp$) dependence of $T_x \sim t_\perp^{\phi}$ gives the crossover exponent $\phi = 1-\alpha$. ϕ is non-universal since α depends on the bare interaction g_2. It follows from (9) that a strong anisotropy $t_\perp/E_F \ll 1$ and sizeable coupling (α) are the necessary ingredients to lower the single particle crossover temperature.

Few remarks are in order. i) In the above procedure of renormalization we have neglected the effect of supplementary terms generated by the partial trace operation (Eq.4). We can show by a rescaling argument[9] that all these new terms (three-body interaction, interchain tunneling of two particles etc...) are not relevant in the RG sense and can therefore be ignored. ii) For $g_2/2\pi v_F \ll 1$, $\phi \simeq 1 - (g_2/2\pi v_F)^2 + \ldots$ and this is compatible with the previous perturbative result of Schuster[11] and its second order multiplicative RG extension made by Progodin and Firsov[12]. However, these treatments are valid only for very small couplings ($\alpha \ll 1$). Moreover, they neglect the partial trace of the transverse degrees of freedom for $E's$ $]T_x, W_\perp]$ and this "freezes" unphysically the growth of $\xi_\perp$ in this range of energy (temperature). From the renormalization transformations (5), the Green function at T_x is given by $g_0 = Z_1^{-1}(T_x)[i\omega_m - \varepsilon_{//}(q) + 2Z_1^{-1}(T_x) t_\perp(q_\perp)]^{-1}$ and $4Z_1^{-1}(T_x)t_\perp$ play the role of an effective bandwidth[12] in the transverse direction. iii) From (5), the 1D corrections to the vertex and the coupling stop also at T_x. Indeed, one can check by using the pertubative results of refs. 10 and 12 that if the zero sound bubble and the self energy graphs of figure 1 are calculated with the renormalized Green function (5-a) and vertex (5-b) their logarithmic divergences at $E \lessgtr E'$ stop precisely at T_x, indicating a split-off of the two channels of correlations at that temperature. So, even if the crossover criteria given in (8) does not make any explicit reference to the 1D zero sound divergence

at $2K_f$ which enter in all relevant quantities, it appears to be fully consistent with its analytic properties as a function of $t_\perp$.

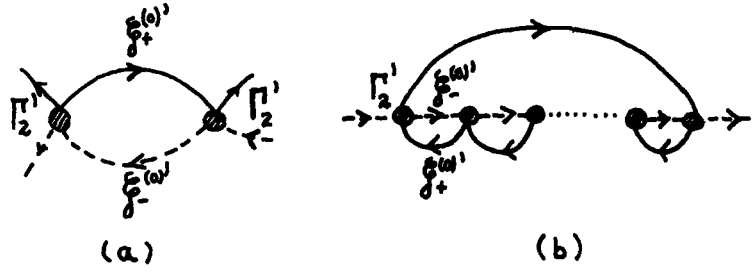

FIGURE 1 Renormalized pertubation theory for E<E'. The 1D2K_f zero sound bubble graph (a) and the one-particle self-energy graph (b) stop theirs logarithmic divergences at T_x.

One can generalize the above results for the cases where the transverse spatial dimension $D_\perp$ is greater than 1. For a 2D lattice of chains with the nearest neighbor interaction $t_\perp$ taken as uniform an extra factor of 2 appears in the formula for T_x and ϕ becomes the 1D→3D crossover exponent. One can show rigorously that the results for T_x and ϕ are also exact for a complete lattice of chains ($D_\perp \to \infty$) with a fixed transverse bandwidth[14]. The extension to a more general choice of 1D couplings is also straightforward. In fact, MRG calculations for 1D electron gas model[2] with $g_1 \neq 0$, g_2 and g_3 ($g_1 - 2g_2 > |g_3|$) show unambigously the absence of gaps and scaling to T-L like behavior as $T \to 0$[2]. In absence of gaps, Z_1^{-1} have also the form given in (6)[2]. The exact expressions of α is not known so far. Usually one can take T-L expression of g_i's with the fixed point (T=0) values of the couplings: $g_1^* \approx g_3^* \approx 0$ and $g_2^* \approx [(g_1/2 - g_2)^2 - g_3^2]^{1/2}$. In any case, if the couplings remain weak ($g_i < W_{11}$), we can safely assume that $0 < \alpha < 1$ for T_x. This gapless model has been extensively studied in connection to the observed properties of $(TMTSF)_2X$ family of organic superconductors[4,5] and this deserves to be further analyzed in the context of the present work.

IV- APPLICATION TO $(TMTSF)_2X$ COMPOUNDS

Evidence for important Coulomb interactions and gapless metallic phase in $(TMTSF)_2X$ compounds have justified[4] the interest given to the T-L models. A gapless metallic phase also suggests that the transverse electron hopping can be an important mechanism for the interchain coupling[4]. Quasi-one-dimensionality in these compounds is usually found[5] to be given by the band anisotropy ratio

$t_\perp/E_F \approx 1/10 \ldots\ldots 1/30$ with $t_\perp \approx 100 \ldots\ldots 300\,K$.
According to the above results, T_x can be strongly reduced from its bare value $T_x^o \approx 30 \ldots\ldots 80\,K$ if the value of α becomes appreciable. Unfortunately, the precise values of α for all compounds are difficult to predict microscopically. However, it is universally admitted that the couplings are not too strong ($g_i < W_{||}$) but not too small either[4], so that α can take any sizeable values within the range $0 < \alpha < 1$. In absence of a rigourous determination of α and consequently of T_x for each compound, one must pay attention to experiments which can exhibit low dimensional features in the range $T < T_x^o$, in order to established or not a decrease of T_x. Recent NMR experiments [15,16] made on the $(TMTSF)_2CLO_4$ metallic phase have effectively revealed an important enhancement of the nuclear relaxation rate T_1^{-1} for $T < 25\,K$ followed by its sudden saturation at $T \approx 8\,K$ [16]. It has been shown[16] that such an enhancement of T_1^{-1} can be predicted from a T-L electron gas model ($g_1 > 0$) and the effect of $t_\perp$ was to stop the enhancement precisely at T_x. Therefore, these data indicate the presence of 1D cooperative phenomena for $T \ll T_x^o$ and strongly suggest the value $T_x \approx 8\,K$ for the perchlorate compound. From the above expression of T_x, this would imply $\alpha = 1/4 \ldots\ldots 1/2$ that is, an appreciable drop of the density of states at the Fermi level due to collective effects and this must be put together with the similar interpretations given in the context of the tunneling [17.a], infrared [17.b] and heat conductivity [17.c] experiments.

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