Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

From Two Coupled Chains to Quasi-One-Dimensional Organic Conductors

Hideo Yoshioka [a] & Yoshikazu Suzumura [a]
[a] Department of Physics, Nagoya University, Nagoya, 464-01, Japan

Version of record first published: 24 Sep 2006.

To cite this article: Hideo Yoshioka & Yoshikazu Suzumura (1996): From Two Coupled Chains to Quasi-One-Dimensional Organic Conductors, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 285:1, 229-234

To link to this article: http://dx.doi.org/10.1080/10587259608030806

Mol. Cryst. Liq. Cryst., 1996, Vol. 285, pp. 229–234
Reprints available directly from the publisher
Photocopying permitted by license only

FROM TWO COUPLED CHAINS TO QUASI-ONE-DIMENSIONAL ORGANIC CONDUCTORS

HIDEO YOSHIOKA and YOSHIKAZU SUZUMURA
Department of Physics, Nagoya University, Nagoya 464-01, Japan

Abstract Electronic states of two coupled chains of interacting electron systems are investigated by means of phase Hamiltonian, and phase transition of quasi-one-dimensional organic conductors are discussed from the point of view of the two chains.

INTRODUCTION

Charge transfer salts which consist of two TMTSF electron donors and a monovalent anion such as PF_6^-, AsF_6^-, ClO_4^- and so on, are known to be typical quasi-one-dimensional (quasi-1D) electron systems. The salts show various phase transition characteristic in low dimension.[1] For example, $(TMTSF)_2PF_6$ exhibits metallic behavior down to about 20K, below which the salt undergoes metal-insulator (M-I) transition to an insulator of spin density wave (SDW) state in ambient pressure. By applying the pressure, critical temperature of the M-I transition decreases and superconducting (SC) phase appears at the critical temperature of 0.9K for 12 kbar.[2] It has been considered that the competition of the SDW state and the SC state results from the fact that the nesting condition originated from quasi-1D band structure is essential to formation of the SDW state but not of the SC state.

Two chains of interacting electron systems coupled by interchain hopping are basic models of the above quasi-1D conductors. In order to understand the various phase transition in the conductors, we investigate two kinds of models of the two chains by use of phase Hamiltonian based on bosonization method. The first one is the model with both the intrachain and interchain forward scattering (MODEL I),[3] and the second one consists of the intrachain forward scattering and the intrachain backward scattering (MODEL II).[4] Recently, it has been reported that the ground state of the two chains of electron systems with repulsive intrachain interaction is given by SC state with interchain and in phase pairing in the case of the weak interaction.[5, 6, 7, 8, 9] However, this result seems to be inconsistent with the phase diagram of the above quasi-1D system. It is because the low pressure leads to the

SDW state due to the good nesting condition, while the two chains show the SC state in spite of the condition of the perfect nesting. We give an answer to such a problem by use of the renormalization group approach, and understand the phase transition of the quasi-1D systems from the point of view of the two coupled chains.

MODEL I

We first diagonalize the kinetic terms in the Hamiltonian in order to take account of the deviation of the fermi wavenumber due to the interchain hopping. Next we apply Abelian bosonization method to the electronic states near the new fermi points and express the Hamiltonian in terms of the phase variables. Thus the Hamiltonian, $\mathcal{H} = \mathcal{H}_T + \mathcal{H}_R$, is represented as follows,[3]

$$\mathcal{H}_T = \frac{v_\rho}{4\pi}\int \mathrm{d}x \left\{\frac{1}{\eta_\rho}(\partial_x\theta_+)^2 + \eta_\rho(\partial_x\theta_-)^2\right\} + \frac{v_F}{4\pi}\int \mathrm{d}x \left\{(\partial_x\phi_+)^2 + (\partial_x\phi_-)^2\right\}, \quad (1)$$

$$\begin{aligned}\mathcal{H}_R &= \frac{v_F}{4\pi}\int \mathrm{d}x \left\{(\partial_x\tilde{\theta}_+)^2 + (\partial_x\tilde{\theta}_-)^2 + (\partial_x\tilde{\phi}_+)^2 + (\partial_x\tilde{\phi}_-)^2\right\} \\ &+ \frac{v_F(g_2 - g_2')}{\pi\alpha^2}\int \mathrm{d}x \left\{\cos\sqrt{2}\tilde{\theta}_- - \cos(2q_0x - \sqrt{2}\tilde{\theta}_+)\right\} \\ &\qquad \times \left\{\cos\sqrt{2}\tilde{\phi}_- + \cos\sqrt{2}\tilde{\phi}_+\right\}, \end{aligned} \quad (2)$$

where $v_\rho = v_F\sqrt{(1+2g_2+2g_2')(1-2g_2-2g_2')}$, $\eta_\rho = \sqrt{(1-2g_2-2g_2')/(1+2g_2+2g_2')}$ and $q_0 = 2t/v_F$. Here v_F, α^{-1} and t are the fermi velocity, the upper cutoff of the wavenumber and the interchain hopping, respectively, and g_2 (g_2') is a normalized matrix element of the intrachain (interchain) forward scattering between oppositely moving electrons. The phases, $\theta_\pm$ and $\phi_\pm$, describe the fluctuations of the total charge and the total spin, respectively, while $\tilde{\theta}_\pm$ and $\tilde{\phi}_\pm$ express the transverse fluctuations of the charge and the spin degrees of freedom. Therefore $\mathcal{H}_T$ with gapless excitations expresses the total charge and spin fluctuations, and $\mathcal{H}_R$ including complex nonlinear terms represents the transverse charge and spin fluctuations.

According to Finkel'stein and Larkin,[10] the Hamiltonian $\mathcal{H}_R$ has a fixed point of the strong coupling and then the nonlinear terms, which do not include the misfit parameter, grow. In this case, the treatment of the mean field (MF) for $\mathcal{H}_R$ is useful. We express $\mathcal{H}_R$ in terms of the new fermion fields, $\bar{\psi}_i$ ($i = 1 \sim 4$),[3] and utilize the MF method. Then $\mathcal{H}_R$ is expressed as follows,

$$\begin{aligned}\mathcal{H}_R &= v_F\int \mathrm{d}x \left\{\bar{\psi}_1^\dagger(-\mathrm{i}\partial_x)\bar{\psi}_1 - \bar{\psi}_2^\dagger(-\mathrm{i}\partial_x)\bar{\psi}_2 + \bar{\psi}_3^\dagger(-\mathrm{i}\partial_x)\bar{\psi}_3 - \bar{\psi}_4^\dagger(-\mathrm{i}\partial_x)\bar{\psi}_4\right\} \\ &+ \pi v_F(g_2 - g_2')\int \mathrm{d}x \left\{\mathrm{i}\bar{\psi}_3^\dagger\bar{\psi}_4^\dagger - \mathrm{i}\bar{\psi}_4\bar{\psi}_3 - \bar{\psi}_4^\dagger\bar{\psi}_3\mathrm{e}^{-\mathrm{i}2q_0x} - \bar{\psi}_3^\dagger\bar{\psi}_4\mathrm{e}^{\mathrm{i}2q_0x}\right\} \\ &\qquad \times \left\{\mathrm{i}\bar{\psi}_1^\dagger\bar{\psi}_2^\dagger - \mathrm{i}\bar{\psi}_2\bar{\psi}_1 + \bar{\psi}_2^\dagger\bar{\psi}_1 + \bar{\psi}_1^\dagger\bar{\psi}_2\right\}, \end{aligned} \quad (3)$$

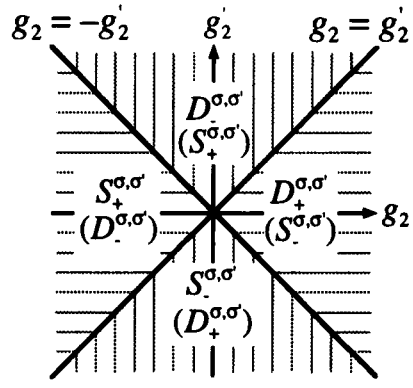

FIGURE 1 Phase diagram on the plain of g_2 and g_2' which shows the most dominant state (the subdominant state in the parenthesis).

$$
\begin{aligned}
\rightarrow \mathcal{H}_R^{MF} &\equiv v_F \int \mathrm{d}x \left\{ \bar{\psi}_1^\dagger (-\mathrm{i}\partial_x) \bar{\psi}_1 - \bar{\psi}_2^\dagger (-\mathrm{i}\partial_x) \bar{\psi}_2 \right\} \\
&+ \frac{\Delta}{2} \int \mathrm{d}x \left\{ \mathrm{i} \bar{\psi}_1^\dagger \bar{\psi}_2^\dagger - \mathrm{i} \bar{\psi}_2 \bar{\psi}_1 + \bar{\psi}_2^\dagger \bar{\psi}_1 + \bar{\psi}_1^\dagger \bar{\psi}_2 \right\} \\
&+ v_F \int \mathrm{d}x \left\{ \bar{\psi}_3^\dagger (-\mathrm{i}\partial_x) \bar{\psi}_3 - \bar{\psi}_4^\dagger (-\mathrm{i}\partial_x) \bar{\psi}_4 \right\} + \Delta' \int \mathrm{d}x \left\{ \mathrm{i} \bar{\psi}_3^\dagger \bar{\psi}_4^\dagger - \mathrm{i} \bar{\psi}_4 \bar{\psi}_3 \right\} \\
&- \frac{\Delta \Delta' L}{2\pi v_F (g_2 - g_2')},
\end{aligned} \tag{4}
$$

where $g_2 \neq g_2'$ and the gaps, Δ and Δ' are self-consistently determined by,

$$
\frac{\Delta}{2} = \pi v_F (g_2 - g_2') \left\{ \mathrm{i} \left\langle \bar{\psi}_3^\dagger \bar{\psi}_4^\dagger \right\rangle - \mathrm{i} \left\langle \bar{\psi}_4 \bar{\psi}_3 \right\rangle \right\}, \tag{5}
$$

$$
\Delta' = \pi v_F (g_2 - g_2') \left\{ \mathrm{i} \left\langle \bar{\psi}_1^\dagger \bar{\psi}_2^\dagger \right\rangle - \mathrm{i} \left\langle \bar{\psi}_2 \bar{\psi}_1 \right\rangle + \left\langle \bar{\psi}_2^\dagger \bar{\psi}_1 \right\rangle + \left\langle \bar{\psi}_1^\dagger \bar{\psi}_2 \right\rangle \right\}. \tag{6}
$$

We calculate correlation functions by using $\mathcal{H}_T$ and $\mathcal{H}_R^{MF}$, and obtain the phase diagram on the plain of g_2 and g_2' shown in Figure 1. In Figure 1, $D_\pm^{\sigma,\sigma'}$ and $S_\pm^{\sigma,\sigma'}$ express the density wave (DW) state with out of phase ordering and the SC state with in phase pairing, respectively, where + (−) denotes intrachain (interchain) ordering. Here σ and σ' express spin indices. In the present case, the state of SDW and charge density wave (singlet superconductivity and triplet superconductivity) are degenerate in the sense that the correlation functions have the same powers. The fact is due to the symmetry between ϕ_+ and ϕ_- in Equation (1) and that between $\tilde{\phi}_+$ and $\tilde{\phi}_-$ in Equation (2). It is noted that, in the repulsive region of $g_2 > |g_2'|$, the SC state remains subdominant though the most dominant state is the DW state.

MODEL II

As is seen in the previous section, the competition between the SDW state and the SC state is not observed in the presence of only the forward scattering. Now

we investigate the competition by taking account of the backward scattering. We consider the case of only the repulsive intrachain interaction.

The interchain hopping leads to two kinds of energy regions, i.e., the high energy region where the excitations are essentially the same as those in the absence of the hopping and the low energy region where the hopping plays an essential role. By applying the renormalization procedure of 1D systems to the high energy region, the effective Hamiltonian available for the low energy region is calculated as,[8, 4]

$$\begin{aligned}
\mathcal{H} &= \frac{v_\theta}{4\pi}\int \mathrm{d}x \left\{\frac{1}{\eta_\theta}(\partial_x\theta_+)^2 + \eta_\theta(\partial_x\theta_-)^2\right\} + \frac{v_\phi}{4\pi}\int \mathrm{d}x \left\{\frac{1}{\eta_\phi}(\partial_x\phi_+)^2 + \eta_\phi(\partial_x\phi_-)^2\right\} \\
&+ \frac{v_F}{4\pi}\int \mathrm{d}x \left\{\frac{1}{\eta_{\tilde\theta}}(\partial_x\tilde\theta_+)^2 + \eta_{\tilde\theta}(\partial_x\tilde\theta_-)^2\right\} + \frac{v_F}{4\pi}\int \mathrm{d}x \left\{\frac{1}{\eta_{\tilde\phi}}(\partial_x\tilde\phi_+)^2 + \eta_{\tilde\phi}(\partial_x\tilde\phi_-)^2\right\} \\
&+ \frac{v_F}{\pi\alpha'^2}g_-\int \mathrm{d}x \cos\sqrt{2}\tilde\theta_- \cos\sqrt{2}\tilde\phi_- + \frac{v_F}{\pi\alpha'^2}g_+\int \mathrm{d}x \cos\sqrt{2}\tilde\theta_- \cos\sqrt{2}\tilde\phi_+ \\
&+ \frac{v_F}{\pi\alpha'^2}g_a^*\int \mathrm{d}x \cos\sqrt{2}\phi_+ \cos\sqrt{2}\tilde\phi_+ + \frac{v_F}{\pi\alpha'^2}g_b^*\int \mathrm{d}x \cos\sqrt{2}\phi_+ \cos\sqrt{2}\tilde\phi_- \\
&- \frac{v_F}{\pi\alpha'^2}g_c^*\int \mathrm{d}x \cos\sqrt{2}\phi_+ \cos\sqrt{2}\tilde\theta_-, \qquad (7)
\end{aligned}$$

where $\alpha' \sim v_F/t > \alpha$, $v_\theta = v_F\sqrt{(1+2g_2-g_1)(1-2g_2+g_1)}$, $v_\phi = v_F\sqrt{(1-g_1^*)(1+g_1^*)}$, $\eta_\theta = \sqrt{(1-2g_2+g_1)/(1+2g_2-g_1)}$, $\eta_\phi = \sqrt{(1+g_1^*)/(1-g_1^*)} > 1$, $\eta_{\tilde\theta} = \eta_{\tilde\phi} = 1$, $g_\pm = g_2 - g_1/2 \pm g_1^*/2$, $g_a^* = g_b^* = g_c^* = g_1^*$. Here g_1 is a matrix element of the backward scattering and g_1^* is a renormalized one given by $g_1/\{1+2g_1\log(v_F/t\alpha)\} \equiv g_1^*$.[11] In the present Hamiltonian, the symmetry of spin degrees of freedom are broken due to the renormalized backward scattering which vanishes in the limit of $t \to 0$. We consider the case of $2g_2 > g_1$ and then $\eta_\theta < 1$.

Properties at temperatures lower than the hopping energy are examined by applying the renormalization group method to Equation (7). The equations of the renormalization group are given as,[4]

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\eta_{\tilde\theta} = \frac{1}{4}(g_-^2 + g_+^2 + g_c^{*2}), \qquad (8)$$

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\eta_{\tilde\phi} = \frac{1}{4}(g_-^2 - g_+^2\eta_{\tilde\phi}^2 - g_a^{*2}\eta_{\tilde\phi}^2 + g_b^{*2}), \qquad (9)$$

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\eta_\phi = -\frac{\eta_\phi^2}{4}(g_a^{*2} + g_b^{*2} + g_c^{*2}), \qquad (10)$$

$$\frac{\mathrm{d}}{\mathrm{d}\ell}g_- = (2 - \frac{1}{\eta_{\tilde\theta}} - \frac{1}{\eta_{\tilde\phi}})g_-, \qquad (11)$$

$$\frac{\mathrm{d}}{\mathrm{d}\ell}g_+ = (2 - \frac{1}{\eta_{\tilde\theta}} - \eta_{\tilde\phi})g_+, \qquad (12)$$

$$\frac{\mathrm{d}}{\mathrm{d}\ell}g_a^* = (2 - \eta_\phi - \eta_{\tilde\phi})g_a^*, \qquad (13)$$

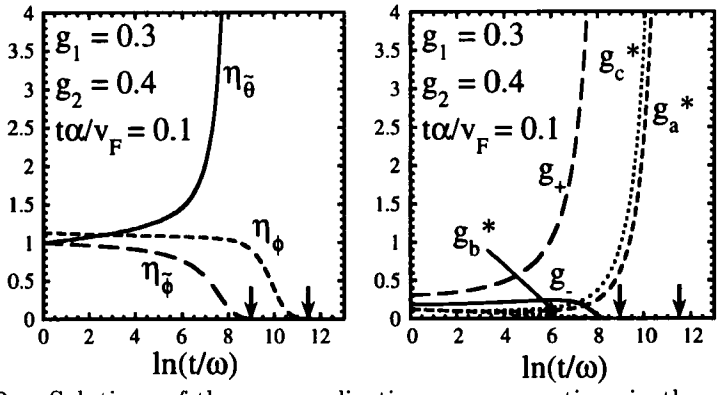

FIGURE 2 Solutions of the renormalization group equations in the case of $g_1 = 0.3$, $g_2 = 0.4$ and $t\alpha/v_F = 0.1$. Here the thick arrow denotes the boundary between the regions I and III (III and II).

$$\frac{\mathrm{d}}{\mathrm{d}\ell} g_b^* = (2 - \eta_\phi - \frac{1}{\eta_{\tilde{\phi}}}) g_b^*, \tag{14}$$

$$\frac{\mathrm{d}}{\mathrm{d}\ell} g_c^* = (2 - \eta_\phi - \frac{1}{\eta_{\tilde{\theta}}}) g_c^*, \tag{15}$$

where $\ell \equiv \ln(t/\omega)$ with ω being the scaling energy. We numerically solve the above equations. The result for $g_1 = 0.3$, $g_2 = 0.4$ and $t\alpha/v_F = 0.1$ is shown in Figure 2.

There are three kinds of regions lower than t, i.e., $t > \omega > \omega_1$ (I), $\omega_1 > \omega > \omega_2$ (III) and $\omega_2 > \omega$ (II), where the locations corresponding to $\ln(t/\omega_1) \simeq 9$ and $\ln(t/\omega_2) \simeq 11.5$ are shown by the thick arrows. In the region I, $\eta_{\tilde{\theta}}$ increases and $\eta_{\tilde{\phi}}$ decreases since g_+ (g_-) tends to the strong (weak) coupling. On the other hand, variations of the nonlinear terms including ϕ_+ and η_ϕ are negligible. In the region III, the gaps for the transverse fluctuations of both charge and spin degrees of freedom appears owing to the relevant g_+. In this region, the variables $\tilde{\theta}_-$ and $\tilde{\phi}_+$ show the relevance and the transverse spin density wave (TSDW) state and the singlet superconducting (SS) state are selected. Since the exponent of the correlation function for the TSDW (SS) state is given by $(\eta_\theta + \eta_\phi^{-1})/2$ ($(\eta_\theta^{-1} + \eta_\phi)/2$) and η_ϕ decreases to zero, the TSDW (SS) state becomes the most dominant and the SS (TSDW) state is subdominant for ω near ω_1 (ω_2). Thus a crossover from the TSDW state to the SS state is seen in the region III. In the region II, the gap of the total spin fluctuation also appears in addition to the above transverse degrees of freedom and the SS state is the most dominant,[5, 6, 7, 8, 9] while the correlation function of the TSDW decays exponentially.

The existence of the region III is essential to relating the result of the two chains with the phase diagram of the quasi-1D conductors as a function of temperature and

pressure. When three-dimensional coupling is taken into account, the crossover from the TSDW state to the SS state in the region III of Figure 2 becomes the actual phase transition. The crossover with fixed ω and increasing t indicates the transition from the SDW state to the SS state with fixed T and increasing pressure in the phase diagram of the quasi-1D organic conductors since the pressure has an effect of increasing t. The present crossover from the SDW state to the SC state is purely due to the increase of t, i.e., the dimensionality. The pressure also leads to the breaking of the nesting condition. This may cause an additional effect of increasing the crossover energy.

SUMMARY

We investigated electronic states of two chains of interacting electron systems coupled by the interchain hopping at low temperatures by use of phase Hamiltonian. In the presence of only the repulsive forward scattering, the dominant state is given by the DW state and the SC state is subdominant. However, the crossover from the SDW state to the SS state is seen in the presence of both the forward and backward scattering. The existence of such a crossover is essential to explaining the phase diagram of SDW vs. SS states in the quasi-1D conductors such as $(TMTSF)_2X$.

This work was partially supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture (No.05640410), and a Grant-in-Aid for Scientific Research on the priority area, Novel Electronic States in Molecular Conductors, from the Ministry of Education, Science and Culture, Japan.

REFERENCES

1. For example, see T. Ishiguro and K. Yamaji, Organic Superconductors (Springer-Verlag, Berlin, 1990).
2. D. Jérome, A. Mazaud, M. Ribault and K. Bechgaard, J. Physique Lett., 41, L95(1980).
3. H. Yoshioka and Y. Suzumura, submitted to J. Phys. Soc. Jpn..
4. H. Yoshioka and Y. Suzumura, submitted to Phys. Rev. B.
5. M. Fabrizio, Phys. Rev. B, 48, 15838(1993).
6. K. Yamaji and Y. Shimoi, Physica C, 222, 349(1994).
7. N. Nagaosa and M. Oshikawa, 1994, cond-mat preprint 9412003.
8. H. J. Schulz, 1994, cond-mat preprint 9412098.
9. L. Balents and M. P. A. Fisher, 1995, cond-mat preprint 9503045.
10. A. M. Finkel'stein and A. I. Larkin, Phys. Rev. B, 47, 10461(1993).
11. J. Sólyom, Adv. Phys., 28, 201(1979).