Confinement of Interchain Hopping by Umklapp Scattering in Two-Coupled Chains

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The effect of umklapp scattering on interchain hopping has been investigated for two-coupled chains of interacting electrons with half-filled band. By analyzing in terms of renormalization group method, we have found that interchain hopping is renormalized to zero and is confined when a gap induced by umklapp scattering becomes larger than a critical value. From a phase diagram calculated on a plane of the interchain hopping and the gap, we discuss a role of the correlation gap which has been studied in metallic state at temperatures above spin density wave state in organic conductors.

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The linear chain conductors, called Bechgaard salts and described by the formula (TMTTF)$_2$X and (TMTSF)$_2$X - where TMTTF and TMTSF stands for tetramethyltetraethiofulvalene and tetramethyltetraserenofulvalene respectively, and X refers to various counter ions - have been, over the years the subject to intensive studies. Early attention has focused on the various broken symmetry (magnetic and superconducting) states but recently the state above the phase transition became the subject of intensive studies. In these salts the transfer integrals are different in different directions and they span a wide range of dimensionality. While the band width along the chain direction is comparable in the various salts, and the bandwidth in the least conduction direction is rather small, the transfer integral in the second best conducting (b) direction increases going from the TMTTF to the TMTSF salts. One central feature of these salts is that there is a transfer of one electron from the TMTTF or TMTSF chain to the X counter ions, and also there is a dimerization along the TMTTF and TMTSF chains and thus these materials can be regarded as having a half-filled electron band, thus umklapp scattering is important.

Various experiments give evidence for a charge gap for the TMTTF salts and a metallic behavior for the TMTSF salts. Recent optical, transport and dielectric experiments, taken together with photoemission measurements, lead to a picture where, with increasing transfer integral $t_b$ a transition occurs from an insulating state where electrons are confined to the individual chains, to a metallic state where the electrons are deconfined. This transition occurs where $t_b$ becomes comparable to the charge gap.

These conductors have been studied theoretically by use of a model of quasi-one-dimensional electron systems having repulsive intrachain interaction without umklapp scattering. The hopping perpendicular to chain becomes relevant even for a small transfer energy, although the hopping is suppressed by one-dimensional fluctuation.

Two-coupled chains has been studied as a basic model which includes intrachain interaction and transverse hopping. For the Tomonaga-Luttinger model with forward scattering, it has been shown that a gap appears in the transverse density fluctuations and that degeneracy of in-phase and out-of-phase pairings of density waves is removed. The model with backward scattering exhibits a phase diagram which is different from that of a single chain. In case of Hubbard model with a repulsive interaction and a incommensurate band, the ground state of two chains is given by the SC state with interchain and in-phase pairing, i.e., d-wave like pairing.

The transverse hopping becomes relevant even for a small transfer energy unless the intrachain interaction is extremely large. On the other hand, it has been maintained that confinement with no coherent single particle hopping occurs in coupled chains of Luttinger liquids for the interchain hopping smaller than a critical value.

In this letter, two-coupled chains with intrachain interaction and half-filled band is considered. The model applies to the normal state of organic conductors, TMTSF and TMTTF salts, for which the importance of umklapp scattering has been pointed out also earlier. We demonstrate a novel fact that the interchain hopping becomes irrelevant and confined with increasing the magnitude of umklapp scattering. The relevance of our result to experiments is also discussed.

We consider two-coupled chains with the intrachain interaction and interchain electron hopping. The kinetic energy parallel to the chain is linearized with the Fermi velocity $v_F \left( \pm v_F \right)$ and Fermi momentum $k_F$ for the right-going (left-going) electron, respectively. The intrachain interactions consist of forward scattering, backward scattering and umklapp scattering whose coupling constants are defined as $g_2$, $g_1$ and $g_3$ respectively. After diagonalization of the term for interchain hopping, the kinetic energy is expressed in terms of bonding state and antibonding state with new Fermi momentum, $k_{F, \pm} \equiv k_F + (\mp t/v_F)$, where $t$ denotes a hopping energy. Applying...
ing the bosonization method to electrons around the new Fermi points, we introduce Bose fields of phase variables, \( \theta_{_{p+}} \) and \( \theta_{_{p-}} \) (\( C_{+} \) and \( C_{-} \)), which express fluctuations for the total (transverse) charge density and spin density respectively.\(^1\) \(^2\) The commutation relation with conjugate phase is given by \( [\theta_{_{p+}}(x), \theta_{_{p-}}(x')] = [\theta_{_{p+}}(x), \theta_{_{p-}}(x')] = [\theta_{_{p+}}(x), \theta_{_{p-}}(x')] = i\pi \sgn(x-x') \). In terms of these phase variables and the bosonization for the field operator\(^1\) \(^2\), our Hamiltonian is given by

\[
\mathcal{H} = \sum_{\nu = \rho, \sigma} \frac{v_\nu}{4\pi} \int dx \left\{ \frac{1}{K_\nu} \left( \partial \theta_{\nu+} \right)^2 + K_\nu \left( \partial \theta_{\nu-} \right)^2 \right\} + \sum_{\nu = C, S} \frac{v_\nu}{4\pi} \int dx \left\{ \frac{1}{K_\nu} \left( \partial \theta_{\nu+} \right)^2 + K_\nu \left( \partial \theta_{\nu-} \right)^2 \right\} \\
+ \frac{2g_2 - g_1}{4\pi^2\alpha^2} \int dx \left\{ \cos \sqrt{2\theta_{C+} - 4tx/v_F} + \cos \sqrt{2\theta_{C-}} \right\} \left\{ \cos \sqrt{2\theta_{S+} - \cos \sqrt{2\theta_{S-}} \right\} \\
+ \frac{g_1}{4\pi^2\alpha^2} \int dx \left\{ \cos \sqrt{2\theta_{\rho+}} \left\{ \cos \sqrt{2\theta_{C+} - 4tx/v_F} - \cos \sqrt{2\theta_{C-} - \cos \sqrt{2\theta_{S+} - \cos \sqrt{2\theta_{S-}} \right\}} \\
+ \frac{g_3}{4\pi^2\alpha^2} \int dx \cos \sqrt{2\theta_{\rho+}} \left\{ \cos \sqrt{2\theta_{C+} - 4tx/v_F} + \cos \sqrt{2\theta_{C-} - \cos \sqrt{2\theta_{S+} + \cos \sqrt{2\theta_{S-}} \right\}}, \tag{1}
\]

where \( v_\nu = v_F \sqrt{1 - (2g_2 - g_1)^2} \), \( v_\sigma = v_F \sqrt{1 - g_1^2} \), \( K_\rho = \frac{[(1 - (2g_2 - g_1))/\{1 + (2g_2 - g_1)\}]^{1/2} K_\sigma = \frac{[(1 + g_1)/\{1 - g_1\}]^{1/2}} \), and \( K_C = K_S = 1 \). The quantity \( \alpha \sim 1/k_F \) is of the order of the lattice constant and \( g_1 = g_2/(2\pi v_F) \) with \( j = 1,2,3 \). In deriving Eq. \([\ref{eq:1}]\), a phase factor of the bosonized field operator, which is added to retain the anticommutation relation, is taken so as to conserve the sign of interaction.\(^3\)

We reexpress the nonlinear term in Eq. \([\ref{eq:1}]\) as \( (v_\nu/\pi\alpha^2)G_{\nu p',\nu'} \cos \sqrt{2\theta_{\nu p'}} \cos \sqrt{2\theta_{\nu p'}} \) where \( \sqrt{2\theta_{\nu p}} = \sqrt{2\theta_{\nu p} - 4tx/v_F} \) for \( \nu = C \) and \( p = + \), and \( \sqrt{2\theta_{\nu p}} = \sqrt{2\theta_{\nu p}} \) otherwise. In the present case, there are twelve coupling constants, which are given by \( G_{C+} = g_2 \), \( G_{C+} = g_2 \), \( G_{C+} = -g_2 \), \( G_{C-} = g_2 \), \( G_{C-} = g_2 \), \( G_{C+} = g_2 \), \( G_{C-} = g_2 \), \( G_{C+} = g_2 \), \( G_{C-} = g_2 \), \( G_{C+} = g_2 \), \( G_{C-} = g_2 \), and \( G_{C+} = g_2 \). The renormalization group method is applied to response functions for SDW, 4Kp–CDW and SC states, which are calculated with the assumption that response function are scaled to the same form for \( \alpha \to \alpha' \). Thus renormalization group equations within the second order are obtained as ( \( \nu = \rho, \sigma \) and \( p, p' = \pm \))

\[
\frac{d}{dl} K_\nu = -\frac{1}{2v_\nu^2} K_\nu^2 \left[ G_{\nu+} G_{\nu+} J_0(y) + G_{\nu+} G_{\nu-} \right. \\
+ G_{\nu+} G_{\nu-} + G_{\nu+} G_{\nu-} \left. \right], \tag{2}
\]

\[
\frac{d}{dl} K_C = \frac{1}{2} \sum_{p = \pm} \left[ \left(-K_C J_0(y) \delta_{p+} + \delta_{p-} \right) \\
+ \{ G_{Cp+} G_{Cp-} + G_{Cp+} G_{Cp-} + G_{Cp+} G_{Cp-} \} \right], \tag{3}
\]

\[
\frac{d}{dl} K_S = \frac{1}{2} \sum_{p = \pm} \left[ \left(-K_S \delta_{p+} + \delta_{p-} \right) \\
+ \{ G_{Sp+} J_0(y) + G_{Sp-} \} \right. \\
+ \{ G_{Sp+} G_{Sp-} + G_{Sp+} G_{Sp-} \} \right], \tag{4}
\]

\[
\frac{d}{dl} G_{C_{\nu+} C_{\nu+}} = \left( \frac{2 - K_\nu - K_C^p}{K_{\nu+} C_{\nu+}} \right) G_{C_{\nu+} C_{\nu+}} \\
- G_{C_{\nu+} C_{\nu+}} G_{C_{\nu+} C_{\nu+}} - G_{C_{\nu+} C_{\nu+}} G_{C_{\nu+} C_{\nu+}} , \tag{5}
\]

\[
\frac{d}{dl} G_{C_{\nu+} S_{\nu+}} = \left( \frac{2 - K_\nu - K_C^p}{K_{\nu+} S_{\nu+}} \right) G_{C_{\nu+} S_{\nu+}} \\
- G_{C_{\nu+} C_{\nu+}} G_{C_{\nu+} S_{\nu+}} G_{C_{\nu+} C_{\nu+}} , \tag{6}
\]

\[
\frac{d}{dl} G_{C_{\nu+} C_{\nu+}} = \left( \frac{2 - K_\nu - K_C^p}{K_{\nu+} C_{\nu+}} \right) G_{C_{\nu+} C_{\nu+}} \\
- \frac{1}{v_\nu^2} G_{\rho+} G_{\rho+} G_{\rho+} - \frac{1}{v_\sigma} G_{\sigma+} G_{\sigma+} G_{\sigma+} \tag{7}
\]

\[
\frac{d}{dl} l(l) = l(l) - \frac{1}{8} \left( G_{C_{\nu+} C_{\nu+}} + G_{C_{\nu+} S_{\nu+}} + G_{C_{\nu+} C_{\nu+}} + G_{C_{\nu+} C_{\nu+}} \right) K_{C} J_0(y) \tag{8}
\]

where \( K_{\nu+} = K_{\nu+}^{p=1} \) for \( p = \pm \), \( \nu_\nu = v_F \nu_F \), \( l(l) = t(l)/(v_\nu \nu^{-1}) \), \( y = 4/4(l) \) and \( J_n(y) \) \((n = 0, 1)\), is the Bessel function. The variable, \( l \), is written explicitly only for \( l(l) \) where \( l(l) = t(t)/e_F \equiv t \) with \( e_F = v_F / \alpha \) and the corresponding energy is given by \( e_F \exp[-l] \). Note that these equations in the zero limit of \( t \) becomes equal to those of one-dimensional case.\(^4\)

We examine both cases of \( g_1 = g_2 \neq 0 \) and \( g_1 = 0, g_2 \neq 0 \) by calculating renormalization group equations for \( K_C(l), K_{C}(l), K_{S}(l), G_{C_{\nu+} C_{\nu+}}(l) \) and \( G_{C_{\nu+} C_{\nu+}}(l) \) with several choices of \( g_2, \hat{g}_2 \) and \( \hat{g}_S \). For the relevant interchain hopping, \( l(l) \) increases rapidly with increasing \( l \) while \( l(l) \) decreases to zero for the irrelevant hopping. The relevant \( l(l) \) corresponds to \( K_{C}(l) \to \infty \) which comes from the rapid oscillation of \( J_0(y) \) in Eq. \([\ref{eq:4}]\). The quantity \( K_{C}(l) \) represents the degree of transverse charge fluctuation. Thus deconfinement (confinement) is obtained when the limiting value of \( K_{C}(l) \) becomes infinite (finite).

In Fig. 1, \( l(l) \) and \( 1/K_{C}(l) \) are shown as a function of \( l \) by solid curve and dotted curve, respectively with the fixed \( g_3 = 0.1, \hat{g}_{hc} \left( = 0.189 \right) \) and 0.3 where \( t = 0.1 \) and \( g_1 = g_2 = 0.3 \). The case for \( g_3 = 0.1 \) (curves \(1 \) and \( 4 \))
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Fig. 1: The \( l \)-dependences of \( \tilde{t}(l) \) and \( 1/K_C(l) \) are shown by solid curve and dotted curve respectively for \( \tilde{g}_3 = 0.1 \) ((1) and (4)), \( \tilde{g}_3 = \tilde{g}_{3c} (= 0.189) \) ((2) and (5)) and \( \tilde{g}_3 = 0.3 \) ((3) and (6)), respectively where \( t = 0.1 \) and \( \tilde{g}_1 = \tilde{g}_2 = 0.3 \). The inset shows the \( \tilde{g}_3 \)-dependence of \( 1/K_C^{\text{asym}} \) which corresponds to the limiting value of \( 1/K_C(l) \).

Fig. 2: The \( \tilde{t} \)-dependence of \( \tilde{g}_{3c} \) for \( \tilde{g}_1 = \tilde{g}_2 = 0.3 \) (solid curve), \( \tilde{g}_1 = \tilde{g}_2 = 0.4 \) (dashed curve) and \( \tilde{g}_1 = 0, \tilde{g}_2 = 0.3 \) (dash-dotted curve). The case of \( g_3 > g_{3c} (g_3 < g_{3c}) \) corresponds to confinement (deconfinement).

shows the result leading to deconfinement. With increasing \( l \), \( \tilde{t}(l) \) increases rapidly and \( 1/K_C(l) \) decreases monotonically to zero. Our solution stops at a value of \( l \) corresponding to \( K_p(l) \simeq 0 \) due to the divergence of some of \( G_{\nu p, \nu' p'}(l) \) since the present treatment is of the second order for the renormalization group equations. The case for \( g_3 = 0.3 \) (curves (3) and (6)) shows a typical behavior for confinement. With increasing \( l \), \( \tilde{t}(l) \) reduces to zero after taking a maximum and \( 1/K_C(l) \) remains finite even at the limiting value of \( l \). There is a crossover from deconfinement to confinement around the location of \( l \) corresponding to the maximum of \( \tilde{t}(l) \) where \( G_{\nu p, \nu' p'}(l) \) becomes of the order of unity. We also obtained that \( G_{\nu p, \nu' p'}(l) \simeq 1/K_C(l) \) for the limiting value, indicating the irrelevance of the misfit parameter and then the interchain hopping. For a critical value given by \( \tilde{g}_3 = \tilde{g}_{3c} \) (curves (2) and (5)), one finds a marginal behavior where both \( \tilde{t}(l) \) and \( 1/K_C(l) \) reduce to zero at the limiting value of \( l \). The \( l \)-dependence of \( K_C(l) \) indicates that there is a transition from deconfinement to confinement as a function of \( \tilde{g}_3 \) in the limit of low energy. In the inset, the \( \tilde{g}_{3c} \)-dependence of \( 1/K_C^{\text{asym}} \) is shown where \( K_C^{\text{asym}} \) is the limiting value of \( K_C(l) \). The location of \( g_{3c} \) is shown by the arrow. For most parameters leading to \( \tilde{g}_3 = \tilde{g}_{3c} \), the present calculation shows common features that a peak height of \( \tilde{t}(l) \) is about 0.82 and \( \omega_m/t \simeq 0.94 \) where \( \omega_m \) is the energy at the peak of \( \tilde{t}(l) \). We note that the Bessel function, \( J_1(y) \), in r.h.s. of Eq. (8) plays a crucial role to obtain such a transition where the effect of second term of Eq. (8) is negligible for the relevant \( \tilde{t}(l) \) and becomes large for the irrelevant \( \tilde{t}(l) \). With increasing \( l \), \( K_p(l) \) decreases to zero where a charge gap is formed for \( K_p(l) \simeq K_p(0)/2 \), e.g., at \( l \simeq 3.25(1.50) \) for \( \tilde{g}_3 = 0.1(0.3) \). The quantity \( K_S(l) \) corresponding to transverse spin fluctuation is also suppressed by umklapp scattering. The behavior of total spin fluctuation indicates the absence of the spin gap even at low energies since \( K_S(l) \) is almost the same as one-dimensional one. Thus one finds that there is a separation of freedoms of charge and spin at energy corresponding to a correlation gap. Note that the decreases of \( K_S(l) \) and \( K_S(l) \) are attributable to the backward scattering. In fact, \( K_S(l) = K_S(l) = 1 \) for both regions of confinement and deconfinement when \( \tilde{g}_1 = 0 \).

In Fig. 2, the \( \tilde{t} \)-dependence of \( \tilde{g}_{3c} \) is shown for \( \tilde{g}_2 = \tilde{g}_1 = 0.3 \) (solid curve), \( \tilde{g}_2 = \tilde{g}_1 = 0.4 \) (dashed curve) and \( \tilde{g}_1 = 0, \tilde{g}_2 = 0.3 \) (dash-dotted curve) where the region for confinement (deconfinement) is given by \( \tilde{g}_3 > \tilde{g}_{3c} \) (\( \tilde{g}_3 < \tilde{g}_{3c} \)). The boundary is determined mainly by the competition between umklapp scattering and interchain hopping. In addition to \( \tilde{g}_3 \), both \( \tilde{g}_3 \) and \( \tilde{g}_1 \) enhance the region for confinement where the effect of the forward scattering is larger than the backward scattering. As \( \tilde{t} \) goes to zero, \( \tilde{g}_{3c} \) reduces to zero and then the confinement does not exist in the absence of umklapp scattering.

Now we examine the correlation gap, \( \Delta \), defined by \( \Delta \equiv \epsilon_p \exp[-l_k] \) where \( l_k \) is evaluated from \( K_p(l_k) = K_p(0)/2 \). We note that such a definition of gap well reproduces a magnitude of gap for the one-dimensional Hubbard model with the weak coupling. It is found that \( \Delta \) is slightly larger than the energy, \( \omega_m \), corresponding to a peak of \( \tilde{t}(l) \) in Fig. 1. In the inset of Fig. 3, \( \Delta \) is shown as a function of \( \tilde{g}_3 \) for \( \tilde{g}_2 = \tilde{g}_1 = 0.3 \) (1), \( \tilde{g}_2 = \tilde{g}_1 = 0.4 \) (2) and \( \tilde{g}_2 = 0.3, \tilde{g}_1 = 0 \) (3) with the fixed \( l = 0.1 \). The quantity \( \Delta \), which is determined mainly by \( \tilde{g}_3 \), is enhanced also by \( \tilde{g}_2 \) and \( \tilde{g}_1 \). The \( l \)-dependence of \( \Delta \) is small as is seen from curve (4) which is calculated.
Fig. 3: The phase diagram of confinement (region (I)) and deconfinement (region (II)) on the plane of the interchain transfer energy, $t_b = \tilde{t}/2$ and the correlation gap, $\Delta$. The solid, dashed and dash-dotted curves denote boundaries which are obtained from respective curves in Fig. 2. In the inset, the correlation gap, $\Delta$ is shown as a function of $g_3$ for $\tilde{g}_2 = \tilde{g}_1 = 0.3$, $\tilde{t} = 0.1$ (1), $\tilde{g}_2 = \tilde{g}_1 = 0.4$, $\tilde{t} = 0.1$ (2), $\tilde{g}_2 = 0.3$, $\tilde{g}_1 = 0$, $\tilde{t} = 0.1$ (3) and $\tilde{g}_2 = \tilde{g}_1 = 0.3$, $\tilde{t} = 0.01$ (4), respectively.

for $\tilde{g}_2 = \tilde{g}_1 = 0.3$ and $\tilde{t} = 0.01$. Here we introduce $t_b$ defined as the transfer energy perpendicular to chain for quasi-one-dimensional system where $t_b = \tilde{t}/2$ from the definition of our Hamiltonian. In terms of $\Delta$ and $t_b = \tilde{t}/2$, the phase diagram is shown in Fig. 3 where region (I) and region (II) correspond to confinement and deconfinement, respectively. Three boundaries given by the solid curve, the dashed curve and the dash-dotted curve are evaluated from the corresponding curves in Fig. 2. It turns out that the ratio of the correlation gap to the perpendicular transfer energy is $\Delta/t_b = 1.8 \sim 2.3$ for the interval range of 0.01 $< t_b/\epsilon_F < 0.4$. This value is in excellent agreement with experiments which indicate a transition from a confined insulator to a deconfined metal for between 1.5 and 2. The critical value of $\Delta$ for the confinement decreases for the large $\tilde{g}_2$ and $\tilde{g}_1$.

The dominant state, which is found with decreasing $\omega(= \epsilon_F \exp[-\tilde{t}])$ and for the fixed $\tilde{g}_3$ and $\tilde{g}_2 = \tilde{g}_1 > 0$, is examined by calculating response functions for SDW with the intrachain and out-of-phase pairing and $4k_F$-CDW with the intrachain and in-phase pairing and SC state with the interchain and in-phase pairing. When $\Delta \lesssim \tilde{t}$ (i.e., $\tilde{g}_3 > \tilde{g}_{3c}$), there is a crossover from confinement to confinement in SDW state at energy given by $\omega \simeq \omega_m(< \Delta)$. Further, the SDW state moves into the confined $4k_F$-CDW state at lower energies. When $\Delta \gtrsim \tilde{t}$, all the states are deconfined and SDW state is replaced by $4k_F$-CDW state at energy much lower than $\Delta$.

The SC state is possible for the region of deconfinement with $\tilde{g}_3 \ll \tilde{t}$ and finite energy. We note that SC state is also found in other region of $2\tilde{g}_2 - \tilde{g}_1 \sim |\tilde{g}_3|$, where the umklapp scattering becomes irrelevant.

In conclusion, we have found, by examining the effect of umklapp scattering on the interchain hopping in two-coupled chains, that the interchain hopping becomes irrelevant resulting in the transition from deconfinement to confinement when correlation gap induced by umklapp scattering becomes larger than the interchain hopping. This result supports Giamarchi’s assertion of the irrelevant hopping by umklapp scattering but differs slightly from that by Kishine and Yonemitsu who have obtained the state with reduced but finite interchain hopping.

Finally we comment on the metallic state above the deconfinement transition, which is highly unusual: there is a small Drude weight and a charge gap remaining, while the spin excitations are gapless. The state is similar to that of a doped Hubbard chain. In a simple minded picture single electron transitions between the chains lead to deviations to $1e$/$\text{unit cell}$ for both chains - and thus to a situation also encountered by doping - but whether interchain electron transfer leads to features seen by experiments remains to be seen.

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