

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 a half-filled band. By analyzing in terms of the 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 that has been studied in the metallic state at temperatures above the spin-density-wave state in organic conductors. [S0163-1829(98)52324-7]

The linear-chain conductors, called Bechgaard salts and described by the formula $(\text{TMTTF})_2X$ and $(\text{TMTSF})_2X$ —where TMTTF and TMTSF stand for tetramethyltetrafulvalene and tetramethyltetraselenofulvalene, respectively, and X refers to various counterions—have been, over the years, the subject of 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.¹ While the bandwidth 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.^{2,3} One central feature of these salts is a transfer of one electron from the TMTTF or TMTSF chain to the X counterions, as well as a dimerization along the TMTTF and TMTSF chains. Thus these materials can be regarded as having a half-filled electron band, and therefore 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,⁴ taken together with photoemission measurement⁵ 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.⁶

These conductors have been studied theoretically by using a model of quasi-one-dimensional electron systems having repulsive intrachain interaction without umklapp scattering. The hopping perpendicular to the chain becomes relevant even for a small transfer energy,⁷ although the hopping is suppressed by one-dimensional fluctuation.⁸ Two coupled chains have been studied as a basic model that 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.⁹⁻¹² The model with backward scattering exhibits a phase diagram that is different from that of a single chain. In the case of the Hubbard model with a repulsive interaction and an incommensurate band, the ground state of two chains is given by the superconducting (SC) state with interchain and in-phase pairing, i.e., d -wave-like pairing.^{10,13,14} The transverse hopping becomes relevant even for a small transfer energy unless the intrachain interaction is extremely large.¹⁰ 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.¹⁵⁻¹⁷

In this paper, two coupled chains with intrachain interaction and a half-filled band are 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 earlier.^{18,19} We demonstrate 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 ($-v_F$) and Fermi momentum k_F for the right-moving (left-moving) 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 the 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 the bosonization method to electrons around the new Fermi points, we introduce Bose fields of phase variables, $\theta_{\rho+}$ and $\theta_{\sigma+}$ (θ_{C+} and θ_{S+}), which express fluctuations for the total (transverse) charge density and spin density, respectively.¹² The commutation relation with conjugate phase is given by $[\theta_{\rho+}(x), \theta_{\rho-}(x')] = [\theta_{\sigma+}(x), \theta_{\sigma-}(x')] = [\theta_{C+}(x), \theta_{C-}(x')] = [\theta_{S+}(x), \theta_{S-}(x')] = i\pi \text{sgn}(x-x')$. In terms of these phase variables and the bosonization for the field operator,²⁰ our Hamiltonian is given by

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

where $v_\rho = v_F \sqrt{1 - (2\tilde{g}_2 - \tilde{g}_1)^2}$, $v_\sigma = v_F \sqrt{1 - \tilde{g}_1^2}$, $K_\rho = [\{1 - (2\tilde{g}_2 - \tilde{g}_1)\} / \{1 + (2\tilde{g}_2 - \tilde{g}_1)\}]^{1/2}$, $K_\sigma = [(1 + \tilde{g}_1) / (1 - \tilde{g}_1)]^{1/2}$, and $K_C = K_S = 1$. The quantity α ($\sim 1/k_F$) is of the order of the lattice constant and $\tilde{g}_j = g_j / (2\pi v_F)$ with $j = 1, 2$, and 3 . In deriving Eq. (1), a phase factor of the bosonized field operator, which is added to retain the anticommutation relation, is taken in order to conserve the sign of interaction.²¹

We reexpress the nonlinear term in Eq. (1) as $(v_F/\pi\alpha^2)G_{\nu p, \nu' p'} \cos\sqrt{2}\bar{\theta}_{\nu p} \cos\sqrt{2}\bar{\theta}_{\nu' p'}$ where $\sqrt{2}\bar{\theta}_{\nu p} = \sqrt{2}\theta_{\nu p} - 4tx/v_F$ for $\nu = C$ and $p = +$, and $\sqrt{2}\bar{\theta}_{\nu p} = \sqrt{2}\theta_{\nu p}$ otherwise. In the present case, there are 12 coupling constants, which are given by $G_{C+, S+} = \tilde{g}_2 - \tilde{g}_1$, $G_{C+, S-} = -\tilde{g}_2$, $G_{C-, S+} = \tilde{g}_2$, $G_{C-, S-} = -\tilde{g}_2 + \tilde{g}_1$, $G_{\sigma+, C+} = -G_{\sigma+, C-} = -G_{\sigma+, S+} = -G_{\sigma+, S-} = \tilde{g}_1$, and $G_{\rho+, C+} = G_{\rho+, C-} = -G_{\rho+, S+} = G_{\rho+, S-} = \tilde{g}_3$. The renormalization group method is applied to response functions for spin-density-wave (SDW), $4k_F$ charge-density-wave (CDW), and SC states, which are calculated with the assumption that response functions are scaled to the same form for $\alpha \rightarrow \alpha' = \alpha e^{dl}$.^{22,23} Thus, renormalization group equations within the second order are obtained as ($\nu = \rho, \sigma$, and $p, p' = \pm$)

$$\begin{aligned}
\frac{d}{dl} K_\nu = & -\frac{1}{2\tilde{v}_\nu^2} K_\nu^2 [G_{\nu+, C+}^2 J_0(y) \\
& + G_{\nu+, C-}^2 + G_{\nu+, S+}^2 + G_{\nu+, S-}^2], \quad (2)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dl} K_C = & \frac{1}{2} \sum_{p=\pm} [\{-K_C^2 J_0(y) \delta_{p,+} + \delta_{p,-}\} \\
& \times \{G_{Cp, S+}^2 + G_{Cp, S-}^2 + G_{\rho+, Cp}^2 + G_{\sigma+, Cp}^2\}], \quad (3)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dl} K_S = & \frac{1}{2} \sum_{p=\pm} [\{-K_S^2 \delta_{p,+} + \delta_{p,-}\} \{G_{C+, Sp}^2 J_0(y) \\
& + G_{C-, Sp}^2 + G_{\rho+, Sp}^2 + G_{\sigma+, Sp}^2\}], \quad (4)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dl} G_{\nu+, Cp} = & (2 - K_\nu - K_C^p) G_{\nu+, Cp} \\
& - G_{\nu+, S+} G_{Cp, S+} - G_{\nu+, S-} G_{Cp, S-}, \quad (5)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dl} G_{\nu+, Sp} = & (2 - K_\nu - K_S^p) G_{\nu+, Sp} - G_{\nu+, C+} G_{C+, Sp} J_0(y) \\
& - G_{\nu+, C-} G_{C-, Sp}, \quad (6)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dl} G_{Cp, Sp'} = & (2 - K_C^p - K_S^{p'}) G_{Cp, Sp'} - \frac{1}{\tilde{v}_\rho} G_{\rho+, Cp} G_{\rho+, Sp'} \\
& - \frac{1}{\tilde{v}_\sigma} G_{\sigma+, Cp} G_{\sigma+, Sp'}, \quad (7)
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dl} \tilde{t}(l) = & \tilde{t}(l) - \frac{1}{8} (G_{C+, S+}^2 + G_{C+, S-}^2 + G_{\rho+, C+}^2 \\
& + G_{\sigma+, C+}^2) K_C J_1(y), \quad (8)
\end{aligned}$$

where $K_\nu^p = K_\nu^{\pm 1}$ for $p = \pm$, $\tilde{v}_\nu = v_\nu/v_F$, $\tilde{t}(l) = t(l)/(v_F\alpha^{-1})$, $y = 4\tilde{t}(l)$, and $J_n(y)$, ($n=0,1$), is the Bessel function. The variable l is written explicitly only for $\tilde{t}(l)$ where $\tilde{t}(0) = t/\epsilon_F \equiv \tilde{t}$ with $\epsilon_F = v_F/\alpha$ and the corresponding energy is given by $\epsilon_F \exp[-l]$. Note that these equations in the zero limit of t become equal to those of the one-dimensional case.²⁴

We examine both cases of $\tilde{g}_1 = \tilde{g}_2 \neq 0$ and $\tilde{g}_1 = 0, \tilde{g}_2 \neq 0$ by calculating renormalization group equations for $K_\rho(l)$, $K_\sigma(l)$, $K_C(l)$, $K_S(l)$, and $G_{\nu p, \nu' p'}(l)$ with several choices of $\tilde{g}_2, \tilde{g}_1, \tilde{g}_3$, and \tilde{t} . For the relevant interchain hopping, $\tilde{t}(l)$ increases rapidly with increasing l while $\tilde{t}(l)$ decreases to zero for the irrelevant hopping. The relevant $\tilde{t}(l)$ corresponds to $K_C(l) \rightarrow \infty$, which comes from the rapid oscillation of $J_0(y)$ in Eq. (3). 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, $\tilde{t}(l)$ and $1/K_C(l)$ are shown as a function of l by solid curves and dotted curves, respectively, with the fixed $\tilde{g}_3 = 0.1$, \tilde{g}_{3c} ($= 0.189$) and 0.3 , where $\tilde{t} = 0.1$ and $\tilde{g}_1 = \tilde{g}_2 = 0.3$. The case for $\tilde{g}_3 = 0.1$ [curves (1) and (4)] 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 $K_\rho(l) \approx 0$ due to the divergence of some of $G_{\nu p, \nu' p'}(l)$ since the present treatment is of the second order for the renormaliza-

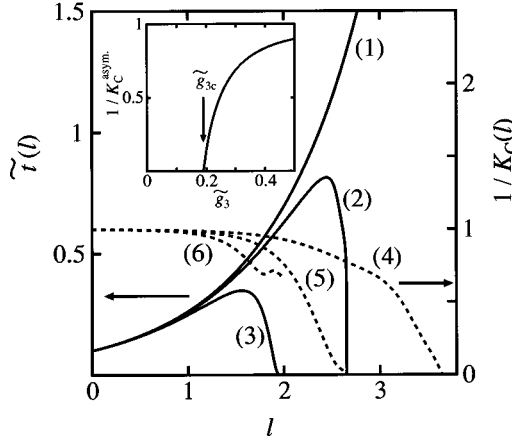


FIG. 1. The l dependences of $\tilde{t}(l)$ and $1/K_C(l)$ are shown by solid curves and dotted curves, respectively, for $\tilde{g}_3=0.1$ [(1) and (4)], $\tilde{g}_3=\tilde{g}_{3c}(=0.189)$ [(2) and (5)], and $\tilde{g}_3=0.3$ [(3) and (6)], respectively, where $\tilde{t}=0.1$ and $\tilde{g}_1=\tilde{g}_2=0.3$. The inset shows the \tilde{g}_3 dependence of $1/K_C^{\text{asym}}$, which corresponds to the limiting value of $1/K_C(l)$.

tion group equations. The case for $\tilde{g}_3=0.3$ [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 $G_{\rho+,vp}(l)$ becomes of the order of unity. We also obtained $G_{\rho+,c+}(l)/G_{\rho+,c-}(l)\approx 1/K_C(l)$ 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}_3 dependence of $1/K_C^{\text{asym}}$ is shown where K_C^{asym} is the limiting value of $K_C(l)$. The location of \tilde{g}_{3c} is shown by the arrow. For most parameters leading to $\tilde{g}_3=\tilde{g}_{3c}$, the present calculation shows a common feature in that a peak height of $\tilde{t}(l)$ is about 0.82 and $\omega_m/t\approx 0.94$, where ω_m is the energy at the peak of $\tilde{t}(l)$. We note that the Bessel function $J_1(y)$ in the right-hand side of Eq. (8) plays a crucial role in obtaining such a transition where the effect of the 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 , $K_\rho(l)$ decreases to zero where a charge gap is formed for $K_\rho(l)\approx K_\rho(0)/2$, e.g., at $l\approx 3.25(1.50)$ 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 $K_\sigma(l)$ is almost the same as the 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 $K_\sigma(l)$ and $K_S(l)$ are attributable to the backward scattering. In fact, $K_\sigma(l)=K_S(l)=1$ 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 $\tilde{g}_2=0.3, \tilde{g}_1=0$ (dash-dotted curve).

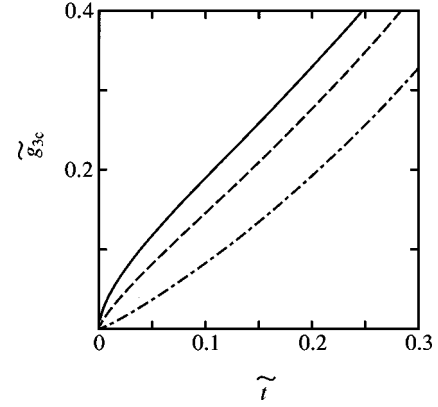


FIG. 2. The \tilde{t} dependence of \tilde{g}_{3c} for $\tilde{g}_1=\tilde{g}_2=0.3$ (solid curve), $\tilde{g}_1=\tilde{g}_2=0.4$ (dashed curve), and $\tilde{g}_1=0, \tilde{g}_2=0.3$ (dash-dotted curve). The case of $\tilde{g}_3>\tilde{g}_{3c}$ ($\tilde{g}_3<\tilde{g}_{3c}$) corresponds to confinement (deconfinement).

$=0.3, \tilde{g}_1=0$ (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}_2 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 Δ defined by $\Delta\equiv\epsilon_F\exp[-l_g]$, where l_g is evaluated from $K_\rho(l_g)=K_\rho(0)/2$. We note that such a definition of gap reproduces well a magnitude of gap for the one-dimensional Hubbard model with weak coupling.²⁵ It is found that Δ is slightly larger than the energy ω_m corresponding to a peak of $\tilde{t}(l)$ in Fig. 1. In the inset of Fig. 3, Δ 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

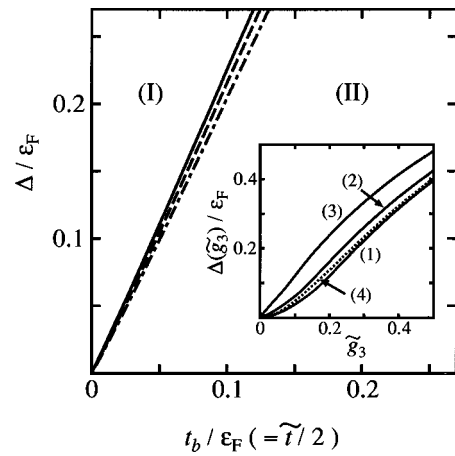


FIG. 3. The phase diagram of confinement [region (I)] and deconfinement [region (II)] on the plane of the interchain transfer energy $t_b(=\tilde{t}/2)$ and the correlation gap Δ . The solid, dashed, and dash-dotted curves denote boundaries that are obtained from respective curves in Fig. 2. In the inset, the correlation gap Δ is shown as a function of \tilde{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.

the fixed $\tilde{t}=0.1$. The quantity Δ , which is determined mainly by \tilde{g}_3 , is enhanced also by \tilde{g}_2 and \tilde{g}_1 . The \tilde{t} dependence of Δ is small as seen from curve (4) which is calculated 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 the chain for a quasi-one-dimensional system where $t_b=t/2$ from the definition of our Hamiltonian. In terms of Δ and $t_b(=t/2)$, the phase diagram is shown in Fig. 3 where regions (I) and (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. The result is 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 $0.01 < t_b/\epsilon_F < 0.1$. This value is in excellent agreement with experiments⁵ that indicate a transition from a confined insulator to a deconfined metal between 1.5 and 2. The critical value of Δ for the confinement decreases for the large \tilde{g}_2 and \tilde{g}_1 .

The dominant state, which is found with decreasing ω ($=\epsilon_F \exp[-l]$) 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, for $4k_F$ CDW with the intrachain and in-phase pairing, and for SC state with the interchain and in-phase pairing. When $\Delta \geq t$ (i.e., $\tilde{g}_3 > \tilde{g}_{3c}$), there is a crossover from deconfinement to confinement in the SDW state at energy given by $\omega \approx \omega_m (< \Delta)$. Further, the SDW state moves into the confined $4k_F$ CDW state at lower energies. When $\Delta \leq t$, all the states are deconfined and the

SDW state is replaced by the $4k_F$ CDW state at energy much lower than Δ . The SC state is possible for the region of deconfinement with $\tilde{g}_3 \ll \tilde{t}$ and finite energy. We note that the SC state is also found in the other region of $2\tilde{g}_2 - \tilde{g}_1 < -|\tilde{g}_3|$, where the umklapp scattering becomes irrelevant.¹⁸

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 the correlation gap induced by umklapp scattering becomes larger than the interchain hopping. This result supports Giamarchi's assertion¹⁹ of irrelevant hopping by umklapp scattering but differs slightly from that by Kishine and Yonemitsu²⁶ 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.²⁷ In a simple picture, single-electron transitions between the chains lead to deviations to 1 electron/unit cell for both chains—and thus to a situation also encountered by doping—but whether interchain electron transfer leads to the features viewed by experiments remains to be seen.

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