Mechanism of confinement in low-dimensional organic conductors

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Confinement-deconfinement transition in quarter-filled two-coupled chains comprising dimerization, repulsive interactions and interchain hopping has been demonstrated by applying the renormalization group method to the bosonized Hamiltonian. The confinement given by the irrelevant interchain hopping occurs with increasing umklapp scattering which is induced by the dimerization leading to effectively half-filling. It is shown that the transition originates in a competition between a charge gap and the renormalized interchain hopping.

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\section{Introduction}

In low-dimensional organic conductors, repulsive interactions play an important role for electronic states with a gap or a pseudo gap. The anisotropy in electric conductivity is enhanced by interactions since the induced pseudo gap around the Fermi surface of a single chain precludes electrons from hopping between chains\cite{3}. There are several arguments as to whether or not the electrons are confined to a chain by the repulsive interaction. Away from half-filling, the confinement needs a large magnitude of the interaction even for the small limit of the interchain hopping\cite{6,7} since the effect of the interchain hopping is much larger than that of the intra-chain interaction. However, in the case of half-filling, the electrons can be confined by the interaction with a moderate strength due to umklapp scattering which induces the charge gap\cite{8,9}.

Bechgaard salts of organic conductors, TMTSF and TMTTF, can be regarded as effectively half-filling due to dimerization\cite{6,7}. The optical experiments have shown the finite Drude weight for the TMTSF salts but not for the TMTTF salts although the correlation gap exists in both salts\cite{8}. This indicates the transition from an insulating state with the electrons confined to chains to a metallic state with deconfined electrons when the correlation gap becomes larger than the interchain hopping\cite{8,9}. In the present study, such a transition is elucidated by applying the renormalization group (RG) method to a model of quarter-filled two-coupled chains with dimerization.

\section{Formulation}

We consider quarter-filled two-coupled chains given by

\[ H = -2t_{\perp} \sum_{j,\sigma} \left( c_{j+1\sigma}^\dagger c_{j\sigma} + h.c. \right) + U \sum_{j,l} n_{j\uparrow} n_{j\downarrow}, \]

where \( t, t_{\perp}, t_{d} \) and \( U \) denote energies for the intrachain hopping, the interchain hopping, dimerization and on-site repulsion, respectively. \( n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma} \). The quantity \( c_{j\sigma} \) denotes the annihilation operator of the electron at the \( j \)-th site of the \( \ell \)-th chain (\( \ell = 1, 2 \)) with spin \( \sigma (\uparrow, \downarrow) \). We use the Fourier transform, \( c_{j\sigma} = N^{-1/2} \sum_{k} e^{i k \mathbf{r}_{j}} \exp(i k j \sigma) \) with the total number of sites \( N \) and the lattice constant \( a \). First, the \( t_{d} \)-term is diagonalized to obtain two bands in the reduced zone, \( -\pi/2a < k < \pi/2a \), and the lower band becomes effectively half-filled, which is described by fermion operators, \( a_{k\sigma} \), and is examined in the present study. Next, diagonalizing the \( t_{\perp} \)-term by \( \alpha_{k\sigma\pm} = (\mp d_{k\sigma} + \bar{d}_{k\sigma})/\sqrt{2} \), the kinetic term is written as \( \mathcal{H}_{K}^d = \sum_{k,\sigma} \varepsilon(k, \sigma) a_{k\sigma}^\dagger a_{k\sigma} \).\( (\zeta = \pm) \) with \( \varepsilon(k, \pm) = -2t_{d} \cos^2 k a + t_{d}^{-1} \sin^2 k a/1 + 2t_{1} \). Thus we have the following effective Hamiltonian\cite{11}

\[ \mathcal{H}_{K}^d = \sum_{k,\sigma} \varepsilon(k, \sigma) a_{k\sigma}^\dagger a_{k\sigma} \]

The kinetic energy with the linearized dispersion around the Fermi surface, \( k_{F} \pm = k_{F} \mp t_{\perp}/v_{F} \), is expressed as \( \mathcal{H}_{K}^d = \sum_{k,p,\sigma,\zeta} v_{F}(p_{k} - k_{p}) a_{k\sigma\zeta}^\dagger a_{k\sigma\zeta} \) with \( p(= +, -) \) denoting right moving (left moving) electrons and \( v_{F} = \sqrt{2} t_{a} \left[ 1 - (t_{d}/t_{a})^2 \right] /1 + (t_{d}/t_{a})^2 \) in which the \( t_{\perp} \)-dependence of the velocity is discarded. Coupling constants of interactions corresponding to forward scattering with the same and opposite directions (\( g_{1} \) and \( g_{2} \)), backward scattering (\( g_{1} \)) and Umklapp scattering (\( g_{1} \)) are given by \( g_{1} = g_{2} = g_{1} = U a, g_{3} \propto U a(t_{d}/t) \) and \( g_{1} = g_{2} \), \( g_{1} = 0 \) where \( \parallel \) and \( \perp \) denote interactions for the same spin and opposite spin.

Applying the bosonization method to electrons around the new Fermi points, we introduce Bose fields of phase variables, \( \theta_{\sigma\pm} \) and \( \theta_{\sigma\perp} \)\cite{12}, which express fluctuations for the total (transverse) charge density and spin density, respectively\cite{12}. The commutation relation with conjugate phase variables is given by \( [\theta_{\sigma\pm}(x), \theta_{\sigma\perp}(x')] = i\pi \delta_{\sigma\sigma'} \text{sgn}(x - x') \). In terms of these
phase variables, our Hamiltonian is given by
\[ \mathcal{H} = \sum_{\nu=\rho,\sigma,C,S} \frac{\psi}{4\pi} \int dx \left[ \frac{1}{K_{\nu}} (\partial_{\psi_{\nu}})^2 + K_{\nu} (\partial_{\theta_{\nu}})^2 \right] + \frac{g_{\nu}}{4\pi^2 a^2} \int dx \left[ \cos(\sqrt{2}\theta_{\nu} + 8t_\perp x/\psi_{\nu}) + \cos \sqrt{2}\theta_{\sigma} \right] \left[ \cos \sqrt{2}\theta_{S} - \cos \sqrt{2}\theta_{S} \right] + \frac{g_{\nu}}{4\pi^2 a^2} \int dx \left[ \cos(\sqrt{2}\theta_{\nu} + 8t_\perp x/\psi_{\nu}) - \cos \sqrt{2}\theta_{\nu} - \cos \sqrt{2}\theta_{S} + \cos \sqrt{2}\theta_{S} \right] + \frac{g_{\nu}}{2\pi^2 a^2} \int dx \sin \sqrt{2}\theta_{\nu} \left[ \cos(\sqrt{2}\theta_{\nu} + 8t_\perp x/\psi_{\nu}) - \cos \sqrt{2}\theta_{\nu} - \cos \sqrt{2}\theta_{S} + \cos \sqrt{2}\theta_{S} \right], \] (2)

where \( \psi_{\nu} = \theta_{\nu} \) except for \( \psi_{C+} = \theta_{C+} - (8t_\perp x/\psi_{\nu})/\sqrt{2} \) and \( \psi_{\nu} = \theta_{\nu} - \pi/(2\sqrt{2}) \). The RG equations for \( K_{\nu} = K_{\nu}(l), t_\perp = t_\perp(l) \) and \( G_{\nu,\nu',\nu''} = G_{\nu,\nu',\nu''}(l) \) are given, up to the second order as, \[ \frac{d}{dl} t_\perp = \frac{1}{8} K_C (G_{2,C+}^2 + G_{\sigma,C+}^2 + G_{\tilde{\sigma},C+}^2) J_1(8t_\perp), \] (4)
\[ \frac{d}{dl} K_{\nu} = -\frac{1}{2\nu} K_{\nu}^2 [G_{\nu,C+}^2 + G_{\nu,S+}^2 + G_{\nu,S-}^2] J_1(8t_\perp), \] (5)
\[ \frac{d}{dl} K_C = -\frac{1}{2} \sum_{p=\pm} \left[ (K_C^2 J_0(8t_\perp) \delta_{p,+} - \delta_{p,-}) (G_{p,C+}^2 + G_{p,C+}^2 + G_{p,C+}^2) \right], \] (6)
\[ \frac{d}{dl} K_S = -\frac{1}{2} \sum_{p=\pm} \left[ (G_{\tilde{\sigma},S+}^2 + \delta_{p,-}) (G_{p,S+}^2 + G_{p,S+}^2) \right] + \frac{G_{\sigma,S+}^2 + G_{\tilde{\sigma},S+}^2 J_0(8t_\perp) + G_{\sigma,S-}^2)}{2}, \] (7)
\[ \frac{d}{dl} G_{\nu,C+} = [2 - K_{\nu} - K_{\nu}^2] G_{\nu,C+} - G_{\nu,S+} G_{\nu,C,S+} - G_{\nu,S-} G_{\nu,C,S-}, \] (8)
\[ \frac{d}{dl} G_{\nu,S+} = [2 - K_{\nu} - K_{\nu}^2] G_{\nu,S+} - G_{\nu,S+} G_{\nu,C,S+} - G_{\nu,S-} G_{\nu,C,S-}, \] (9)

\[ \frac{d}{dl} G_{\nu,S-} = [2 - K_{\nu} - K_{\nu}^2] G_{\nu,S-} - G_{\nu,S+} G_{\nu,C,S+} - G_{\nu,S-} G_{\nu,C,S-}. \]

The term \( K_{\nu}(l) \) in the r.h.s. of eq. (4) reduces to zero due to a factor \( J_1(8t_\perp) \). Figure 2 displays the corresponding \( l \)-dependence of coupling constants. The main figure shows coupling constants for forward and backward scatterings with \( G_{C+} \) (curve (1)), \( G_{C-} \) (curve (2)), \( G_{\sigma,+} \) (curve (3)), \( G_{\sigma,-} \) (curve (4)), \( G_{\tilde{\sigma},+} \) (curve (5)), \( G_{\tilde{\sigma},-} \) (curve (6)), \( G_{\sigma,+} \) (curve (7)) and \( G_{\tilde{\sigma},-} \) (curve (8)) while the inset shows those for the umklapp scattering with \( G_{\nu,C+} \) (curve (9)), \( G_{\nu,C-} \).
(curve (10)), \(-G_{\rho^+-S^+}\) (curve (11)) and \(G_{\rho^+-S^-}\) (curve (12)). Coupling constants \(G_{\rho^++C^-}\) and \(-G_{\rho^+-S^+}\) increase rapidly and give rise to the trigger of relevance of the coupling constant \(G_{\rho^+-S^+}\) as seen also in the one-dimensional chain. Note that the relevance of coupling constants \(G_{C^--S^+}\), \(-G_{\rho^++C^-}\) and \(-G_{\sigma^+-S^+}\) is also obtained in the absence of umklapp scattering. The relevant behaviors found from the zero limit of \(K_{\rho}, K_{\sigma}, 1/K_{\rho}\) and \(K_S\) exhibit the phase locking of \(\theta_{\rho^+}, \theta_{\sigma^+}, \theta_{C^-}\) and \(\theta_{S^+}\), which are given by \(\sqrt{2}\theta_{\rho^+} = \pi/2\), \(\sqrt{2}\theta_{\sigma^+} = 0\), \(\sqrt{2}\theta_{C^-} = 0\) and \(\sqrt{2}\theta_{S^+} = \pi\) from relevant behaviors of curves (3), (6), (7), (10) and (11). Other coupling constants, which are expected to decrease, are still large due to the second order perturbation. The change of the sign of \(G_{\rho^+-S^+}\) in the renormalization process comes from the relevance of \(\theta_{\sigma^+}\) and \(\theta_{S^+}\). The effect of \(t_\perp\) on coupling constants becomes large at low energies where the splitting of magnitudes becomes noticeable for the forward scattering (between curves (1) and (4) and between curves (2) and (3)), the backward scattering (curves (5), (6), (7) and (8)), and the umklapp scattering (curves (9), (10), (11) and (12)).

In Fig. 3, the \(l\)-dependence of \(t_\perp\) is shown for the fixed \(t_{d}/t = 0.05\), \(t_{d,c}/t(\approx 0.082)\) and 0.1. The increase of \(t_d\) leads to the suppression of \(t_\perp(l)\). The case of \(t_{d}/t = 0.05\) shows the relevant behavior, which corresponds to deconfinement. The quantity \(t_\perp(l)\) for \(t_{d}/t = 0.1\) does not increase monotonically but decreases to zero after taking a maximum indicating confinement. The quantity \(t_\perp(l)\) with a critical magnitude of \(t_{d} = t_{d,c}\) denotes the behavior between the confinement and the deconfinement. For comparison, we show the dotted curve (the dashed curve which is calculated for \(U = 0\) (\(U/t = 5\), \(t_{d}/t = 0.05\) but \(g_3 = 0\) as a special choice of parameter) where the analytical expression for the dotted curve is given by \(t_\perp(l) = t_\perp e^t\). Note that the dashed curve is different from the case of \(U/t = 5\) and \(t_d = 0\). The dashed curve is evaluated to obtain \(t^\text{eff,0}_\perp\), which denotes the interchain hopping renormalized only by the intrachain interaction, i.e., without the umklapp scattering. The effective interchain hopping \(t^\text{eff,0}_\perp\) is defined by \(t^\text{eff,0}_\perp = t \exp[-t^\text{eff,0}_\perp]\) where \(t_\perp(t^\text{eff,0}_\perp)/t = 1\) for \(g_3 = 0\). The quantity \(t^\text{eff,0}_\perp/t\) becomes unity for \(U = 0\) or \(t_\perp/t = 1\). The inset denotes the \(t_\perp\)-dependence of \(t_{d,c}\) for the fixed \(U/t = 3, 4,\) and 5.

In Fig. 4, the \(l\)-dependence of \(K_{\rho}(l)\) for \(U/t = 5\) with the fixed \(t_{d}/t = 0.05\) and 0.1 where \(t_\perp = 0\) for the dashed curve and \(t_\perp = 0.1\) for the solid curve. The arrow denotes \(l_{\Delta}\) defined by \(K_{\rho}(l_{\Delta}) = K_{\rho}/2\). The inset exhibits the charge gap: \(\Delta_0^{l_{\Delta}}\) for \(t_{d}/t = 0\) (dashed curve) and \(\Delta_{\rho}\) for \(t_\perp = 0.1\) (solid curve).
The boundary between confinement (\(t_d > t_{d,c}\)) and deconfinement (\(t_d < t_{d,c}\)) depends appreciably on \(U\), which gives rise to the enhancement of the confined region on the plane of \(t_\perp\) and \(t_d\). The limiting form for small \(t_\perp\) is given by \(t_{d,c}/t \propto (t_\perp/t)^{\rho} \) with the \(U\)-dependent \(\rho\).

The \(l\)-dependence of \(K_\rho(l)\) is shown by solid curve for the fixed \(t_d/t = 0.05\) and 0.1 in Fig. 4. The charge gap is defined by \(\Delta_\rho = v_F \alpha^{-1} \exp[-l_\Delta] \) with \(K_\rho(l_\Delta) = K_\rho/2\) and \(v_F \alpha^{-1} = t(\pi/\sqrt{2})(1 - (t_d/t)^2)/(1 + (t_d/t)^2)^{1/2}\). The dashed curve, which denotes \(K_\rho(l)\) for \(t_\perp = 0\), leads to the charge gap, \(\Delta^{1D}_\rho\), for one-dimensional (1D) case in the presence of dimerization, \(t_d\). The charge gap is suppressed slightly by the interchain hopping since \(K_\rho(l)\) for the solid curve decreases slowly compared with that for the dashed curve, i.e., \(l_\Delta\) is increased by \(t_\perp\). Such a behavior is understood from eq. (5) with \(\nu = \rho\), in which the first term of the r.h.s. becomes small due to the Bessel function suppressed by the large \(t_\perp\). The inset exhibits the charge gap as a function of \(t_d\) with the fixed \(U/t = 3, 4\) and 5 where the solid (dashed) curve corresponds to the case of \(t_\perp/t = 0.1\) (0). Note that the dashed curve is given by \(\Delta^{1D}_\rho \propto W^2(g_3/W)^{1/(2 - 2K_\rho)}\) [10].

In Fig. 5, the \(t_\perp\)-dependence of \(t^{\text{eff}}_\perp\) with \(U/t = 5\) (\(U/t = 3\)) is shown by the solid (dotted) curve for \(t_d/t = 0\) (1), 0.05 (2) and 0.1 (3) \(t_d/t = 0\) (4), 0.05 (5) and 0.1 (6)], where the effective interchain hopping \(t^{\text{eff}}_\perp\), including the effect of the dimerization, is estimated by \(t^{\text{eff}}_\perp = t \exp[-l_\Delta]\) with \(t_\perp(l_{\text{eff}})/t = 1\) [4]. The curves (1) and (4) for small \(t_\perp/t\) well reproduce the analytical result given by \(t^{\text{eff}}_\perp/t_\perp \propto (t_\perp/t)^{\alpha_0/(1 - \alpha_0)}\) with the \(U\)-dependent quantity \(\alpha_0 = (K_\rho + K_{\rho}^{-1} + K_\sigma + K_{\sigma}^{-1} - 4)/4\) [1]. Comparing the slope of curve (1) with that of curve (4), one finds that the renormalization of \(t_\perp\) increases by the intrachain interaction \(U\). With decreasing \(t_d/t\), the ratio \(t^{\text{eff}}_\perp/t_\perp\) decreases rapidly and becomes zero for \(t_\perp\) less than a critical value of \(t_\perp\) indicated by the arrow.

From the inset of Fig. 3 and that of Fig. 4, we obtain the phase diagram of confinement (I) and deconfinement (II) on the plane of \(t_\perp\) and \(\Delta_\rho\). In Fig. 6, the boundary between these two states is shown for \(U/t = 3\) (dashed curve), 4 (dotted curve) and 5 (solid curve). The boundary is rather straight and the \(U\)-dependence becomes small compared with that of the inset of Fig. 3. It has been claimed previously that such a behavior indicates the competition between the charge gap and the interchain hopping \(t_\perp\) [4, 11]. However such a statement is not clear enough since the boundaries depend on the choice of \(U\). This problem can be remedied by the following treatment. We take \(\Delta^{1D}_\rho(t^{\text{eff}}_\perp)\) in stead of \(\Delta_\rho(t_\perp)\) as the vertical (horizontal) axis on the phase diagram where \(\Delta^{1D}_\rho\) is obtained from the dashed curve of the inset of Fig. 4. The resultant boundaries are shown in the inset of Fig. 6, where the good coincidence is obtained among these three curves. Thus it is concluded that the boundary between confinement and deconfinement is determined by the competition between the one-dimensional charge gap (i.e., in the absence of the interchain hopping) and the interchain hopping renormalized only by the intrachain interaction (i.e., without the umklapp scattering).

§4. Discussion

We have examined the mechanism of confinement in terms of quarter-filled two-coupled chains with dimerization as a model of low dimensional systems. The confinement occurs when the charge gap induced by the umklapp scattering becomes larger than the interchain hopping renormalized by the intrachain hopping. It has been found that the ratio for \(U/t = 5\) (\(U/t = 3\) and 0.05 <
Fig. 7. The phase diagram of confinement (I) and deconfinement (II) on the plane of \( t_{\perp} \) and \( \Delta \rho \). The main figure denotes the boundary for \( U/t = 5 \) and \( t_d/t = 0.05 \) with the fixed nearest-neighbor interaction: \( V/t = 0, 0.5 \) and 1. In the inset, the dotted (dashed) curve denotes the boundary for the fixed \( t_d/t = 0.1 \) while the solid curve denotes the boundary for the another case of the Hubbard model at half-filling with \( t_d/t = 0.05 \).

\[ t_{\perp}/t < 0.2 \] is given by \( \Delta_{\rho}^{1D}/t_{\perp}^{\text{eff},0} \simeq 1.8 \) (\( \Delta_{\rho}^{1D}/t_{\perp}^{\text{eff},0} \simeq 1.9 \)) and \( 1.1 \lesssim \Delta_{\rho}/t_{\perp} \lesssim 1.3 \) (\( 1.3 \lesssim \Delta_{\rho}/t_{\perp} \lesssim 1.5 \)).

Here we discuss the effect of nearest neighbor interaction (\( V \)), for the small \( V \), in which the commensurability energy may be negligibly small \([4,5]\). In this case, \( V \) does not contribute to both the backward scattering and the umklapp scattering even in the presence of the dimerization (\( t_d \)). The effect of \( V \) appears in the forward scattering where the coupling constant is expressed as \( g_{2\parallel} = g_{2\parallel} = 2V \) and \( g_{2\perp} = g_{4\perp} = (U + 2V)a \). In Fig. 7, the boundary of confinement-deconfinement transition with \( U/t = 5 \) is shown for \( V/t = 0, 0.5 \) and 1 where \( V \) enhances the confined region.

Finally we comment on the case of two-coupled chain with the conventional half-filled Hubbard model where the phase diagram is shown in the inset of Fig. 7. Compared with those of Fig. 6, the ratio \( \Delta_{\rho}/t_{\perp} \) (\( \simeq 1.7 \) for \( t_{\perp}/t = 0.1 \)) is slightly large and the boundary (solid curve) is rather straight. Such a result is compared with the boundaries for the fixed \( t_d/t = 0.05 \) and 0.1, which are shown by the dotted curve and dashed curve, respectively. With increasing the dimerization, the slope of the boundary becomes steep and moves toward the solid curve since the large dimerization may lead the system to half-filling.

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