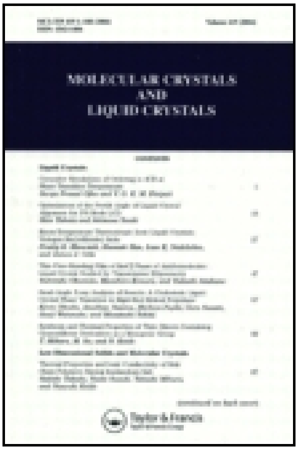

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# Charge Gap and Interchain Correlation in Quasi-One-Dimensional Dimerized Organic Conductors

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# Charge Gap and Interchain Correlation in Quasi-One-Dimensional Dimerized Organic Conductors

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We study the relation between the charge gap and the interchain one-body correlation function in quasi-one-dimensional dimerized organic conductors at quarter filling, by applying the density matrix renormalization group method to a three-chain extended Hubbard model. The charge gap increases with the degree of dimerization in the intrachain hopping integrals. When the charge gap is larger than the interchain hopping integral, the interchain hopping correlation is strongly suppressed, as observed in the $(TMTTF)_2X$ salts.

*Keywords:* charge gap; interchain coherence; dimerization; organic conductors

## INTRODUCTION

**The variety of electronic phases in the temperature-pressure phase diagram of the $(TMTTF)_2X$ and $(TMTSF)_2X$ salts[1] has been regarded as due to decreasing dimerization[2] and increasing three-dimensionality[3] with applied pressure. The wave number of the spin density wave (SDW) is suggested to change from commensurate in the $(TMTTF)_2Br$ salt[4], which is located on the "low-pressure" side, to incommensurate in the $(TMTSF)_2PF_6$ salt[5,6], which is located on the "high-pressure" side of the phase diagram. Above the SDW transition temperatures, the photoexcitations are confined into the chains in $(TMTTF)_2Br$,**

while deconfined in $(TMTSF)_2PF_6$[7]. Among theoretical studies, we have pointed out, with a two-loop renormalization-group (RG) approach to an infinite-chain system, that interchain one-particle coherence is much more easily suppressed by electron correlation when the dimerization produces a charge gap and that interchain two-particle coherence (i.e., long-range order) is then relatively easily restored as dimensionality increases[8]. Similar suppression of interchain motion is presented with a one-loop RG approach to a two-chain bosonized system also[9]. These perturbative methods capture the tendency toward the suppression of the interchain coherence from the high-temperature side. Here, in order to study the relation between the charge gap and the interchain one-body correlation function in the ground state, we adopt the density matrix renormalization group (DMRG) method[10].



## THREE-CHAIN EXTENDED HUBBARD MODEL

Since the even-chain systems have a spin gap, we use, as a first step toward quasi-one-dimensional systems, a three-chain extended Hubbard model,

$$H=-t_1\sum_{i=1}^{Lx/2}\sum_{j=1}^{3}\sum_{\sigma=\uparrow,\downarrow}(c^{+}_{2i-1,j,\sigma}c_{2i,j,\sigma}+\text{h.c.})-t_2\sum_{i=1}^{Lx/2-1}\sum_{j=1}^{3}\sum_{\sigma=\uparrow,\downarrow}(c^{+}_{2i,j,\sigma}c_{2i+1,j,\sigma}+\text{h.c.})$$
$$-t_b\sum_{i=1}^{Lx}\sum_{j=1}^{2}\sum_{\sigma=\uparrow,\downarrow}(c^{+}_{i,j,\sigma}c_{i,j+1,\sigma}+\text{h.c.})+U\sum_{i=1}^{Lx}\sum_{j=1}^{3}n_{i,j,\uparrow}n_{i,j,\downarrow}+V\sum_{i=1}^{Lx-1}\sum_{j=1}^{3}n_{i,j}n_{i+1,j}\ ,$$

where $n_{i,j,\sigma}=c^{+}_{i,j,\sigma}c_{i,j,\sigma}$, $n_{i,j}=\Sigma_\sigma\ n_{i,j,\sigma}$, and $c^{+}_{i,j,\sigma}$ ($c_{i,j,\sigma}$) creates (annihilates) an electron with spin $\sigma$ on the $i$th site of the $j$th chain. The intrachain hopping integrals $t_1$ and $t_2$ are larger than the interchain hopping integral $t_b$. Here $U$ represents the on-site repulsion strength, and $V$ the intrachain nearest-neighbor

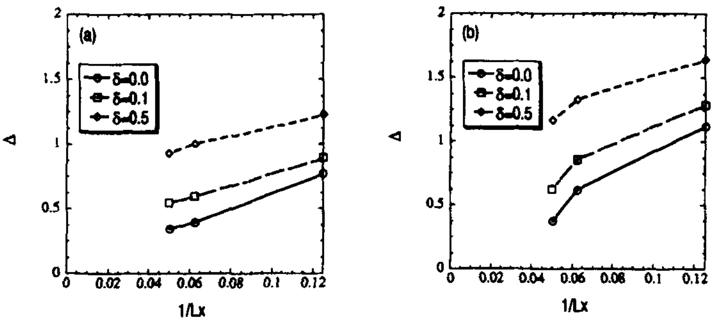


FIGURE 1 Charge gap $\Delta$ for $\delta=0$ (solid line), 0.1 (dash-dotted line), 0.5 (dashed line) and (a) $V=1$, (b) $V=2$. Other parameters are $t_b=0.1$, $U=4$, and $(L_x, m)=(8, 100), (16, 120), (20, 150)$.

repulsion strength. The degree of dimerization is defined as $\delta=(t_1-t_2)/(t_1+t_2)$. In order to compare the results with those in the perturbative calculations, we fix the Fermi velocity in the chain direction, i.e., $t=t_1t_2[(t_1^2+t_2^2)/2]^{-1/2}=1$. The $(TMTTF)_2X$ and $(TMTSF)_2X$ salts generally correspond to $(\delta, t_b)=(0.2, 0.04)$ and (0.05, 0.1), respectively[11]. We adopt the open boundary condition for the $L_x$x3 lattice and consider quarter filling (i.e., $L_x$x3/4 electrons for each spin). In the DMRG calculations, the number of states kept, $m$, is taken up to 150 for $L_x$ up to 20. Since the calculated wave function depends on the initial guess, we iterate sweeps in the finite system algorithm from several initial states having the spin rotational symmetry, though the wave functions converge to broken-symmetry states.

## RESULTS

The charge gap $\Delta$ is calculated from the equation, $2\Delta=E(L_x3/4-1, L_x3/4-1)+$

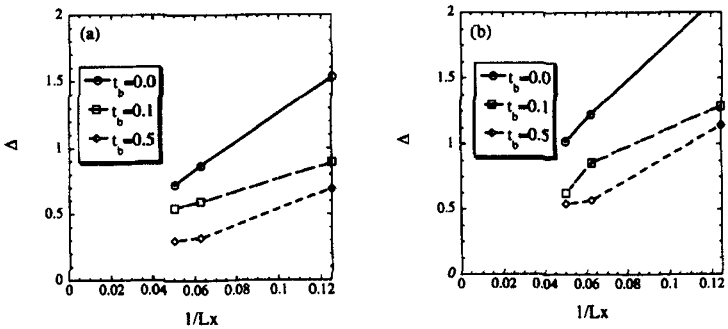


FIGURE 2 Charge gap $\Delta$ for $t_b$=0 (solid line), 0.1 (dash-dotted line), 0.5 (dashed line) and (a) $V$=1, (b) $V$=2. Other parameters are $\delta$=0.1, $U$=4, and $(L_x, m)$=(8, 100), (16, 120), (20, 150).

$E(L_x \times 3/4+1, L_x \times 3/4+1)-2E(L_x \times 3/4, L_x \times 3/4)$, where $E(n_\uparrow, n_\downarrow)$ is the ground state energy for $n_\uparrow$ up- and $n_\downarrow$ down-spin electrons. For $t_b=\delta=0$ and $V<U/2$, $\Delta$ is known to vanish in the $L_x \to \infty$ limit. For $t_b=0$, a finite value of $\delta$ causes the umklapp process, which results in a finite $\Delta$[2]. The charge gap $\Delta$ is expected to survive for small $t_b$ when $\delta$ is large enough[8,9]. The results shown in Figs. 1 and 2 are consistent with the expectation so far. In the $L_x \to \infty$ limit, $\Delta$ should vanish for $\delta=0$ in Fig. 1. For $U=4$ and $V=2$ in Fig. 1(b), the extrapolation to the $L_x \to \infty$ limit is not good partly because it is expected to be near the quantum phase transition to an insulator (located near $V=U/2$ for $t_b=\delta=0$). Furthermore, the $L_x=8n$ and $L_x=8n+4$ series would lie on different lines as the $L_x=4n$ and $L_x=4n+2$ series at half filling, so that the extrapolation is not smooth. Figure 1 suggests that $\Delta$ increases with $V$, as naively expected.

So far, the $t_b$ dependence of $\Delta$ has not been studied well. Figure 2 shows

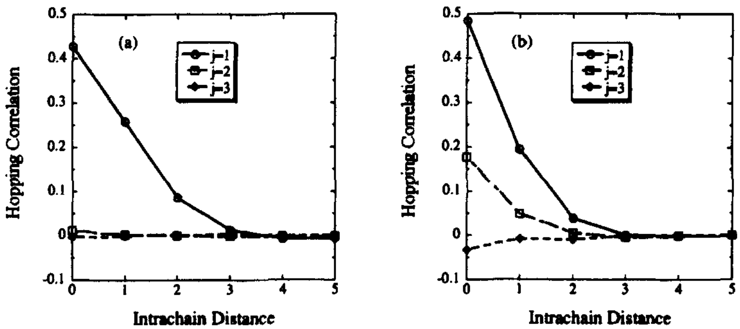


FIGURE 3 Hopping correlation $\Sigma_\sigma < c^+_{Lx/2,j',\sigma}\ c_{Lx/2-i,j,\sigma} >$ as a function of $i$ for $j'=1$ with $j=1$ (solid line), $j=2$ (dash-dotted line), $j=3$ (dashed line) and (a) $t_b=0.1$, (b) $t_b=0.5$. Other parameters are $\delta=0.1$, $U=4$, $V=1$, and $(L_x, m)=(20, 120)$.

that $\Delta$ decreases as $t_b$ increases. For $t_b=0.5$ already, the $L_x=8n$ series of $\Delta$ seems to vanish in the $L_x\rightarrow\infty$ limit. The charge gap $\Delta$ may disappear for smaller $t_b$. Here, the data for $t_b=0$ are exact. Thus, the extrapolation of the $L_x=8n$ series of $\Delta$ for $t_b=0.1$ (from the two data points) to the $L_x\rightarrow\infty$ limit is overestimated. Below we compare the interchain one-body correlation function for different $\delta$ and $t_b$, thus for different $\Delta$ at finite $L_x$. It is found that they show different behavior roughly according to $t_b$ larger or smaller than $\Delta$ at finite $L_x$.

It is interesting to observe how the interchain one-particle coherence is restored when $t_b$ increases. Figure 3 shows the hopping correlation function $\Sigma_\sigma < c^+_{Lx/2,j',\sigma}\ c_{Lx/2-i,j,\sigma} >$ as a function of the intrachain distance $i$ and the chain index $j$. It decays exponentially as the intrachain distance increases because of a finite $\Delta$. When the interchain hopping correlation is compared with the intrachain hopping correlation, the former is strongly suppressed for $t_b=0.1$, but it is almost half of the latter for $t_b$=0.5. The charge gaps $\Delta$ of these finite systems are 0.5 and 0.3, respectively. It is concluded that the interchain one-particle coherence is strongly suppressed when $t_b$ is smaller than $\Delta$.

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