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2007 J. Phys.: Condens. Matter 19 145228

(http://iopscience.iop.org/0953-8984/19/14/145228)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 145228 (6pp) doi:10.1088/0953-8984/19/14/145228

Effect of interchain frustration in quasi-one-dimensional conductors at half-filling

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Received 31 August 2006
Published 23 March 2007
Online at stacks.iop.org/JPhysCM/19/145228

Abstract

We examine the effect of frustrated interchain hoppings $t_{\perp 1}$ and $t_{\perp 2}$ on one-dimensional Mott insulators. By applying an $N_\perp$-chain two-loop renormalization-group method to the half-filled quasi-one-dimensional Hubbard model, we show that the system remains insulating even for the large $t_{\perp 1}$ as far as $t_{\perp 2} = 0$ and vice versa, whereas a metallic state emerges by increasing both interchain hoppings. We also discuss the metallic behaviour suggested in the quasi-one-dimensional organic compound (TTM-TTP)I_3 under high pressure.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Recently, the quasi-one-dimensional (Q1D) organic compound (TTM-TTP)I_3, which is characterized by a half-filled HOMO band due to presence of the monovalent anion I_3, has attracted much attention following the discovery of an anomalous metallic behaviour at high pressure [1–3]. At ambient pressure, the system exhibits an insulating behaviour below $T_{\rm MI} = 120$ K and can be regarded as a Mott insulator [1, 2]. Quite recently, Yasuzuka *et al* [3] performed resistivity measurements at sufficiently high pressure up to 8 GPa and reported that the metal–insulator transition temperature can be suppressed down to $T_{\rm MI} = 20$ K at $P = 8$ GPa. A metallic ground state was predicted to occur for pressure above 10 GPa.

From a theoretical point of view, the 1D half-filled Hubbard model with the onsite Coulomb repulsion U can be considered as a minimal model to describe a Mott insulator. A large number of analytical and numerical results have been accumulated so far, and in one dimension the exact ground state of the model is known to be Mott insulating for all positive values of interaction $U > 0$. Thus one can expect that a higher-dimensionality effect due to the intercolumn (i.e. interchain) electron transfer plays a key role in the appearance of the predicted metallic behaviour in (TTM-TTP)I_3. From the crystal structures, one can find that

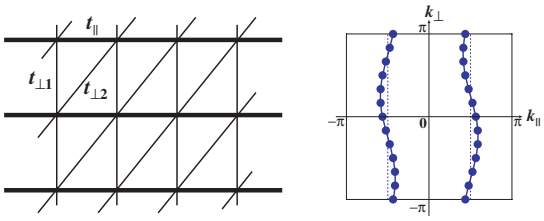

Figure 1. Left: lattice geometry of the present model. Right: the corresponding Fermi surface where the case for $N_\perp = 12$ and $t_{\perp 1} = t_{\perp 2}$ is shown.

the interchain network in (TTM-TTP)I_3 is not so simple since the lattice structure is not simply rectangular. The figures extracted from the extended Hückel calculations [4, 5] indicate that there are two kinds of interchain transfer integral. Both are of the same order of magnitude; that is, the interchain network is frustrated. So we adopt half-filled 1D Hubbard chains coupled by the frustrated interchain hoppings $t_{\perp 1}$ and $t_{\perp 2}$. The lattice geometry is shown in figure 1. We apply a recently developed two-loop renormalization-group (RG) method to this Q1D Hubbard model and show that the system becomes metallic only when the interchain network introduces frustration. We also discuss the metallic state suggested by the resistivity measurements on the (TTM-TTP)I_3 compound [3].

2. Model and renormalization group equations

We consider the quasi-one-dimensional half-filled Hubbard model in which electrons move on a triangular lattice (figure 1). The transfer integrals are highly anisotropic: $t_\parallel \gg |t_{\perp 1}|, |t_{\perp 2}|$ ($t_\parallel (>0)$ is the transfer integral along chains and $t_{\perp 1}$ and $t_{\perp 2}$ are those between chains). Our Hamiltonian is given by $H = H_0 + H_{\rm I}$ where

$$H_0 = -t_\parallel \sum_{j,l,s} \left(c^\dagger_{j,l,s} c_{j+1,l,s} + \text{H.c.} \right) - t_{\perp 1} \sum_{j,l,s} \left(c^\dagger_{j,l,s} c_{j,l+1,s} + \text{H.c.} \right) - t_{\perp 2} \sum_{j,l,s} \left(c^\dagger_{j,l,s} c_{j+1,l+1,s} + \text{H.c.} \right) - \mu \sum_{j,l,s} c^\dagger_{j,l,s} c_{j,l,s}, \tag{1}$$

$$H_{\rm I} = U \sum_{j,l} n_{j,l,\uparrow} n_{j,l,\downarrow}. \tag{2}$$

The operator $c_{j,l,s}$ denotes electron annihilation on the jth site in the lth chain with spin s, and $n_{j,l,s} = c^\dagger_{j,l,s} c_{j,l,s} - \frac{1}{2}$. The system size along chains (L) is considered to be sufficiently large and the site index j, which runs $j = 1, \ldots, L$, is to be understood as an integral in the thermodynamic limit. The chain index runs $l = 1, \ldots, N_\perp$, and we consider the system with finite number of chains $N_\perp$, where the periodic boundary condition is imposed: $c_{j,N_\perp+1,s} = c_{j,1,s}$.

By applying the Fourier transformation, the kinetic term can be rewritten as $H_0 = \sum_{\boldsymbol{k},s} \varepsilon(\boldsymbol{k}) c^\dagger_{\rm s}(\boldsymbol{k}) c_{\rm s}(\boldsymbol{k})$, where $\boldsymbol{k} \equiv (k_\parallel, k_\perp)$ and the energy dispersion is given by

$$\varepsilon(\boldsymbol{k}) = -2t_\parallel \cos k_\parallel - 2t_{\perp 1} \cos k_\perp - 2t_{\perp 2} \cos(k_\parallel + k_\perp) - \mu. \tag{3}$$

The transverse momentum is given by $k_\perp = (2\pi/N_\perp)n$ where $n = -(N_\perp/2)+1, \ldots, (N_\perp/2)$. For small interchain hopping $|t_{\perp i}| \ll t_\parallel$, the system has an open Fermi surface (figure 1) where the Fermi surface can be identified by the transverse momentum $k_\perp$ [6]. By focusing on the

lowest-order terms of the interchain hopping $t_{\perp 1}$ and $t_{\perp 2}$, the Fermi surfaces for right- and left-moving electrons are given by ($p = +/- = R/L$)

$$k_{\mathrm{F}}^{p}(k_{\perp}) = +p\frac{\pi}{2} + p\frac{t_{\perp 1}}{t_{\parallel}}\cos k_{\perp} - \frac{t_{\perp 2}}{t_{\parallel}}\sin k_{\perp}, \tag{4}$$

and the chemical potential is $\mu = \mathrm{O}(t_{\perp i}^{2})$. The Fermi surface is symmetric with respect to $\boldsymbol{k} \leftrightarrow -\boldsymbol{k}$. By considering the weak-interacting case, we linearize the dispersion near the Fermi energy. By further neglecting the $k_{\perp}$ dependence of the velocity, the linearized dispersion is given in a simple form: $\varepsilon_{p}(\boldsymbol{k}) = pv[k_{\parallel} - k_{\mathrm{F}}^{p}(k_{\perp})]$ with $v = 2t_{\parallel}$.

Based on this dispersion relation, we apply the perturbative RG method and clarify the appearance of the metallic state due to frustration from interchain hopping. In the weak-coupling RG approach, a 1D Mott insulating behaviour follows from the relevance of electronic Umklapp scattering, which has a bare finite amplitude at half-filling [7]. The dimensionality effects on a 1D Mott insulator have also been examined numerically by the dynamical mean-field approach extended to include one-dimensional fluctuations (the so-called chain-DMFT) [8, 9] and by a field-theoretical method coupled to an RPA approach to interchain hopping [10]. Fermi surface nestings, however, which are non-perturbative effects in $t_{\perp}$ and are crucial to the description of weak coupling 1D Mott insulators, are not taken into account in these approaches. In the present $N_{\perp}$-chain RG approach, these Fermi surface effects are included [11, 12]. In order to clarify the metallic behaviour theoretically, one has to examine the properties of the one-particle Green's function, i.e., the self-energy corrections, whose singular contributions only appear beyond the one-loop level of the RG. In the present paper, we apply the recently developed two-loop RG theory [6] to the present half-filled Q1D Hubbard chains.

Here we briefly recall the formulation of the two-loop RG method for the Q1D systems. The detailed formulation is given in [6] and we adopt the same notations. We first introduce the coupling constants $g_{1\perp}$, $g_{2\perp}$, $g_{\parallel}$, $g_{3\perp}$, and $g_{3\parallel}$, which represent the backward scattering with opposite spins ($g_{1\perp}$), the forward scattering with opposite spins ($g_{2\perp}$), the forward scattering with the same spins ($g_{\parallel}$), the Umklapp scattering with opposite spins ($g_{3\perp}$), and the Umklapp scattering with the same spins ($g_{3\parallel}$). Furthermore, the coupling constants are differently renormalized depending on the external momenta of the vertex and have the explicit transverse-momentum (i.e., patch-index) dependence. To take these effects into account, we introduce the transverse-momentum dependence of the coupling constants in the initial g-ology Hamiltonian. In terms of the Hubbard interaction U, the magnitude of the couplings are given by $g_{1\perp(q_{\perp},k_{\perp 1},k_{\perp 2})} = g_{2\perp(q_{\perp},k_{\perp 1},k_{\perp 2})} = g_{3\perp(q_{\perp},k_{\perp 1},k_{\perp 2})} = U$ and $g_{\parallel(q_{\perp},k_{\perp 1},k_{\perp 2})} = g_{3\parallel(q_{\perp},k_{\perp 1},k_{\perp 2})} = 0$. To simplify the notation in the following, we will suppress the $\perp$ index of transverse momenta. As in the 1D case, the physical picture becomes transparent by introducing a new set of couplings: $g_{\rho(q,k_1,k_2)} \equiv (g_{2\perp(q,k_1,k_2)} + g_{\parallel(q,k_1,k_2)})$, $g_{\sigma(q,k_1,k_2)} \equiv (g_{2\perp(q,k_1,k_2)} - g_{\parallel(q,k_1,k_2)}) = g_{1\perp(q,k_1,k_2)}$, $g_{c(q,k_1,k_2)} \equiv g_{3\perp(q,k_1,\pi-k_2)}$, and $g_{cs(q,k_1,k_2)} \equiv g_{3\parallel(q,k_1,\pi-k_2)}$, where g_{ρ} and g_{c} (g_{σ} and g_{s}) are the coupling constants representing the charge (spin) degrees of freedom. The RG equations, which are not shown explicitly, are derived by scaling the bandwidth cutoff Λ as $\Lambda_l = \Lambda \mathrm{e}^{-l}$, where l is the scaling parameter. The most important quantity in the present analysis is the renormalization factor $z_{k_{\perp}}$, which is determined by the two-loop self-energy corrections. The explicit form of the RG equation for the wavefunction renormalization is

$$\frac{\mathrm{d}}{\mathrm{d}l}\ln z_{k} = -\frac{1}{2N_{\perp}^{2}}\sum_{q,k'} G_{\Sigma n(q,k,k')}^{2} J_{1(q,k,k')} - \frac{1}{2N_{\perp}^{2}}\sum_{q,k'} G_{\Sigma u(q,k,k')}^{2} J'_{1(q,k,k')}, \tag{5}$$

where $G_{\Sigma n}^{2}$ and $G_{\Sigma u}^{2}$ denote the coupling constants

$$G_{\Sigma n(q,k,k')}^{2} \equiv \tfrac{1}{2}\left[G_{\rho(q,k,k')}^{2} + 3\,G_{\sigma(q,k,k')}^{2}\right], \tag{6}$$

$$G_{\Sigma u(q,k,k')}^{2} \equiv G_{c(q,k,k')}^{2} + G_{c(\pi-q+k+k',k,k')}^{2} - G_{c(q,k,k')}G_{c(\pi-q+k+k',k,k')} \tag{7}$$

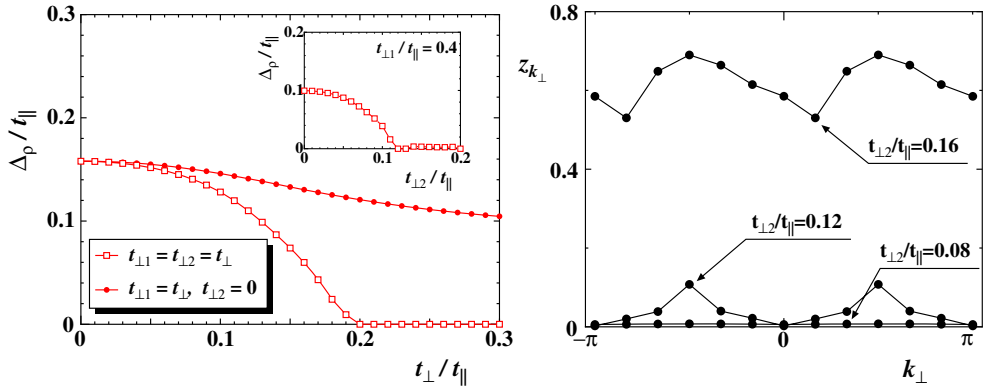

Figure 2. Left: charge gap Δ_ρ as a function of $t_\perp$ for $U/t_\parallel = 2$, $N_\perp = 12$. The $t_{\perp 2}$ dependence of Δ_ρ with fixed $t_{\perp 1}/t_\parallel = 0.4$ is shown in the inset. Right: the wavefunction renormalization factor $z_{k_\perp}(l = 7)$ for $U/t_\parallel = 2$, $N_\perp = 12$, $t_{\perp 1}/t_\parallel = 0.4$ with several $t_{\perp 2}/t_\parallel$.

with $G_\nu = g_\nu/(2\pi v)$. The quantities $J_{1(q,k,k')}$ and $J'_{1(q,k,k')}$ are nonuniversal cutoff functions of $t_{\perp i}/\Lambda$.

3. Results

The $t_\perp$ dependence of the charge gap is shown in figure 2 for the cases with ($t_{\perp 1} = t_{\perp 2} = t_\perp$) and without ($t_{\perp 1} = t_\perp$ and $t_{\perp 2} = 0$) frustration. The criterion for the occurrence of energy gaps is the same as in [6]: $\Delta_\nu = \Lambda e^{-l_\nu}$, where $G_{\nu+}(l_\nu) = O(1)$. The results for the rectangular lattice ($t_{\perp 2} = 0$) are also shown where the system is always insulating even for large $t_{\perp 1}$ [6]. In the case with frustration, the charge gap is strongly reduced; for the parameters used in the model, it is found to vanish at $t_\perp/t_\parallel \approx 0.2$. This collapse of the charge gap occurs when the interchain hopping becomes comparable with the charge gap at $t_\perp = 0$, which behaviour is reminiscent for the deconfinement transition suggested in the quasi-one-dimensional Mott insulators [8, 9]. The charge gap for large interchain hopping shows large size ($N_\perp$) dependence for the frustrated case, while it is almost $N_\perp$ independent for the case without frustration. This size dependence for large interchain hopping implies that the metallic state appears as a result of frustrated interchain hopping in the large-$N_\perp$ limit. The emergence of the metallic behaviour can be attributed to nesting deviations of the Fermi surface that prevent the normal state from becoming unstable towards a spin-density-wave formation. The Fermi surface would be perfectly nested if $t_{\perp 1} \neq 0$ and $t_{\perp 2} = 0$, or $t_{\perp 1} = 0$ and $t_{\perp 2} \neq 0$. In the former case, the nesting vector is $\boldsymbol{Q} = (\pi, \pi)$ whereas, in the latter case, $\boldsymbol{Q} = (\pi, 0)$.

The metallic behaviour can also be confirmed from the wave function renormalization factor $z_{k_\perp}$. The $k_\perp$ dependence of $z_{k_\perp}(l)$ with $l = 7$ for several values of $t_{\perp 2}$ with fixed $t_{\perp 1}/t_\parallel$ is shown in figure 2. For the rectangular lattice ($t_{\perp 2} = 0$), this quantity takes a small value and has very weak $k_\perp$ dependence, consistent with the existence of an insulating state. On the other hand, it takes sizable values and shows a strong $k_\perp$ dependence for strong interchain frustration. The quantity $z_{k_\perp}$ presents a broad maximum around $k_\perp \approx \pm\pi/2$, which behaviour implies that the Fermi pockets [10] or 'cold' regions [11, 12] appear around $\boldsymbol{k} \approx (k_F^p(\pm\pi/2), \pm\pi/2)$.

4. Summary and discussion

In summary, we have examined the effect of the interchain frustration for half-filled Q1D Hubbard chains by applying an $N_\perp$-chain two-loop RG method. We have analysed both the

$t_\perp$ dependence of the Mott gap and the quasi-particle weight $z_{k_\perp}$. The lattice geometry of the system is crucial to the Mott insulating behaviour, and the metallic state is obtained only when the network of interchain hopping sufficiently frustrates the nesting conditions.

Finally we discuss the metallic state that was suggested to occur in the Q1D organic compound (TTM-TTP)I_3 under high pressure [3]. The estimated magnitude of the Coulomb repulsion between electrons on the same HOMO orbital is $U = 0.57$ eV [1]. From band calculations, the transfer integrals adopted for (TTM-TTP)I_3 are $t_\parallel = 260$ meV, $t_{\perp 1} = 9$ meV, and $t_{\perp 2} = 6$ meV. As shown in figure 2, the interchain frustration is crucial to inducing a metallic state in the present half-filled system. However, the hydrostatic pressure would enhance not only the interchain hopping but also the intrachain hopping $t_\parallel$; thus the strength of the interaction $U/t_\parallel$ (and in turn the magnitude of the charge gap) is effectively reduced. Quantitatively the latter effect would dominate the overall pressure dependence of the transition temperature in (TTM-TTP)I_3 [3]. Our analysis implies that the insulator–metal transition itself is dominated by the interchain frustration and is not controlled by a naive change in the bandwidth. In (TTM-TTP)I_3 at ambient pressure, a non-magnetic state has been reported below the metal–insulator transition temperature, but such a spin state is not reproduced in the present analysis. In order to discuss the spin state in (TTM-TTP)I_3, we have to take into account the inhomogeneity of charge in a single molecule, and that needs further investigation. However, we believe that the scenario of the present paper would capture the mechanism of the metalization and that the spin properties are determined by secondary effects of frozen charge fluctuations.

The Mott transition in an anisotropic triangular lattice in two dimensions has also been addressed by numerical path-integral renormalization-group techniques [13] and the transition from an insulator without magnetic ordering to a paramagnetic metal has been suggested by changing the hopping parameters. Our approach is restricted to the small interchain hopping region; however, the result of the metal–insulator transition would be consistent with the numerical results since the metallic state is observed for finite frustration. The phase boundary of the metal–insulator transition would connect to the ones obtained by the numerics, where the parameter correspondences are $t_\parallel \to t$, $t_{\perp 1} \to t$, and $t_{\perp 2} \to t'$. We have focused the present analysis on the metallic behaviour and did not study the magnetic properties. In order to clarify the magnetic ordering, we have to investigate the susceptibility of various symmetry-broken states based on the RG formalism. Such an analysis on symmetry-broken states will be reported in the future.

Acknowledgments

One of the authors (MT) thanks S Yasuzuka for valuable discussions and for showing him the experimental results prior to publication. He also thanks T Kawamoto for providing him with the revised data of the extended Hückel calculations on the (TTM-TTP)I_3. This work was supported in part by a Grant-in-Aid for Scientific Research on Priority Areas of Molecular Conductors (No 15073213) from the Ministry of Education, Science, Sports, and Culture, Japan.

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