Collapse of Charge Ordering Due to Disorder in Quasi One-Dimensional Electron Systems

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Abstract. Effects of disorder on charge ordering (CO) is investigated for one-dimensional (1D) and quasi 1D extended Hubbard model with infinite on-site repulsion at quarter filling. Only the forward scattering due to disorder is taken into account. In the 1D model, the resistivity due to Umklapp scattering that is an origin of CO is shown to be suppressed by the forward scattering. In addition, we obtain that the CO transition temperature \(T_{CO}\) for quasi 1D model becomes smaller with increasing strength of the forward scattering.

1. Introduction and model
Charge ordered (CO) states, in which inhomogeneous but regular charge arrangement is realized, has been found in strongly correlated electron systems such as transition metal oxides\[1\] and molecular conductors\[2\]. Such a charge arrangement occurs in order to gain the repulsive nearest neighbor and/or next nearest neighbor Coulomb interaction. Therefore, the state has been analyzed based on the extended Hubbard (EH) model with the off-site interaction as well as the on-site one\[3\]. On the other hand, disorder has been also known to lead to charge localization, so called Anderson localization. However, effect of disorder and that of mutual interaction compete with each other because the charge pattern by the former is random whereas the latter gives rise to the regular charge arrangement. In the present study, we investigate the effects of disorder on CO of one-dimensional (1D) and quasi-1D electron systems.

We consider the EH chains at quarter filling coupled by the interchain interaction \(V_\perp\)[4, 5, 6]. The case with the infinite on-site repulsion is discussed\[7\], and then the model is expressed by the spinless Fermion system as

\[
\mathcal{H} = \sum_l \mathcal{H}_l + V_\perp \sum_{j,j',l} n_{j,l} n_{j',l'},
\]

\[
\mathcal{H}_l = -t \sum_j \left( c_{j+1,l}^\dagger c_{j,l} + \text{h.c.} \right) + V \sum_j n_{j+1,l} n_{j,l},
\]

where \(c_{j,l}^\dagger\) is the creation operator of the spinless Fermion at the \(j\)-th cite in the \(l\)-th chain and \(n_{j,l} = c_{j,l}^\dagger c_{j,l}\). The quantities \(t\) and \(V\) express the hopping and the mutual interaction between the nearest neighbor site in the chain, respectively. In Eq. (1), \((l,l')\) denotes a pair of the adjacent chains. The term expressing the interchain interaction is treated by the interchain meanfield approximation, \(n_{j,l} n_{j',l'} \rightarrow \langle n_{j,l} \rangle n_{j',l'} + n_{j,l} \langle n_{j',l'} \rangle - \langle n_{j,l} \rangle \langle n_{j',l'} \rangle\). Assuming CO with...
two-fold periodicity as \( \langle n_{j,t} \rangle = (-1)^{j+t}n \), we obtain the effective 1D model, which is expressed by the bosonized form \([4]\),

\[
H = \frac{\nu}{4\pi} \int dx \left\{ \frac{1}{2K} (\partial_x \theta)^2 + 2K (\partial_x \phi)^2 \right\} + \frac{\nu G}{\pi a^2} \int dx \cos 2\sqrt{2}\theta - \frac{zV_n n}{\pi a} \int dx \sin 2\sqrt{2}\theta, \tag{3}
\]

where the phase variables satisfy the commutation relation, \([\theta(x), \partial_y \phi(y)] = -2\pi i \delta(x-y)\), and \( a \) is the lattice spacing. Here, \( z \) means the number of the adjacent chains and \( G = V a/(2\pi \nu) \). The order parameter of CO is given self-consistently by \( n = \langle \sin \sqrt{2}\theta \rangle/\pi \) where \( \langle \cdots \rangle \) means thermal average. In the following, we consider the case \( 0 \leq V \leq 2t \) where the strictly 1D chain is in the metallic state with the velocity of excitation and the exponent having the following expression, \( v = \pi t a / \sqrt{1 - (V/2t)^2} \cos^{-1}(V/2t) \) and \( K = [4 - (4/\pi) \cos^{-1}(V/2t)]^{-1} \). On the other hand, the infinitesimally small \( V_\perp \) makes the system insulating and gives rise to the finite \( T_{CO} \)[4].

As an impurity potential, we take into account of the forward scattering. Though the forward scattering does not lead to charge localization, it will be shown to play a key role for the formation of CO. The Hamiltonian reads,

\[
H_{\text{imp}} = \frac{1}{\sqrt{2}\pi} \int dx \tilde{u}(x) \partial_x \theta, \tag{4}
\]

where \( \tilde{u}(x) \) is the random field satisfying \( \langle \tilde{u}(x) \tilde{u}(y) \rangle_{\text{imp}} = (\nu_F / \tau_f) \delta(x-y) \) with \( \tau_f \) and \( \nu_F \) being the relaxation time of the forward scattering and the Fermi velocity, respectively\([8]\). Here, \( \langle \cdots \rangle_{\text{imp}} \) expresses the average in terms of the impurity configuration. Equation (4) can be absorbed in the free part of the bosonic Hamiltonian by defining \( \theta = \theta + ((2\sqrt{2}K/v) f^x dx' \tilde{u}(x'))[9] \).

\[\text{2. Resistivity}\]

At first, we consider the strictly 1D system where \( V_\perp = 0 \). The dynamical conductivity \( \sigma(\omega) \), which is expressed by the memory function \( M(\omega) \), is written as follows\([10, 11]\),

\[
\sigma(\omega) = -i \chi^R(0) \frac{1}{\omega + M(\omega)}, \tag{5}
\]

\[
M(\omega) = -\frac{1}{\chi^R(0)} \frac{\langle F_\omega F \rangle}{\omega} - \langle F_\omega F \rangle_{\omega=0}, \tag{6}
\]

where

\[
\langle A; A \rangle_\omega = -i \int dx \int_0^\infty dt e^{i(\omega+in)t} \langle [A(x,t), A(0,0)] \rangle,
\]

with \( \eta \to +0 \). In Eq. (6), \( F = [j, \mathcal{H}] \) with \( j = \sqrt{2}vK \partial_x \phi/\pi \) being the current operator and \( \chi^R(0) = \langle \langle j; j \rangle \rangle_{\omega=0} = -2vK/\pi \).

In the presence of impurity forward scattering, the quantity \( F(x,t) \) is given by \( F(x,t) \propto \sin \left\{ 2\sqrt{2}\theta(x,t) - (8K/v) f^x dx' \tilde{u}(x') \right\} \). The formula leads to the following expression;

\[
\langle F(x,t) F(0,0) \rangle_{\text{imp}} = \exp \left\{ -\frac{\nu_F}{2\tau_f} \left( \frac{8K}{v} \right)^2 |x| \right\} \langle F(x,t) F(0,0) \rangle_{a=0}. \tag{8}
\]

Thus, the Memory function becomes smaller compared with that in the absence of impurity forward scattering. As a result, the resistivity \( \rho(T) = iM(0)/\chi^R(0) \) is suppressed. In Fig. 1, the obtained resistivity \( \rho(T) \) in arbitrary unit (a) and the normalized one \( \rho(T)/\rho_0(T) \) (b) are
shown as a function of temperature $T$ for several choices of $a/(v_F \tau_f)$. Here, the quantity $\rho_0(T)$ is the resistivity in the absence of disorder [11, 6],

$$\rho_0(T) = \frac{a \pi}{4} \frac{1}{(\chi R(0))^2} \left( \frac{8KvG}{\pi a} \right)^2 \left( \frac{2\pi aT}{v} \right)^{16K-3} B^2(4K, 4K),$$

(9)

where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$. As is easily observed in Fig. 1, suppression becomes significant when the temperature is lowered.

3. CO transition temperature

Next, we discuss the CO transition temperature $T_{CO}$ of the quasi 1D system, which is determined by the following equation,

$$1 = \frac{zV_\perp}{\pi^2 a} \int_0^{T_{CO}} dx \int_0^T d\tau \langle \sin \{ \sqrt{2}\tilde{\theta}(x, \tau) - \frac{4K}{v} \int_0^x dx' \tilde{u}(x') \} \sin \{ \sqrt{2}\tilde{\theta}(0, 0) - \frac{4K}{v} \int_0^0 dx' \tilde{u}(x') \} \rangle_{imp}$$

$$= \frac{zV_\perp}{\pi^2 a} \int_0^{T_{CO}} dx \exp \left\{ - \frac{v}{2\tau_f} \left( \frac{4K}{v} \right)^2 |x| \right\} \int_0^T d\tau \langle \sin \sqrt{2}\tilde{\theta}(x, \tau) \sin \sqrt{2}\tilde{\theta}(0, 0) \rangle.$$  

(10)

In the calculation of the second line in Eq. (10), the term $\cos 2\sqrt{2}\tilde{\theta}$ in Eq. (3) is safely neglected because the term is renormalized to zero in the low energy limit for $0 \leq V \leq 2t$. In the case of $1/\tau_f \rightarrow 0$, the infinitesimal $V_\perp$ leads to the finite $T_{CO}$, namely the critical value of the interchain interaction for appearance of CO at the finite temperature, $V_\perp^c$, is equal to zero. As is easily seen in Figs. 2 (a) and (b), the impurity forward scattering suppresses $T_{CO}$. In addition, the critical value $V_\perp^c$ becomes finite for $0 \leq V < 2t$ as is shown in Fig. 2 (a). In case of $V = 2t$, $T_{CO}$ shows exponential dependence as a function of $(zV_\perp/t)^{-1}$ (see the inset of Fig. 2 (b)), and $V_\perp^c = 0$. Actually, for $T_{CO} \ll K^2(v_F/v)\tau_f^{-1}$, we can obtain the analytical expressions; for $0 \leq V < 2t$,

$$T_{CO} = \frac{v}{a} \left( 1 - \frac{V_\perp^c}{V_\perp} \right)^{1/(4K-1)},$$

(11)

$$zV_\perp^c = (4K - 1) \times 8\pi^2K^2vF^2v\tau_f^{-1},$$

(12)
and for $V = 2t$,

$$T_{CO} = \frac{v}{a} \exp \left\{ -\frac{\pi^2 (v_F/v)}{2 zV/t} \right\}. \quad (13)$$

4. Summary

In the present paper, we took into account of the forward scattering due to disorder and calculated the resistivity of quarter filled 1D EH model originated from Umklapp scattering, and the transition temperature of CO of quasi 1D EH chains coupled by the interchain interaction. We obtained that both quantities are suppressed by the impurity forward scattering. Thus, it was found that the forward scattering due to the impurity potential has a role for destroying CO though the scattering does not give rise to the charge localization. The backward scattering due to the impurity potential, which is ignored in the present study, leads to Anderson localization. The competition between CO and Anderson localization is an interesting problem which is left for future work.

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