Electronic States in Half-Filled Correlated System
with Alternating Potential

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The effect of an alternating potential on a one-dimensional half-filled Hubbard model with repulsive interaction has been examined by applying the renormalization group method to the bosonized Hamiltonian. The electronic state, which is determined by the competition between alternating potential and umklapp scattering, is calculated where the relevance and the irrelevance of the alternating potential leads to the band insulator and the Mott insulator respectively. The excitation gaps for charge and spin fluctuations are calculated for both states.

KEYWORDS: charge gap, half-filling, alternating potential, umklapp scattering, Mott insulator

§1. Introduction

An insulator with mixed ionic-covalent character in the presence of electron correlation is of interest since the large repulsive interaction leads to a Mott insulator due to umklapp scattering at half-filling.

The effect of electron correlation on such an insulator has been studied in some materials which consist of two-kinds of atoms per cell. In the perovskite oxide compounds, BaTiO$_3$, where the ferroelectricity is usually discussed based on the lattice distortion, the covalency plays an important role due to the following fact. The first principle calculation shows that Ba$^{2+}$Ti$^{2.89+}$O$_{3.63}$$^{3-}$ and then the valence is reduced significantly from the formal valence.\textsuperscript{1} Such a prediction is consistent with the XPS experiment.\textsuperscript{2} Further the effect of correlation is also claimed by the fact that dynamical effective charges for oxygen and titanium are large due to the covalence.\textsuperscript{3,4}

In terms of exact diagonalization, the effect of the electron correlation has been examined for a one-dimensional half-filled Hubbard model with alternating potential, which is caused by two kinds of atoms and induces the difference of the site energy.\textsuperscript{5,6} When the repulsive interaction increases or the level separation decreases, the band (ionic-covalent) insulator undergoes a transition into the Mott insulator followed by a jump of electron numbers of each lattice sites. In addition to
the electron-lattice interaction, the electronic polarizability is strongly enhanced near the phase boundary due to the correlation.\textsuperscript{7}

Polarization induced by a sublattice displacement, has been examined for a one-dimensional two-band Hubbard model at half-filling.\textsuperscript{4,8} The number of parameters is reduced by setting equal values of the Hubbard $U$ on two kinds of atoms of oxygen and generic cation, while the site energies are different. At a critical value of interaction corresponding to a transition from a band insulator to a Mott insulator, the static ionic charge is continuous but the polarization and the dynamic charge are discontinuous showing the Berry’s phase\textsuperscript{9} associated with the macroscopic polarization as the primary order parameter. The discontinuity disappears by removing the finite-size effect, i.e., displacing the coarse mesh in order to avoid the $k = 0$ singular point and taking the large number of $k$-points where $k$ is the quasicell momenta.

The model which is the same as ref.\textsuperscript{4} but has the infinite length, has been explored by use of mean-field approximation in order to clarify the nature of electronic states and the relation of the Berry’s phase to the phase transition.\textsuperscript{10} The ground state has antiferromagnetic ordering for large repulsive interaction indicating a magnetic instability while the state is nonmagnetic for small interaction. There exists the gap to the charge excitations independently of the value of repulsive interaction while the system is replaced by antiferromagnet with gapless spin excitations in strong coupling regime and has a gap to all excitations in the opposite limit. Although the magnetic state with the gapless spin excitation is known for the conventional Hubbard model with the repulsive interaction, it is not clear if such an excitation still exists even for the small limit of the alternating potential. Therefore the method beyond the mean-field theory is needed to study the model with the infinite length.

In order to treat strictly one-dimensional fluctuations and electron correlation, we apply, in the present paper, a method of the bosonization to the system, which is the same as refs.\textsuperscript{4} and \textsuperscript{10}. Further, the renormalization group method is utilized where the electronic states of the band insulator and the Mott insulator are determined by the relevance and the irrelevance of alternating potential. In §2, formulation for deriving the renormalization group equations is given in terms of the phase variable, which is based on the bosonization. In §3, the transition from the band insulator to the Mott insulator is calculated as the function of on-site electron-electron interaction and the energy difference between two-sites. In §4, summary is given and the effect of the alternation of the electron hopping energy given by the Su-Schrieffer-Heeger model\textsuperscript{11} is briefly discussed.

\section{Formulation}

The Hamiltonian of one-dimensional half-filled Hubbard model with the alternating potential is given by

\begin{equation}
\mathcal{H} = -t \sum_{j,\sigma} \left( c_{j,\sigma}^\dagger c_{j+1,\sigma} + \text{h.c.} \right) + W_0 \sum_{j,\sigma} (-1)^j n_{j,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow},
\end{equation}

where $c_{j,\sigma}^\dagger$ creates a fermion of spin $\sigma$ at site $j$, $n_{j,\sigma}$ is the number of an electron of spin $\sigma$ at site $j$, and $W_0$ is the strength of the alternating potential.
where \( c_{j,\sigma}^\dagger \) denotes a creation operator for the electron at the \( j \)-th site with spin \( \sigma (= \uparrow, \downarrow) \). \( n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma} \). Quantities \( t, W_0 \) and \( U \) are energies for the transfer integral, the alternating potential and the on-site electron-electron Coulomb repulsive interaction, respectively.

First, eq. (1) is rewritten by use of the Fourier transform, \( c_{k,\sigma} = 1/\sqrt{N} \sum_j e^{-ikR_j} c_{j,\sigma} \), where \( R_j \) is the location of the \( j \)-th lattice site and \( N \) is the total number of the lattice site. The first and second terms of eq. (1) are expressed as, \( \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + W_0 \sum_{k>0,\sigma} \left( c_{k,\sigma}^\dagger c_{k-\pi/a,\sigma} + c_{k-\pi/a,\sigma}^\dagger c_{k,\sigma} \right) \) where \( \varepsilon_k = -2t \cos ka \) and \( a \) is the lattice constant. The dispersion of the kinetic energy, \( \varepsilon_k \), around the Fermi momentum is linearized as \( v_F (pk - k_F) \), where \( v_F (= 2ta) \) and \( k_F (= \pi/2a) \) denote the Fermi velocity and the Fermi momentum, respectively. The fermion operator around the Fermi momentum is rewritten as \( c_{k,p,\sigma} (= c_{k+pF,\sigma} ) \), where \( p (= + \text{ and } -) \) denotes the branch for the right moving and left moving electrons. The third term of eq. (1) is rewritten as \((L = Na)\)

\[
\mathcal{H}_{\text{int}} = \frac{g_1}{L} \sum_{k_1,k_2,q,p} c_{k_1,p,\uparrow}^\dagger c_{k_2,-p,\downarrow} c_{k_2+q,p,\downarrow} c_{k_1-q,-p,\uparrow} + \frac{g_2}{L} \sum_{k_1,k_2,q,p} c_{k_1,p,\uparrow}^\dagger c_{k_2,-p,\downarrow} c_{k_2+q,-p,\downarrow} c_{k_1-q,p,\uparrow} + \frac{g_3}{L} \sum_{k_1,k_2,q,p} c_{k_1,p,\uparrow}^\dagger c_{k_2,p,\downarrow} c_{k_2+q,-p,\downarrow} c_{k_1-q,-p,\uparrow} + \frac{g_4}{L} \sum_{k_1,k_2,q,p} c_{k_1,p,\uparrow}^\dagger c_{k_2,p,\downarrow} c_{k_2+q,p,\downarrow} c_{k_1-q,-p,\uparrow},
\]

where \( g_1 = g_2 = g_3 = g_4 = Ua \) and these quantities denote coupling constants for the backward scattering \((g_1)\), forward scattering between the opposite branch \((g_2)\), umklapp scattering \((g_3)\) and forward scattering within the same branch \((g_4)\), respectively.

Next the bosonization method\(^{[3]}\) is applied to eq. (1). The phase variables, \( \theta_{\rho \pm} \) and \( \theta_{\sigma \pm} \), expressing fluctuations of the charge density and spin density are given by

\[
\theta_{\rho \pm}(x) = \frac{1}{\sqrt{2}} \sum_{q \neq 0} \frac{\pi i}{qL} e^{-\frac{\pi i}{2qL} |q|} \sum_{k,\sigma} \left( c_{k+q,\pm,\sigma}^\dagger c_{k,\pm,\sigma} \pm c_{k+q,\pm,\sigma} c_{k,-\sigma}^\dagger \right), \quad (3)
\]

\[
\theta_{\sigma \pm}(x) = \frac{1}{\sqrt{2}} \sum_{q \neq 0} \frac{\pi i}{qL} e^{-\frac{\pi i}{2qL} |q|} \sum_{k,\sigma} \left( c_{k+q,\pm,\sigma}^\dagger c_{k,\pm,\sigma} \pm c_{k+q,\pm,\sigma} c_{k,-\sigma}^\dagger \right), \quad (4)
\]

where \( \sigma = +(-) \) corresponds to \( \uparrow(\downarrow) \) and \([\theta_{\nu \pm}(x), \theta_{\nu' \pm}(x')] = i\pi \delta_{\nu,\nu'} \text{sgn}(x - x') \). By using these phase variables, we rewrite the field operator, \( \psi_{p,\sigma}(x) (= L^{-1} \sum_k e^{ipk_F x + ikx} c_{k,p,\sigma} ) \), as

\[
\psi_{p,\sigma} = \frac{1}{\sqrt{2\pi \alpha}} \exp(ipk_F x + i\Theta_{p,\sigma}) \exp(i\pi \Xi_{p,\sigma}), \quad (5)
\]

\[
\Theta_{p,\sigma} = \frac{1}{2} [p \theta_{p,\uparrow} + \theta_{p,-} + \sigma(p \theta_{\sigma,\uparrow} + \theta_{\sigma,-})], \quad (6)
\]

where \( \alpha \) is of the order of the lattice constant. The phase factor in eq. (5), is chosen as \( \Xi_{p,\uparrow} = p(\hat{N}_{+,+} + \hat{N}_{-,+})/2 \) and \( \Xi_{p,-} = (\hat{N}_{+,+} + \hat{N}_{-,+}) + p(\hat{N}_{+-} + \hat{N}_{-,+})/2 \) with the number operator, \( \hat{N}_{p,\sigma} \), in order to satisfy the anticommutation relation. Such a choice of \( \Xi_{p,\sigma} \) conserves a sign of the
nonlinear terms, which is obtained from the interaction terms of eq. (2). Based on these bosonic fields, eq. (1) is rewritten as\cite{13}

\[
\mathcal{H} = \frac{v_{\nu}}{4\pi} \int dx \left[ \frac{1}{K_{\nu}} (\partial \theta_{\nu+})^2 + K_{\nu} (\partial \theta_{\nu-})^2 \right] + \frac{g_3}{2\pi^2 \alpha^2} \int dx \cos 2\theta_{\nu+} \\
+ \frac{v_{\sigma}}{4\pi} \int dx \left[ \frac{1}{K_{\sigma}} (\partial \theta_{\sigma+})^2 + K_{\sigma} (\partial \theta_{\sigma-})^2 \right] + \frac{g_1}{2\pi^2 \alpha^2} \int dx \cos 2\theta_{\sigma+} \\
+ \frac{2W_0}{\pi \alpha} \int dx \cos \theta_{\nu+} \cos \theta_{\sigma+} ,
\]

where \( v_{\nu} = [(2\pi v_F + g_4)^2 - g_3^2]^{1/2} / 2\pi, \) \( K_{\nu} = [(2\pi v_F + g_4 - g_2)/(2\pi v_F + g_4 + g_2)]^{1/2}, \) \( v_{\sigma} = [(2\pi v_F - g_4)^2 - g_1^2]^{1/2} / 2\pi \) and \( K_{\sigma} = [(2\pi v_F - g_4 + g_1)/(2\pi v_F - g_4 - g_1)]^{1/2}. \)

Now we derive renormalization group equations by examining response functions, \( R_A(x_1 - x_2, \tau_1 - \tau_2) \equiv (T_{\nu} \mathcal{O}_A(x_1, \tau_1) \mathcal{O}_A^\dagger(x_2, \tau_2)), \) where \( \tau_j \) is the imaginary time and \( \mathcal{O}_A \) denotes several kinds of order parameters. Response functions are evaluated perturbatively by expanding nonlinear terms of eq. (7). From the assumption that response functions are invariant for \( \alpha \to \alpha' = \alpha e^{4\alpha} \)\cite{14,15}, renormalization group equations for \( K_{\nu}, K_{\sigma}, g_3, g_1 \) and \( W_0 \) are derived as (Appendix A)

\[
\frac{d}{dl} K_{\nu}(l) = -2 G_3^2(l) K_{\nu}^2(l) - G_W^2(l) K_{\nu}^2(l) ,
\]

\[
\frac{d}{dl} K_{\sigma}(l) = -2 G_1^2(l) K_{\sigma}^2(l) - G_W^2(l) K_{\sigma}^2(l) ,
\]

\[
\frac{d}{dl} G_3(l) = \left[ 2 - 2K_{\nu}(l) \right] G_3(l) - G_W^2(l) ,
\]

\[
\frac{d}{dl} G_1(l) = \left[ 2 - 2K_{\sigma}(l) \right] G_1(l) - G_W^2(l) ,
\]

\[
\frac{d}{dl} G_W(l) = \left[ 2 - K_{\nu}(l)/2 - K_{\sigma}(l)/2 \right] G_W(l) \\
- G_3(l) G_W(l) - G_1(l) G_W(l) ,
\]

where initial conditions are chosen as \( K_{\nu}(0) = K_{\nu} \) (\( \nu = \rho \) and \( \sigma \)), \( G_3(0) = g_3/2\pi v_F, \) \( G_1(0) = g_1/2\pi v_F \) and \( G_W(0) = W_0/(v_F \alpha^{-1}). \) For the simplicity, we replaced \( v_{\rho} \) and \( v_{\sigma} \) by \( v_F, \) in eqs. (8)-(12) since the deviation of the numerical factor is small.

The calculation of \( K_{\sigma}(l) \) in eq. (9) is performed by the following procedure. When we substitute \( K_{\sigma}(l) = 1 + G_1(l) \) for r.h.s. of eqs. (9) and (11) and retain the coupling constants up to the second order, eq. (9) becomes equal to eq. (11). In this case, the fixed point of \( K_{\sigma}(l) \) with \( W_0 = 0 \) is given by unity showing the validity of the SU(2) symmetry, i.e. \( K_{\sigma}(\infty) = 1. \) Therefore eqs. (9) and (11) are treated by such an expanded form for \( K_{\sigma}(l) > 1 \) while we use the original form of eq. (9) for \( K_{\sigma}(l) < 1. \)

We note the electronic states obtained from eq. (12). In the absence of the \( U \)-term, the state of eq. (1) has a gap, \( 2W_0, \) at \( k = \pm k_F \) of the band while that of eq. (1) with \( W_0 = 0 \) exhibits a charge gap, \( \Delta_{\rho}, \) due to half-filling corresponding to a Mott gap. Both of these cases are insulating states. The former is the band insulator with the relevant \( G_W(l), \) which increases infinity for large \( l. \) The
latter is the Mott insulator with the relevant $G_3(l)$. In the presence of both $U$-term and $W_0$-term, there are two cases of the relevant $G_W(l)$ and the irrelevant $G_W(l)$. We use the terminology of the band insulator for the relevant $G_W(l)$ and the Mott insulator for the irrelevant $G_W(l)$ although the latter case denotes actually a crossover to the Mott state, i.e., the spin gap decreases rapidly to zero as shown in the next section.

Here we examine the order parameters, which are characteristic of these insulating states. Since the phase of $\theta_{\sigma+}$ is locked at $\pi$ or $0$ ($\pm \pi/2$) for the relevant (irrelevant) $G_W(l)$, we can consider the order parameter of the band insulator (the Mott insulator) as $\langle \cos \theta_{\sigma+} \rangle$ ($\langle \sin \theta_{\rho+} \rangle$). The finite value of $\langle \cos \theta_{\rho+} \rangle$ denotes the ionic state since the $W_0$-term of eqs. (1) and (7) is proportional to the difference between electron numbers of two kinds of lattice sites. As for the locking of $\theta_{\sigma+}$, the effect of the $W_0$-term is much stronger than that of the $g_1$-term in eq. (7), because the $g_1$-term becomes irrelevant for $W_0 = 0$. Thus we always have the finite value of $\langle \cos \theta_{\sigma+} \rangle$. We note that the quantity $\langle \cos \theta_{\rho+} \rangle$ $\langle \cos \theta_{\sigma+} \rangle$ is negative due to the positive value of $W_0$ in eq. (7) and that there is a degeneracy of a state with the positive $\langle \cos \theta_{\rho+} \rangle$ and the negative $\langle \cos \theta_{\sigma+} \rangle$ and a state with the negative $\langle \cos \theta_{\rho+} \rangle$ and the positive $\langle \cos \theta_{\sigma+} \rangle$. For studying these properties, we calculate response functions, $R_{\cos \theta_{\rho+}}(r_1 - r_2) = \langle T_\tau \cos \theta_{\rho+}(r_1) \cos \theta_{\rho+}(r_2) \rangle$ ($\nu = \rho$ and $\sigma$). By use of the renormalization group technique, these response functions are derived as (Appendix A)

$$R_{\cos \theta_{\rho+}}(r) = \exp \left[ - \int_0^{\ln(r/\alpha)} dl \left( K_\rho(l) + 2G_3(l) \right) \right],$$

$$R_{\cos \theta_{\sigma+}}(r) = \exp \left[ - \int_0^{\ln(r/\alpha)} dl \left( K_\sigma(l) + 2G_1(l) \right) \right],$$

where $r = (x^2 + (v_F \tau)^2)^{1/2}$. For the band insulator the limiting values of both $R_{\cos \theta_{\rho+}}(r)$ and $R_{\cos \theta_{\sigma+}}(r)$ are finite, while only that of $R_{\cos \theta_{\sigma+}}(r)$ becomes finite for the Mott insulator.

§3. **Band insulator vs. Mott insulator**

For the calculation of characteristic energy in terms of renormalization group equations, it is crucial to determine the magnitude of the cutoff parameter, $\alpha$, which is chosen conventionally as $\alpha = a/\pi^{2/3}$. We estimate $\alpha$ from the response function for charge density wave with a momentum close to $2k_F$ as follows. Such a response function with $W_0 = U = 0$ can be calculated explicitly by both the conventional method and the bosonization method (Appendix B). From the comparison of these two quantities for the half-filled band, we obtain $\alpha \simeq \pi/(1.273a)$. Thus characteristic energy corresponding to $l$ is given by $v_F \alpha^{-1} \exp[-l]$.

In Fig. 1, quantities $K_\rho(l)$(solid curve), $K_\sigma(l)$(dashed curve), $G_3(l)$(dot-dashed curve) and $G_W(l)$(dotted curve) are shown as a function of $l$ for $U/t = 2$ and $W_0/t = 1$. With increasing $l$, $G_W(l)$ increases monotonically and then becomes relevant leading to the band insulator. The change of sign of $G_3(l)$ occurs at $l \simeq 2.1$ due to the relevant $G_W(l)$. The positive $G_3(l)$ originates in the umklapp scattering, $g_3$, and the negative $G_3(l)$ comes from the higher harmonics induced by the
Fig. 1. The $l$-dependence of coupling constants, $K_\rho(l)$, $K_\sigma(l)$, $G_3(l)$ and $G_W(l)$, with fixed $U/t = 2$ and $W_0/t = 1$. The 2-dot-dashed curve denotes $K_\rho(l)$ for $W_0/t = 0$.

Fig. 2. The $l$-dependence of coupling constants, $K_\rho(l)$, $K_\sigma(l)$, $G_3(l)$ and $G_W(l)$, with fixed $U/t = 4$ and $W_0/t = 1$ where the notations are the same as Fig. 1.
$W_0$-term. With increasing $l$, $K_\rho$ decreases monotonically since both $G_3(l)$ and $G_W(l)$ reduce $K_\rho(l)$. The reduction of $K_\rho(l)$ by $G_W(l)$ is understood from the fact that $K_\rho(l)$ is suppressed noticeably compared with the case of $W_0 = 0$ (2-dot-dashed curve). The $l$-dependence of $G_1(l)$ is similar to that of $G_3(l)$, i.e., the positive $G_1(l)$ changes the sign with increasing $l$. With increasing $l$, $K_\rho(l)$ and $K_\sigma(l)$ merge each other and their magnitudes are reduced to zero. This behavior indicates the formation of both charge gap, $E_g$, and spin gap, $\Delta_\sigma$, which originate in the $W_0$-term.

In Fig. 2, the numerical result for $U/t = 4$ and $W_0/t = 1$ is shown where the notations are the same as Fig. 1. The behavior of $K_\sigma(l)$, $G_3(l)$ and $G_W(l)$ is quite different compared with that of Fig. 1 although that of $K_\rho(l)$ is qualitatively the same. The difference between $K_\rho(l)$ (solid curve) and that of $W_0 = 0$ (2-dot-dashed curve) is very small due to the irrelevant $G_W(l)$. The effect of the $W_0$-term reducing the charge gap is seen from the fact that $K_\rho(l)$ in the presence of $W_0$ (solid curve) is slightly larger than that of $W_0 = 0$ (2-dot-dashed curve). With increasing $l$, $G_W(l)$ takes a maximum and decreases to zero. Thus the effect of $W_0$ becomes negligibly small for the large $l$ (i.e., small energy). Such an irrelevant $G_W(l)$ leads to a state similar to the Mott insulator induced by the umklapp scattering. The quantity $G_3(l)$ is always positive and increases monotonically from the initial value $g_3$. The $l$-dependence of $K_\sigma(l)$ is similar to that with $W_0 = 0$, i.e., $K_\sigma(l) \geq 1$ in the range of Fig. 2. However a small spin gap does exist since $K_\sigma(l)$ reduces to zero for the large $l$.

Based on the calculation given by Figs. 1 and 2, it turns out that there is a critical value of $U = U_c$, where the band insulator is obtained for $U < U_c$ and the Mott insulator is obtained for $U > U_c$. In Fig. 3, the $U$-dependence of excitation gap and $|\langle \cos \theta_{\nu+} \rangle|$ is shown. The charge gap ($E_g$) and spin gap ($\Delta_\sigma$) are evaluated by the formula, $E_g = v_F \alpha^{-1} \exp[-l_\rho]$ and $\Delta_\sigma = v_F \alpha^{-1} \exp[-l_\sigma]$ where $l_\nu$ ($\nu = \rho$ and $\sigma$) is chosen as $K_\nu(l_\nu) = 0.3$. Such a choice is reasonable since, in the absence of $W_0 = 0$, the charge gap of the present calculation (dotted curve) coincides well with the exact one (dot-dashed curve). The $U$-dependence of $E_g$ and $\Delta_\sigma$ is shown by solid curve and dashed curve, respectively. The arrow denotes the location for a critical value of $U_c/t \simeq 3.0$, which separates the band insulator from the Mott insulator. There is a minimum of $E_g$ (solid curve) where the corresponding $U$ is slightly smaller than $U_c$. Such a minimum arises from a competition between the $W_0$-term and the $g_3$-term. For large $U$, the magnitude of $E_g$ moves close to $\Delta_\rho$ (dotted curve), which denotes the charge gap in the absence of $W_0$. With increasing $U$, the spin gap $\Delta_\sigma$ decreases but takes a finite value even for $U > U_c$. For small $U$, one finds $E_g \simeq \Delta_\sigma$ indicating that the difference between the magnitude of the charge gap and that of the spin gap is negligibly small. Thus it turns out that the behavior of the charge gap is quite different from that of spin gap.

In the inset of Fig. 3, the $U$-dependence of $|\langle \cos \theta_{\nu+} \rangle|$ and $|\langle \cos \theta_{\sigma+} \rangle|$ is shown by solid curve (1) and dashed curve (2), respectively where the arrow denotes $U = U_c$. The quantity $\langle \cos \theta_{\nu+} \rangle$ ($\nu = \rho$ and $\sigma$), is defined by $\langle T_\nu \cos \theta_{\nu+}(x) \cos \theta_{\nu+}(0) \rangle \rightarrow \langle \cos \theta_{\nu+} \rangle^2$ for $|x| \rightarrow \infty$. In the context of the present calculation, such a value is calculated from the minimum value of response function due
to the second order renormalization group equation. With increasing $U/t$, $|\langle \cos \theta_{\rho^+} \rangle|$ decreases and is reduced to zero at $U = U_c$, corresponding to the transition from the band insulator to the Mott insulator, where the locking of phase for the former (latter) state is given by $\theta_{\rho^+} = \pi$ or $0$ ($\theta_{\rho^+} = \pm \pi/2$). The finite value of $\langle \cos \theta_{\rho^+} \rangle$ corresponds to the relevance of $G_W(l)$, i.e., the band insulator. In contrast to $\langle \cos \theta_{\rho^+} \rangle$, we find that $\langle \sin \theta_{\rho^+} \rangle$ becomes finite for the irrelevance of $G_W(l)$, i.e., $U > U_c$ due to the change of the locked $\theta_{\rho^+}$ from $0$ to $\pm \pi/2$. The quantity $|\langle \cos \theta_{\sigma^+} \rangle|$ decreases but remains finite even for $U > U_c$ showing the similarity to $\Delta_{\sigma}$. We note that $|\langle \cos \theta_{\rho^+} \rangle| \propto \sqrt{|W_0|}$ for $U = 0$ and small $|W_0|/t \lesssim 2$. Such a result is compatible with the fact that the conventional band gap with $U = 0$, is proportional to $W_0$. Then the present calculation is valid for $W_0/t \lesssim 2$. The $U$-dependence of $E_g$ and $\langle \cos \theta_{\rho^+} \rangle$ ($\Delta_{\sigma}$ and $\langle \cos \theta_{\sigma^+} \rangle$) shows that a transition (a crossover) from the band insulator to the Mott insulator appears due to the competition between the alternating potential and the electron-electron interaction.

From the calculation of $U_c$ similar to Fig. 3 with several choices of $W_0$, a phase diagram of the band insulator and Mott insulator is shown on the plane of $U/t$ and $W_0/t$ in Fig. 4. Since the the boundary between these two states is convex downward, the effect of $W_0$ is much larger than $U$ for small $U$. The boundary, which is well reproduced by a formula, $\exp[-2\pi t/U]$, for small $U/t,$
indicates a fact that the characteristic energy for the competition is not $U$ but the charge gap $\Delta_\rho$.
In the inset, the same phase diagram is shown on the plane of $\Delta_\rho/t$ and $W_0/t$. From the result that $W_0/\Delta_\rho = 1.6 \sim 1.7$ for $0.3 < \Delta_\rho/t < 2.0$, it is found that the boundary between the band insulator and Mott insulator is determined by the competition between $\Delta_\rho$ and $W_0$.

§4. Summary and Discussion

In the present paper, we have examined the effect of the alternating potential, $W_0$, on a one-dimensional half-filled Hubbard model with the repulsive interaction, $U$. The property of the model with the infinite length is calculated by use of the methods of bosonization and renormalization group. With increasing $U$, a second order phase transition followed by the continuous change of the order parameters occurs from the band insulator into the Mott insulator at $U_c$ where the former (latter) corresponds to the relevant (irrelevant) $G_W(l)$. Such a transition is demonstrated from the fact that $\langle \cos \theta_{\rho^+} \rangle$ becomes zero for $U \rightarrow U_c - 0$. The band insulator denotes the ionic state since $\langle \cos \theta_{\rho^+} \rangle \neq 0$ in addition to $\langle \cos \theta_{\sigma^+} \rangle \neq 0$. Phases of the band insulator are locked at $\theta_{\rho^+} = \pi$ (or 0) and $\theta_{\sigma^+} = 0$ (or $\pi$) respectively. For the Mott insulator, phases are locked at $\theta_{\rho^+} = \pi/2$ or $-\pi/2$ and $\theta_{\sigma^+} = 0$ or $\pi$ due to the presence of the spin gap even if $G_W(l)$ is irrelevant. The charge gap, $E_g$, takes a minimum and the spin gap $\Delta_\sigma$ exhibits a crossover around the transition point of $U = U_c$. The phase diagram of band insulator and Mott insulator has been obtained on the plane of $U$ and $W_0$. 

Fig. 4. Phase diagram for the band insulator and the Mott insulator on the plane of $U/t$ and $W_0/t$. The inset shows the same phase diagram on the plane of $\Delta_\rho/t$ and $W_0/t$. 

$U/t$

$W_0/t$

Band Insulator

Mott Insulator

$\Delta_\rho/t$

$W_0/t$
Here we compare the boundary calculated in the present paper with those obtained by the numerical diagonalization. In ref. [4], in which the same model is treated, the boundary between band insulator and Mott insulator is calculated as $U_c/t \simeq 2.27$ for $W_0/t \simeq 0.57$ while our result shows $U_c/t \simeq 2.4$ for $W_0/t = 0.57$. In refs. [5] and [6] which introduced two kinds on-site potentials $U_B < U_A$ in addition to the present model, they obtained $U_{Bc}/t \simeq 2.5, 3.4$ and $5.4$ for $W_0/t \simeq 0.67, 1.0$ and $2.0$ while the present results show $U_{c}/t \simeq 2.5, 3.0$ and $4.2$ for $W_0/t = 0.67, 1.0$ and $2.0$ respectively. A quantitative coincidence between their numerical calculations and ours are found for $W_0/t \lesssim 1$. Further we note a fact deduced from the present result that $\langle \cos \theta_{\rho+} \rangle = 0$ at $U = U_c$. Close to $U = U_c$, the free energy as a function of $\langle \cos \theta_{\rho+} \rangle$ takes a double minimum for the band insulator due to the degeneracy with respect to $\theta_{\rho+} = 0$ and $\pi$ while it takes a single minimum for the Mott insulator. Thus the charge fluctuation is strongly enhanced around $U = U_c$ as seen in the second order phase transition. Such a fact could be related to the enhancement of the dynamical charge [4] and the increase of localization length [8] at the critical point.

Finally we discuss about the effect of dimerization where the corresponding Hamiltonian is given by

$$-t_d \sum_{j,\sigma} \left[ (-1)^j c_{j,\sigma}^\dagger c_{j+1,\sigma} \right]. \tag{15}$$

In terms of phase variable, eqs. (5) and (6), one can replace eq. (15) as

$$\frac{4t_d}{\pi \alpha} \int dx \sin \theta_{\rho+} \cos \theta_{\sigma+}. \tag{16}$$

Equation (16) is compatible with the $g_3$-term in eq. (7) since the energy gain of the former is obtained for $\theta_{\rho+} = \pi/2$ and $\theta_{\sigma+} = \pi$ (or $\theta_{\rho+} = -\pi/2$ and $\theta_{\sigma+} = 0$) while that of the latter is obtained for $\theta_{\rho+} = \pm \pi/2$. By noting that $t_d$-term and the $W_0$-term have the same periodicity with $2\pi$ as a function of $\theta_{\rho+}$, these two terms coexist for the relevant $G_W(l)$. In this case, the phase is determined so as to minimize two energies of $t_d$-term and $W_0$-term. We can incorporate eq. (16) into renormalization equations and find that $t_d$-term is always relevant and that there exists a boundary between the relevant $G_W(l)$ and the irrelevant $G_W(l)$. Based on these consideration, we can expect following. Although the qualitative feature is the same as that with $t_d = 0$, there are noticeable facts that the spin gap is strongly enhanced due to the relevant $t_d$ and that the critical value $U_c$ decreases due to the enhancement of umklapp scattering by $t_d$.

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Appendix A: Derivation of the renormalization group equations

A.1 Coupling Constants

The renormalization group equations are derived in a way similar to Giamarchi and Schulz. By treating the nonlinear terms in eq. (7) as the perturbation, the response function, \( R_\rho(x, \tau) \equiv \langle T_\tau \exp[i\theta_\rho^+(x, \tau)] \exp[-i\theta_\rho^+(0, 0)] \rangle \), is calculated up to the third order as

\[
R_\rho(r_1 - r_2) = \left\langle e^{i[\theta_\rho^+(r_1) - \theta_\rho^+(r_2)]} \right\rangle_0 \\
+ \frac{1}{2} G_3^2 (2\pi)^2 \sum_{\epsilon, \epsilon'} \int \frac{d^2r_3 d^2r_4}{\alpha^2} \left\{ \left\langle e^{i[\theta_\rho^+(r_1) - \theta_\rho^+(r_2) + \epsilon\theta_\rho^+(r_3) - \epsilon\theta_\rho^+(r_4)]} \right\rangle_0 \\
- \left\langle e^{i[\theta_\rho^+(r_1) - \theta_\rho^+(r_2)]} \right\rangle_0 \left\langle e^{i[2\theta_\rho^+(r_3) - 2\theta_\rho^+(r_4)]} \right\rangle_0 \right\}
\]

+ \frac{1}{2} G_3^2 (2\pi)^2 \sum_{\epsilon, \epsilon', \epsilon''} \int \frac{d^2r_3 d^2r_4 d^2r_5}{\alpha^2} \left\{ \left\langle e^{i[\theta_\rho^+(r_1) - \theta_\rho^+(r_2) + \epsilon\theta_\rho^+(r_3) - \epsilon\theta_\rho^+(r_4) - \epsilon'\theta_\rho^+(r_5)]} \right\rangle_0 \\
- \left\langle e^{i[\theta_\rho^+(r_1) - \theta_\rho^+(r_2)]} \right\rangle_0 \left\langle e^{i[2\theta_\rho^+(r_3) - 2\theta_\rho^+(r_4) - \theta_\rho^+(r_5)]} \right\rangle_0 \right\}
\]

+ \frac{1}{2} G_3^2 (2\pi)^2 \sum_{\epsilon, \epsilon'} \int \frac{d^2r_3 d^2r_4 d^2r_5}{\alpha^2} \left\{ \left\langle e^{i[\theta_\rho^+(r_1) - \theta_\rho^+(r_2) + \epsilon\theta_\rho^+(r_3) - \epsilon\theta_\rho^+(r_4) - \epsilon'\theta_\rho^+(r_5)]} \right\rangle_0 \\
- \left\langle e^{i[\theta_\rho^+(r_1) - \theta_\rho^+(r_2)]} \right\rangle_0 \left\langle e^{i[2\theta_\rho^+(r_3) - 2\theta_\rho^+(r_4) - \theta_\rho^+(r_5)]} \right\rangle_0 \right\}
+ \cdots ,
\]  

where \( r = (x, v_F \tau) \) and \( \langle \cdots \rangle_0 \) denotes an average over the harmonic parts including \( K_\rho \) or \( K_\sigma \) in eq. (7). Scaling equations for coupling constants up to the second-order can be calculated from response function, \( R_\rho(r) \), which is expanded up to the third-order for the nonlinear terms. A straightforward calculation of eq. (A-1) yields,

\[
R_\rho(r_1 - r_2) = e^{-K_\rho U(r_1 - r_2)} \\
+ \frac{G_3^2}{(2\pi)^2} \sum_{\epsilon = \pm 1} \int \frac{d^2r_3 d^2r_4}{\alpha^2} e^{-K_\rho U(r_1 - r_2) - 4K_\rho U(r_3 - r_4)} \\
\times \left\{ e^{2K_\rho[U(r_1 - r_3) - U(r_1 - r_4) - U(r_2 - r_3) + U(r_2 - r_4) - U(r_2 - r_4)]} - 1 \right\}
\]

+ \frac{G_3^2}{(2\pi)^2} \sum_{\epsilon = \pm 1} \int \frac{d^2r_3 d^2r_4}{\alpha^2} e^{-K_\rho U(r_1 - r_2) - (K_\rho + K_\sigma) U(r_3 - r_4)} \\
\times \left\{ e^{K_\rho[U(r_1 - r_3) - U(r_1 - r_4) - U(r_2 - r_3) + U(r_2 - r_4) - U(r_2 - r_4)]} - 1 \right\}
\]

- \frac{G_3^2}{(2\pi)^2} \sum_{\epsilon = \pm 1} \int \frac{d^2r_3 d^2r_4 d^2r_5}{\alpha^2} e^{-K_\rho U(r_1 - r_2) + (K_\rho - K_\sigma) U(r_4 - r_5)} e^{-2K_\rho[U(r_3 - r_4) + U(r_3 - r_5)]} \\
\times \left\{ e^{2K_\rho[U(r_1 - r_3) - U(r_2 - r_3)] + \epsilon K_\rho[-U(r_1 - r_4) - U(r_1 - r_5) + U(r_2 - r_4) + U(r_2 - r_5)]} - 1 \right\}
\]
\[-G_1G_W^2 \frac{1}{(2\pi)^3} \sum \int \frac{d^2r_3 d^2r_4 d^2r_5}{\alpha^2} \frac{e^{-K_\rho U(r_1-r_2)-(K_\rho-K_\sigma)U(r_4-r_5)}}{\alpha^2}e^{-2K_\sigma[U(r_4-r_4)+U(r_3-r_5)]} \times \left\{ e^{2K_\rho[U(r_1-r_4)-U(r_1-r_3)-U(r_2-r_4)+U(r_2-r_3)]} - 1 \right\} + \ldots , \tag{A.2} \]

where \( U(r) = \ln(r/\alpha) \) \((r = [x^2 + (v_\rho v_\sigma)^2]^{1/2}) \). We have discarded the difference of velocities, i.e., \( v_\rho = v_\sigma = v_F \). As for third-order with respect to coupling constant in eq. (A.2), three cases of \( r_5 = r_4 + r \), \( r_5 = r_3 + r \) and \( r_5 = r_3 + r \) with small \( r \) are chosen where the expansion of these terms around \( r = 0 \) is rewritten as

\[-G_3G_W^2 \frac{1}{(2\pi)^3} \sum \int \frac{d^2r_3 d^2r_4}{\alpha^2} \frac{e^{-K_\rho U(r_1-r_2)-4K_\rho U(r_3-r_4)}}{\alpha^2} \times \left\{ e^{2K_\rho[U(r_1-r_3)-U(r_1-r_4)-U(r_2-r_3)+U(r_2-r_4)]} - 1 \right\} \int \frac{d^2r}{\alpha^2} e^{-2K_\rho U(r)} \]

\[-2G_3G_W^2 \frac{1}{(2\pi)^3} \sum \int \frac{d^2r_3 d^2r_4}{\alpha^2} \frac{e^{-K_\rho U(r_1-r_2)-(K_\rho+K_\sigma)U(r_3-r_4)}}{\alpha^2} \times \left\{ e^{K_\rho[U(r_1-r_3)-U(r_1-r_4)-U(r_2-r_3)+U(r_2-r_4)]} - 1 \right\} \int \frac{d^2r}{\alpha^2} e^{-2K_\rho U(r)} \]

\[-2G_1G_W^2 \frac{1}{(2\pi)^3} \sum \int \frac{d^2r_3 d^2r_4}{\alpha^2} \frac{e^{-K_\rho U(r_1-r_2)-(K_\rho+K_\sigma)U(r_3-r_4)}}{\alpha^2} \times \left\{ e^{K_\rho[U(r_1-r_3)-U(r_1-r_4)-U(r_2-r_3)+U(r_2-r_4)]} - 1 \right\} \int \frac{d^2r}{\alpha^2} e^{-2K_\rho U(r)} \ldots . \tag{A.3} \]

By comparing eqs. (A.2) with (A.3), it is found that eq. (A.3) has an effect of the renormalization for \( G_3 \)-term and \( G_W \)-term in eq. (A.2). Actually eq. (A.2) can be rewritten by the first three terms with effective coupling constants, which are given by

\[ G_3^{\text{eff}} = G_3 - G_W^2 \int \frac{d^2r}{\alpha^2} \left( \frac{r}{\alpha} \right)^{1+K_\rho-K_\sigma} \tag{A.4} \]

\[ G_W^{\text{eff}} = G_W - G_3 G_W \int \frac{d^2r}{\alpha^2} \left( \frac{r}{\alpha} \right)^{1-2K_\rho} - G_1 G_W \int \frac{d^2r}{\alpha^2} \left( \frac{r}{\alpha} \right)^{1-2K_\sigma} \tag{A.5} \]

On the other hand, the effective quantity of \( K_\rho \) can be calculated from the response function up to the second order for the nonlinear terms. By expanding the exponential in the second and the third terms of eq. (A.2) and using new variables \( r = r_3 - r_4 \) and \( R = (r_3 + r_4)/2 \), eq. (A.2) is rewritten as,

\[ R_\rho(r_1-r_2) = e^{-K_\rho U(r_1-r_2)} \left[ 1 + 2 \frac{G_3^2}{(2\pi)^2} K_\rho^2 J_+(2K_\rho) I_+(r_1-r_2) \right. \]

\[ + \left. \frac{G_W^2}{(2\pi)^2} K_\rho^2 J_+(K_\rho/2 + K_\sigma/2) I_+(r_1-r_2) \right] \tag{A.6} \]

where

\[ I_+(r_1-r_2) = \int d^2R \frac{U(r_1-R) \nabla_{r_2}^2 U(r_2-R)}{U(r_1-r_2)} = 2\pi U(r_1-r_2) \tag{A.7} \]

\[ J_+(K) = \int \frac{d^2r}{\alpha^2} \frac{r^2}{\alpha^2} e^{-2KU(r)} = 2\pi \int_0^\infty \frac{dr}{\alpha} \left( \frac{r}{\alpha} \right)^{3-2K} \tag{A.8} \]

\[ U(r) = \ln(r/\alpha) \]
The scale invariance of eq. (A.6) is shown by reexponentiating eq. (A.6) where the effective quantity of \( K_\rho \) is obtained as
\[
K^{\text{eff}}_\rho = K_\rho - 2G_3^2K_\rho^2 \int \frac{dr}{\alpha} \left( \frac{r}{\alpha} \right)^{3-4K_\rho} - G_W^2 K_\rho^2 \int \frac{dr}{\alpha} \left( \frac{r}{\alpha} \right)^{3-K_\rho-K_\sigma}, \tag{A.9}
\]
For the transformation given by \( \alpha \to \alpha' = \alpha e^{dl} \), these quantities have to be scaled as
\[
K_\rho^{\text{eff}}(K'_\nu, G'_\mu; \alpha') = K_\rho^{\text{eff}}(K_\nu, G_\mu; \alpha), \tag{A.10}
\]
\[
G_3^{\text{eff}}(K'_\nu, G'_\mu; \alpha') = G_3^{\text{eff}}(K_\nu, G_\mu; \alpha) (\alpha'/\alpha)^{2-2K_\rho}, \tag{A.11}
\]
\[
G_W^{\text{eff}}(K'_\nu, G'_\mu; \alpha') = G_W^{\text{eff}}(K_\nu, G_\mu; \alpha) (\alpha'/\alpha)^{2-K_\nu/2-K_\sigma/2}, \tag{A.12}
\]
where \( K'_\nu(\nu = \rho, \sigma) \) and \( G'_\mu(\mu = 3, 1, W) \) denote renormalized quantities. The quantity \( 2K_\rho (K_\rho/2 + K_\sigma/2) \) is a scaling dimension for \( G_3^{\text{eff}} \) (for \( G_W^{\text{eff}} \)), which is obtained from the second (third) term of eq. (A.9). By applying the infinitesimal transform to eqs. (A.9), (A.4) and (A.5), renormalized quantities are expressed as
\[
K'_\rho = K_\rho - 2G_3^2K_\rho^2 dl - G_W^2 K_\rho^2 dl, \tag{A.13}
\]
\[
G'_3 = G_3 + (2 - 2K_\rho)G_3 dl - G_W^2 dl, \tag{A.14}
\]
\[
G'_W = G_W + (2 - K_\rho/2 - K_\sigma/2)G_W dl - G_3 G_W dl - G_1 G_W dl, \tag{A.15}
\]
which lead to eqs. (8), (10) and (12), respectively. The renormalization group equations for \( K_\sigma(l) \) and \( G_1(l) \) can be obtained in a similar way to eqs. (8) and (10) by calculating the response function given by \( \langle T_x \exp[i\theta_\sigma(x, \tau)] \exp[-i\theta_\sigma(0, 0)] \rangle \). We note that, in case of \( W_0/t = 0 \), these equations reduces to to well known equations for half-filled Hubbard model.

### A.2 Response Function

Based on the solution of of eqs. (8)-(12), we examine the response function, \( R_{\cos \theta_{\nu+}}(r_1 - r_2) = \langle T_x \cos \theta_{\nu+}(r_1) \cos \theta_{\nu+}(r_2) \rangle \), which is calculated by writing \( R_{\cos \theta_{\nu+}}(r) = \exp[-K_\rho U(r)] \cdot F_{\cos \theta_{\nu+}}(r). \) The perturbative calculation for \( R_{\cos \theta_{\nu+}} \) leads to
\[
F_{\cos \theta_{\nu+}}(r_1 - r_2) = 1 - \frac{G_3}{2\pi} \int \frac{d^2r_3}{\alpha^2} e^{2K_\rho[U(r_1-r_2)-U(r_1-r_3)-U(r_2-r_3)]} \left[ 2G_3^2 \int \frac{dr}{\alpha} \left( \frac{r}{\alpha} \right)^{3-4K_\rho} + G_W^2 \int \frac{dr}{\alpha} \left( \frac{r}{\alpha} \right)^{3-K_\rho-K_\sigma} \right] K_\rho^2 U(r_1 - r_2), \tag{A.16}
\]
The scaling invariance under the transformation of \( \alpha \to \alpha' = \alpha e^{dl} \) is assumed for the quantity \( F_{\cos \theta_{\nu+}}(r) \), which is expressed as
\[
F_{\cos \theta_{\nu+}}(r, K_\nu, G_\mu; \alpha) = I_{\cos \theta_{\nu+}}(dl, K_\nu, G_\mu) \cdot F_{\cos \theta_{\nu+}}(r, K'_\nu, G'_\mu; \alpha'). \tag{A.17}
\]
The quantity \( I_{\cos \theta_{\nu+}} \) is determined perturbatively. By applying the infinitesimal transform to eq. (A.16), we obtain
\[
F_{\cos \theta_{\nu+}} = 1 - 2G_3 dl + (2G_3^2 + G_W^2) K_\rho^2 U(r_1 - r_2) dl
\]
From eqs. (B.2) and (B.3), it is found that

\[ C \]

For the case with only the first term of eq. (1), eq. (B.1) is calculated as

\[ \text{where} \]

\[ U \]

\[ \text{The terms including the second order of the coupling constants are rewritten as follows. From} \]

\[ \text{We calculate response function of charge density wave with} \]

\[ Q \]

\[ \text{The evaluation by the bosonization method leads to} \]

\[ 1 \]

\[ \text{Thus the reconstructed } F_{\cos \theta_{\rho+}} \text{ is expressed as} \]

\[ \text{The terms including the second order of the coupling constants are rewritten as follows. From} \]

\[ \text{eq. (8), one obtains,} \]

\[ \int_0^{\ln(r/\alpha)} dl \left[ 2G_3^2(l) K_{\rho}^2(l) + G_W^2(l) K_{\rho}^2(l) \right] \ln \left( \frac{r}{\alpha(l)} \right) = K_{\rho}(0) \ln(r/\alpha) - \int_0^{\ln(r/\alpha)} dl K_{\rho}(l), \]

\[ \text{where} \]

\[ \alpha(l) = \alpha e^l. \]

\[ \text{The response function } R_{\cos \theta_{\rho+}} \text{ is expressed as} \]

\[ \text{which leads to eq. (13). In a similar way, another response function leads to eqs. (14).} \]

**Appendix B: Evaluation of cutoff parameter**

We calculate response function of charge density wave with \( Q = 2k_F + q \) and \( k_F = \pi/(2a) \), which is expressed as

\[ \Pi(Q) = \frac{1}{2} \sum_{j,\sigma} \int d\tau \begin{pmatrix} T_{\tau} c_{j,\sigma}^\dagger(\tau) c_{\sigma}^\dagger(0) c_{0,\sigma}(0) c_{0,\sigma}(0) \end{pmatrix} e^{-iQ R_{j} + i\omega_m \tau} \bigg|_{\omega_m \to 0}. \]

For the case with only the first term of eq. (1), eq. (B.1) is calculated as

\[ \Pi(Q) = \frac{1}{2\pi} \int_{-\pi/\alpha}^{0} dk \frac{f(\varepsilon_k + Q) - f(\varepsilon_k)}{\varepsilon_k^2 - \varepsilon_k + Q} \quad \longrightarrow \quad \frac{1}{2\pi v_F} \ln \frac{C}{q_a}, \]

where \( C \approx 1.273\pi \). The evaluation by the bosonization method leads to \( \text{eq. (B.3)} \)

\[ \Pi_B(Q) = \frac{1}{(2\pi \alpha)^2} \int dx \int d\tau \frac{1}{1 + (v_F \tau/\alpha)^2 + (x/\alpha)^2} e^{iQ x - i\omega_m \tau} \bigg|_{\omega_m \to 0} \]

\[ \frac{K_0(qa)}{2\pi v_F} \longrightarrow \frac{1}{2\pi v_F} \ln \frac{1}{qa}. \]

From eqs. (B.2) and (B.3), it is found that \( \alpha \approx a/(1.273\pi) \).
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