Metal-Insulator Transition of the One-Dimensional Extended Hubbard Model

Kazuhiro SANO[a] and Yoshiaki ŌNO[b,c,d]

[a] *Department of Physics Engineering, Mie University, Tsu, Mie 514-8507, JAPAN*
[b] *Department of Physics, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, JAPAN*
[c] *CREST Japan Science and Technology Corporation (JST)*
[d] *Department of Mathematics, Imperial College of Science Technology and Medicine, 180 Queen's Gate, London SW7 2BZ, U.K.*
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Abstract

The metal-insulator transition of the one-dimensional Hubbard model with both on-site U and nearest neighbor V interactions is studied by a combination of the numerical diagonalization method and the renormalization (RG) group method. Substituting the numerical result to the RG equation as the initial condition, we calculate the Luttinger-liquid parameter K_ρ at quarter filling. Comparing the renormalized K_ρ with the known exact result, we find it to be reliable in the strong coupling regime. This approach gives an evident critical point of the metal-insulator transition beyond the usual finite-size scaling for the numerical diagonalization result. The charge gap is also estimated by the numerical diagonalization method in the insulator region.

Keywords: Metal-Insulator transition; Extended Hubbard Model;numerical diagonalization;

The one-dimensional(1D) correlated electron systems have been extensively studied as a simple model of quasi-1D materials. [1, 2] In particular, the 1D extended Hubbard model with on-site repulsive interaction U and nearest neighbor repulsive interaction V is interest for the understanding of the physics of the metal-insulator transition. Here, the Hamiltonian of the 1D extended Hubbard model is

$$H = t\sum_{i,\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + h.c.) + U\sum_i n_{i\uparrow}n_{i\downarrow} + V\sum_{i,\sigma\sigma'} n_{i\sigma}n_{di+1\sigma'},$$

where $c^\dagger_{i\sigma}$ stands for creation operators of a electron with spin σ at site i and $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$. t represents the transfer energy between the nearest neighbor site, which will be set to unity (t=1) in the present study.

It is well known that the 1D extended Hubbard model shows the metal-insulator (M-I) transition at quarter-filling in the region for large U and V. The weak coupling renormalization group method (known as g-ology) and the numerical diagonalization method have clarified the nature of the M-I transition. The g-ology yields the phase diagram of the 1D extended Hubbard model analytically, but this approach is limited to application in the weak coupling limit. [1–4] On the other hand, the numerical approach is useful method to investigate the properties in the strong coupling region. [5] In particular, the numerical diagonalization of a finite-size system has supplied us with reliable and important information. [6–8] However, analysis is difficult for the numerical approach near the phase boundary of the M-I transition because the charge gap which determines the characteristic energy scale of the system becomes exponentially small.

To overcome this difficulty, we consider a combination of the numerical diagonalization method and the renormalization group (RG) method. [9, 10] It will provides us an approach which give high accuracy beyond usual finite size scaling of the numerical diagonalization.

At first, we briefly discuss a general argument for 1D electron systems based on the bosonization theory. In the low

energy limit, an effective Hamiltonian is given by

$$\begin{aligned} H &= H_\sigma + H_\rho \\ &= H_\sigma + \frac{v_\rho}{2\pi}\int_0^L \mathrm{d}x \left[K_\rho(\partial_x\theta_\rho)^2 + K_\rho^{-1}(\partial_x\phi_\rho)^2\right] \\ &+ \frac{2g_{3\perp}}{(2\pi\alpha)^2}\int_0^L \mathrm{d}x \cos[\sqrt{8}\phi_\rho(x)] \end{aligned} \quad (1)$$

where v_ρ and K_ρ are the charge velocity and coupling parameter, respectively. The operator ϕ_ρ and the dual operator θ_ρ represent the phase fields of charge part. $g_{3\perp}$ denotes the amplitude of the umklapp scattering and α is a short-distance cutoff. Here, H_σ is an effective Hamiltonian of spin part and we do not consider it. According to the bosonization theory, the effective Hamiltonian can be separated into the charge and spin parts independently. So, we turn our attention to only the charge part.

At quarter-filling, the $8k_F$ umklapp scattering is crucial to understanding the M-I transition. The effect of the Umklapp term is renormalized under the change of the cutoff $\alpha \to \mathrm{e}^l\alpha$. Within one-loop order, the renormalization group (RG) equations are given by

$$\frac{\mathrm{d}K_\rho(l)}{\mathrm{d}l} = -8G^2(l)K_\rho^2(l), \quad (2)$$

$$\frac{\mathrm{d}G(l)}{\mathrm{d}l} = [2 - 8K_\rho(l)]G(l), \quad (3)$$

where $G(0) = g_{3\perp}/2\pi v_\rho$ and the scaling quantity l is related to the cutoff α. These equations determine the RG flow diagrams and the phase boundary of the system. Roughly speaking, the insulator region appears for $G(l) \gtrsim K_\rho(l)$ or $K_\rho(l) < 0.25$. [3,4]

In the weak-coupling limit, v_ρ, $g_{3\perp}$ and $K_\rho(0)$ are evaluated as $(2\pi v_F + U + 4V)^2 - (U+4V)^{2\,1/2}/2\pi$, $(U - 4V)U^2/(2\pi v_F)^2$ and $1 + (U+4V)/(\pi v_F)^{-1/2}$ respectively at quarter-filling. Here, v_F is given by $2t\sin k_F$. If we substitute these values to the RG equations as the initial conditions, we find that the insulator region appears for $U \gtrsim 7$ at $V = 0$. This wrong result shows that the weak-coupling approximation breaks down in the strong coupling region.

To use the RG equations beyond the weak-coupling region, we adopt the numerical diagonalization result as initial conditions in the RG equations. We diagonalize finite size systems numerically and calculate $K_\rho(L)$ of the L-sites system. Using a relation $l \simeq \ln L$, we substitute $K_\rho(L)$ to $K_\rho(l)$ in the RG equations and solve them numerically . Here, we have to prepare two initial values. We use two values $K_\rho(L_1)$ and $K_\rho(L_2)$ because it is easy for the numerical diagonalization method to calculate $K_\rho(L)$ than $G(L)$. The values $G(l)$ are determined by the solution of the RG equations.

In Fig.1, we show solutions $K_\rho(l)$ of the RG equations as a function of $1/L$ with the numerical diagonalization result for various V in the limit $U \to \infty$. Here, we set $L_1 = 12$ and $L_2 = 16$. The flows of $K_\rho(l)$ seem to connect smoothly with

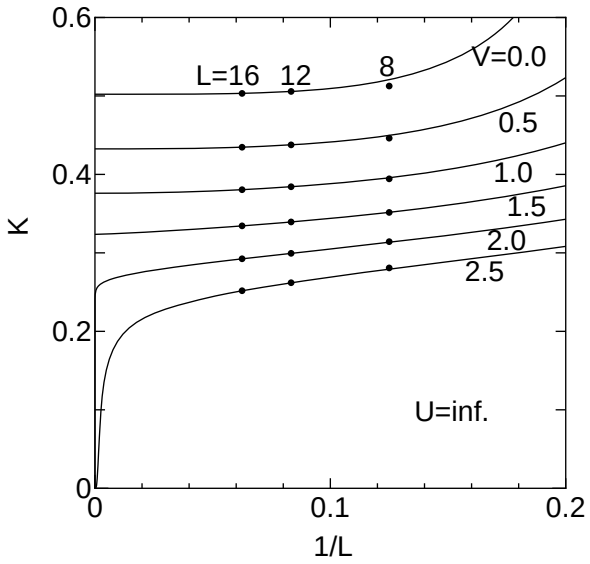

Fig. 1. The RG flows of K_ρ(the broken lines) and the numerical diagonalization results(the sold circles). Although the value $K_\rho(\infty)$ at $V = 2.0$ seems to be $\simeq 0.25$ in the figure, the RG flow converges to $K_\rho(\infty) = 0$.

the numerical result. It suggests that the RG equations give reasonable $K_\rho(\infty)$ from the numerical diagonalization result in the strong-coupling regime. In the limit $U \to \infty$, the 1D extended Hubbard model is mapped on XXZ spin model and the Luttinger-liquid parameter K_ρ is exactly obtained as $\cos(\frac{\pi}{4K_\rho}) = -V/2$. [11] We compare the values K_ρ from our approach and a similar approach by Emery and Noguera with the exact values in Table 1. In our approach, the M-I transition is found at $V \simeq 1.94$; this value is slightly smaller than the exact value $V = 2.0$. However, our result shows good agreement with the exact result as well as the result of Emery and Noguera. It indicates that the combination of the numerical diagonalization and the RG equations gives accurate values of K_ρ near the M-I transition.

Table I. Luttinger-liquid parameter K_ρ in the limit $U \to \infty$.

V	This work	Emery and Noguera	Exact
0.0	0.5022	-	0.5
1.0	0.3765	-	0.375
2/1.75	0.3608	0.3592	0.3604
2/1.5	0.3414	0.3406	0.3414
2/1.25	0.3128	0.3140	0.3144
1.935	0.2566	-	0.2721
2.0	0.0(insulator)	0.262	0.25

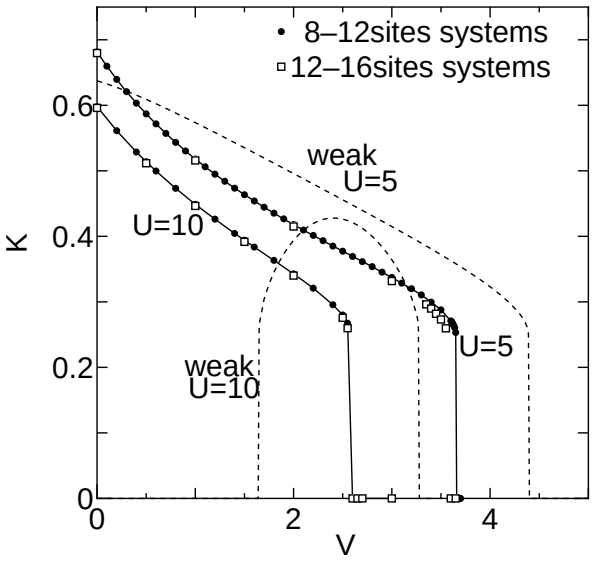

Fig. 2. $K_\rho(L=\infty)$ as a function of V at $U=5$ and 10 with the result of the weak-coupling approximation(the broken lines). The sold circles represent the result of the case $L_1=8$ and $L_2=12$. The open square represent the result of the case $L_1=12$ and $L_2=16$.

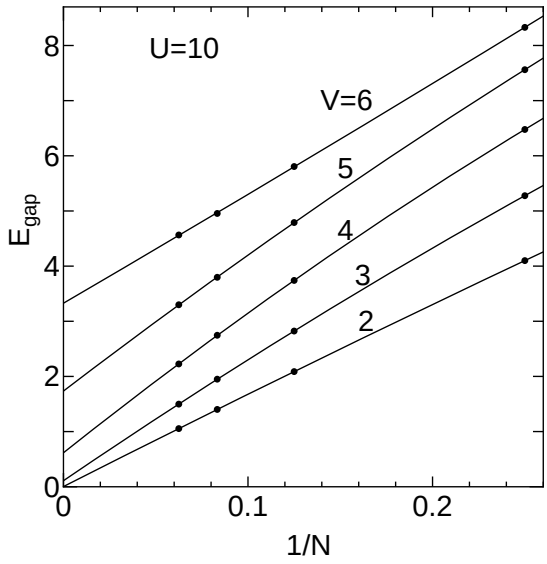

Fig. 3. The charge gap $\Delta_\rho(L)$(The sold circles) as a function of $1/L$ at $U=10$ for various V. The solid lines represent fitted lines to the data(See the text).

In Fig.2, we show $K_\rho(\infty)$ as a function of V with the weak coupling approximation result at $U=5$ and 10. In order to check the size dependence, we calculate $K_\rho(\infty)$ by using the two different initial conditions ($L_1=8$, $L_2=12$) and ($L_1=12$, $L_2=16$). Figure 2 indicates that the size dependence of $K_\rho(\infty)$ is very small. It also shows that the M-I transition occurs at $V\simeq 2.6$ for $U=5$ and at $V\simeq 3.7$ for $U=10$. The result shows good agreement with the phase boundary of the M-I transition in the previous work. [10] It suggests that our approach gives high accurate values of $K_\rho(\infty)$ beyond usual finite size scaling near the M-I transition. On the other hand, the weak-coupling approximation seems to be applicable to the case of $U=5$, but it is not correct for $U=10$ even if qualitatively except the region $1.5\lesssim V\lesssim 3.5$.

Next, we consider the charge gap by the numerical diagonalization method. The charge gap is defined by

$$\Delta_\rho(L)=E(L/2+1)+E(L/2-1)-2E(L/2). \quad (4)$$

where $E(L/2)$ is the total ground state energy of a system with $L/2$ electrons and $E(L/2)$ is calculated up to 16 sites systems. Figure 3 shows $\Delta_\rho(L)$ as a function of $1/L$ for various V at $U=10$. We assume that the size dependence of $\Delta_\rho(L)$ is

$$\Delta_\rho(L)=\Delta_\rho(\infty)+c_1/L+c_2/L^2, \quad (5)$$

where c_1 and c_2 are constants. The charge gap seems to be zero at $V=2$ and very small at $V=3$. It suggests that the M-I transition occurs between $V=2$ and $V=3$. Although it is difficult to estimate precisely the charge gap near the M-I transition, the extrapolated result of the charge gap may be consistent with the RG analysis.

In Fig.4, we show that $\Delta_\rho(\infty)$ as a function of V at $U=5$ and $U=10$. The charge gap increases with V and/or U. When $V/t>>1$, the values $\Delta_\rho(\infty)$ seem to be saturated and close to $U-4$. This result is interpreted as follows. [6–8, 10] In the limit $V/t\to\infty$, the ground state energy $E(L/2)$ is always zero at quarter-filling. If one electron is add to this, the energy is given by $E(L/2+1)=U$. When one electron is removed, two free holes which behave as spin-less fermions appear and they have a kinetic energy $\simeq -4\cos(2\pi/L)$. Therefore, the charge gap is given by $\Delta_\rho(L)\simeq U-4\cos(2\pi/L)$. It also leads the exact transition point $U_c=4$ at $L\to\infty$.

In summary, we consider the M-I transition of the one-dimensional extended Hubbard model by the combination of the numerical diagonalization method and the renormalization (RG) group method at quarter filling. Substituting the Luttinger-liquid parameter K_ρ obtained by the numerical diagonalization to the RG equation, we can fully utilize the information contained in the RG equations. This method provides us the reliable result of K_ρ beyond usual finite size scaling of the numerical diagonalization near the M-I transition. In the insulator region, the charge gap is

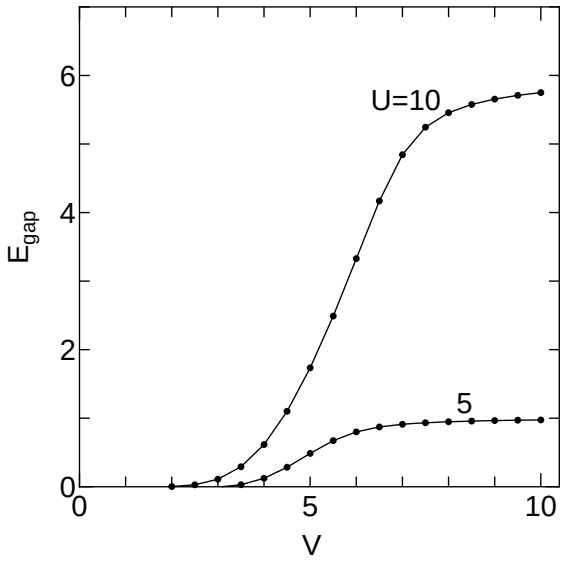

Fig. 4. The charge gap $\Delta_\rho(\infty)$(The sold circles) as a function of V at $U = 5$ and 10.

calculated by the numerical diagonalization method. In the limit $V/t \to \infty$, we discuss the values of the charge gap and the transition point of the M-I transition analytically.

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1) J. Sólyom, Adv. Phys. **28**, 201 (1979).
2) V. J. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. T. Devreese, R. Evrand and V. van Doren, (Plenum, New York, 1979), p.327.
3) M. Tsuchiizu, H. Yoshioka and Y. Suzumura, Physica **B**, (to be published).
4) H. Yoshioka, M. Tsuchiizu and Y. Suzumura, preprint.
5) H. Q. Lin and J. E. Hirsch, Phys. Rev **B33**, 8155 (1985).
6) F. Mila and X. Zotos, Europhys. Lett. **24**, 133 (1993).
7) K. Penc and F. Mila, Phys. Rev. B **49**, 9670 (1994).
8) K. Sano and Y. Ōno, J. Phys. Soc. Jpn. **63**, 1250 (1994).
9) V. J. Emery and C. Noguera, Phys. Rev. Lett. **60**, 631 (1988); They evaluated $G(L)$ by the level splitting of a finite size system and calculated K_ρ from the RG equations in the limit $U \to \infty$.
10) M. Nakamura, cond-mat9909277; He shows the phase boundary of the M-I transition by observing the level crossing of the excitation spectra of finite size systems.
11) A. Luther and Peschel, Phys. Rev. B **9**, 2911 (1974).