Charge gap in the one-dimensional extended Hubbard model at quarter filling

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We propose a different combined approach, which consists of the exact diagonalization, renormalization group, and Bethe ansatz methods, for precise estimates of the charge gap Δ in the one-dimensional extended Hubbard model, with on-site and nearest-neighbor interactions U and V at quarter filling. This approach enables us to obtain the absolute value of Δ, including the prefactor, without ambiguity even in the critical regime of the metal-insulator transition (MIT) where Δ is exponentially small, beyond usual renormalization group methods and/or finite-size scaling approaches. The detailed results of Δ, down to the order of 10^{-10} near the MIT, are shown as contour lines on the U-V plane.

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There has been much theoretical interest in one-dimensional (1D) strongly correlated electron systems, such as the t-J and Hubbard models, as good testing grounds for the concept of the Tomonaga-Luttinger liquid.[1,2] Various methods, such as the weak coupling theory (g-ology), bosonization theory, Bethe ansatz (BA) method, conformal field theory, as well as numerical approaches, have been used to clarify the nature of these models.[3] Among them, combined approaches using the exact diagonalization (ED) and the renormalization group (RG) methods have been extensively developed to investigate the critical behavior near the quantum critical point.[4–9] These approaches enable us to obtain accurate results of the phase boundary for the spin gap and charge gap phases than purely numerical approaches combined with finite-size scaling.

Recently, we have intensively examined the critical behavior near the metal-insulator transition (MIT) in the one-dimensional extended Hubbard model, with the on-site and nearest-neighbor interactions U and V at quarter filling, using a combined approach of the ED and RG methods.[7–9] In this approach, the Luttinger-liquid parameter, K_ρ, is calculated using the ED for finite-size systems, and then substituted into the RG equation as an initial condition to obtain K_ρ in the infinite-size system. The obtained result agrees well with the available exact result for $U=\infty$, even in the critical regime of the MIT, where the characteristic energy becomes exponentially small and the usual finite-size scaling is not applicable. When the system approaches the MIT critical point, $V \to V_c$ for a fixed U, K_ρ behaves as $(K_\rho - \frac{1}{4})^2 = c_K(1 - V/V_c)$, where the critical value V_c and the coefficient c_K are functions of U.[9] This approach also yields the critical behavior of the charge gap Δ in the insulating state near the MIT, where $|\ln \Delta|^{-2} = c_\Delta(V/V_c - 1)$ with the coefficient c_Δ a function of U. In these studies,[7–9] however, the absolute value of Δ including the prefactor was not explicitly obtained.

In general, it is considered difficult for the RG method, or its derivative method, to yield absolute values of physical quantities, including the prefactor. To overcome this difficulty, we added the BA method to our previous combined approach for use in the present study. More explicitly, the BA result in the infinite-size system with $U=\infty$ is connected to the ED result in the finite-size system with finite U through the analysis of the RG solution. This approach enables us to estimate the absolute value of Δ including the prefactor without ambiguity, and is in contrast with previous methods.

The extended Hubbard model is given by the Hamiltonian

$$H = -t\sum_{i,\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + \text{H.c.}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{i,\sigma\sigma'} n_{i\sigma}n_{i+1\sigma'}, \tag{1}$$

where $c_{i\sigma}^{\dagger}$ stands for the creation operator for an electron with spin σ at site i, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. t represents the transfer energy between the nearest-neighbor sites and is set to unity ($t=1$) in the present study. It is well known that this Hamiltonian [Eq. (1)] can be mapped on an XXZ quantum spin Hamiltonian in the limit $U \to \infty$. The nearest-neighbor interaction term V corresponds to the Z component of the antiferromagnetic exchange coupling and the transfer energy t corresponds to the X component. When the Z component is larger than the X component, the system has an *Ising-type* symmetry and an excitation gap exists. For the Hubbard model, this corresponds to the case with $V > 2t$, where the exact result of the charge gap is given by[10]

$$\Delta = 4(\sinh \lambda)\sum_{n=-\infty}^{\infty} \frac{(-1)^n}{2\cosh n\lambda} \tag{2}$$

with

$$\lambda = -\ln[(V/2) - \sqrt{(V/2)^2 - 1}]. \tag{3}$$

On the other hand, in the case with *XY-like* symmetry ($V < 2t$), the system is metallic and the Luttinger-liquid parameter K_ρ is exactly obtained from $\cos\left(\frac{\pi}{4K_\rho}\right) = -V/2$.[11]

To introduce our approach, we briefly discuss a general argument for 1D electron systems based on the bosonization theory.[1–3] According to this theory, the effective Hamiltonian

for the 1D electron systems can be generally separated into charge and spin parts. Therefore, we concentrate only on the charge part and do not consider the spin part for this study. In the low-energy limit, the effective Hamiltonian of the charge part is given by

$$H_\rho = \frac{v_\rho}{2\pi}\int_0^L dx[K_\rho(\partial_x\theta_\rho)^2 + K_\rho^{-1}(\partial_x\phi_\rho)^2] + \frac{2g_{3\perp}}{(2\pi\alpha)^2}\int_0^L dx\cos[2\sqrt{8}\phi_\rho(x)], \quad (4)$$

where v_ρ and K_ρ are the charge velocity and the coupling parameter, respectively. The operator ϕ_ρ and the dual operator θ_ρ represent the phase fields of the charge part. $g_{3\perp}$ denotes the amplitude of the umklapp scattering and α is the short-distance cutoff. Based on the Hamiltonian Eq. (4), the electronic state is described by only the two parameters K_ρ and $g_{3\perp}$, except for the energy scale determined by v_ρ.

At quarter filling, the $8k_F$ umklapp scattering plays a crucial role in the charge gap. The effect of the umklapp term is renormalized under the change of the cutoff $\alpha \to e^\ell \alpha$, where ℓ is the scaling quantity. This process is also considered to be the change of the system size $L \to e^\ell L$. Therefore, the size dependence of K_ρ is described by the RG equations.[7–9] In this work, we adopt Kehrein's formulation as the RG equations[13,14]

$$\frac{dK_\rho(\ell)}{d\ell} = -8\frac{G(\ell)^2 K_\rho(\ell)^2}{\Gamma[8K_\rho(\ell)-1]}, \quad (5)$$

$$\frac{d\log G(\ell)}{d\ell} = [2 - 8K_\rho(\ell)], \quad (6)$$

where $\Gamma(x)$ is the Γ function and $G(l)$ stands for the umklapp effect with $G(0)=g_{3\perp}/(2\pi v_\rho)$. Here, the value of the short-distance cutoff α is selected from the lattice constant of the system and set to unity. This formulation is an extension of the perturbative RG theory and allows us to estimate the charge gap beyond the weak-coupling regime.

To solve the RG equations, we need an initial condition for the two values, $K_\rho(0)$ and $G(0)$. Because it is easy for the ED calculation to obtain $K_\rho(\ell)$ as compared to $G(\ell)$, we eliminate $G(\ell)$ in the RG equations. For this purpose, we integrate Eq. (6) to yield

$$G(\ell) = G(\ell_1)\exp\int_{\ell_1}^{\ell}[2 - 8K_\rho(\ell')]d\ell', \quad (7)$$

where ℓ_1 is a constant. By substituting Eq. (7) into Eq. (5), we obtain the differential equation for $K_\rho(\ell)$ as

$$\frac{dK_\rho(\ell)}{d\ell} = -8\frac{G^2(\ell_1)\exp\left\{\int_{\ell_1}^{\ell}[4 - 16K_\rho(\ell')]d\ell'\right\}K_\rho(\ell)^2}{\Gamma[8K_\rho(\ell)-1]}. \quad (8)$$

Setting $K_\rho(\ell_1)$ as the initial condition, we solve Eq. (8) numerically except for the constant $G(\ell_1)$. The value of $G(\ell_1)$ is determined by comparing the solution $K_\rho(\ell)$ at $\ell=\ell_2$ with the initial value $K_\rho(\ell_2)$. Thus, the solutions for Eqs. (5) and (6) are obtained in full.

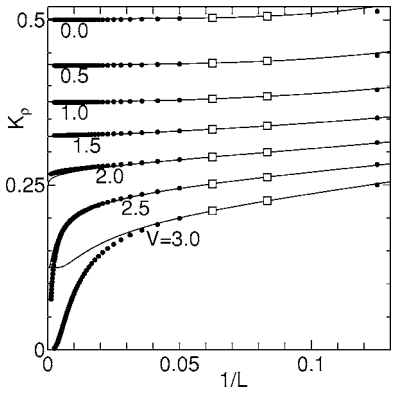

FIG. 1. The size dependence of $K_\rho(L)$ obtained from the RG equations (solid lines) and the exact Bethe ansatz results (filled circles) for various V at $U=\infty$. The open squares are the numerical initial conditions with $L_1=12$ and $L_2=16$ for the RG equations.

Using the relation $\ell \simeq \ln L$, we calculate two initial values, $K_\rho(\ell_1)$ and $K_\rho(\ell_2)$, with L_1- and L_2-site systems by the ED method. In finite-size systems, $K_\rho(L)$ is calculated from the charge susceptibility χ_c and the Drude weight D as

$$K_\rho = \frac{1}{2}(\pi\chi_c D)^{1/2}, \quad (9)$$

with $D=\frac{\pi}{L}\frac{\partial^2 E_0(\phi)}{\partial\phi^2}$, where $E_0(\phi)$ is the total energy of the ground state as a function of magnetic flux $L\phi$, and L is the system size.[3] Here, the magnetic flux is imposed by introducing the following gauge transformation: $c^\dagger_{m\sigma} \to e^{im\phi}c^\dagger_{m\sigma}$ for an arbitrary site m. The uniform charge susceptibility χ_c is obtained from

$$\chi_c = \frac{4/L}{E_0(N+2,L) + E_0(N-2,L) - 2E_0(N,L)}, \quad (10)$$

where $E_0(N,L)$ is the ground-state energy of a system with L sites and N electrons. Here, the filling n is defined by $n=N/L$. We numerically diagonalize the Hamiltonian Eq. (1) up to 16 sites using the standard Lanczos algorithm. In the case where $U=\infty$, we also calculate $E_0(N,L)$ by the Bethe ansatz method[12] for finite-size systems with up to 800 sites. Using the definitions of Eqs. (9) and (10), we calculate K_ρ and χ_c from the ground-state energy of the finite-size system.

In Fig. 1, we show the size dependence of $K_\rho(L)$ obtained from the solutions of the RG equations, together with the exact Bethe ansatz results for various V at $U=\infty$. We chose $L_1=12$ and $L_2=16$ for the numerical initial condition in the RG equations, and we set $L_1=L_2-4$ hereafter. The limit, $K_\rho(L\to\infty)$, of the BA result becomes a finite value for $V\leqslant 2$ and converges to zero for $V>2$. We see that the RG solution is very close to the exact result and the size dependence of $K_\rho(L)$ is well described by the RG equations, with the exception of very large size systems for $V>2$.

In Fig. 2, we show the RG flows of the systems with various V for $U=10$ together with those for $U=\infty$. We observe that the RG flows for $U=10$ and those for $U=\infty$ coin-

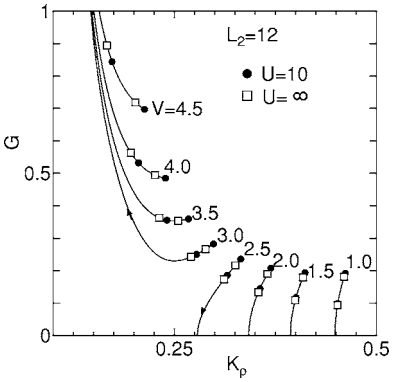

FIG. 2. The RG flow on the $K_\rho - G$ plane for various V at $U=10$ with the numerical initial condition (filled circles). The open squares are the numerical initial conditions at $U=\infty$ fitting to the RG flow for $U=10$.

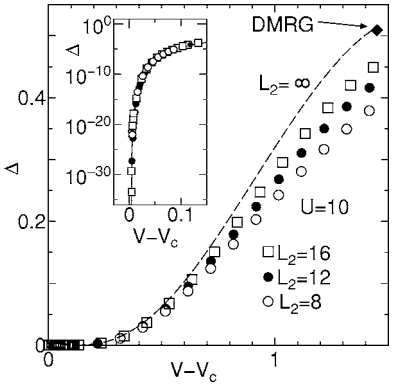

FIG. 3. The charge gap Δ as a function of $V-V_c$ at $U=10$ for $L_2=8$, 12, and 16 together with the extrapolated result (dashed line). The solid diamond is the DMRG result (Ref. 18). Inset shows the semilogarithmic plot of Δ near the MIT.

cide with each other. Based on the Luttinger-liquid theory, it is considered that the systems assigned with the same RG flows also have the same electronic state except for the energy scale v_ρ. If we find a specific RG flow for $U=\infty$ (we call it a reference system) corresponding to that for finite U (an original system), we can connect both systems through the RG flow and derive the properties of the original system from the known result of the reference system. To identify the RG flow, we use a renormalized coupling constant $\tilde{G}(\ell)$ constructed from the product of $G(\ell)$ and the effective energy scale $e^{-\ell(2-8K_\rho)}$. In the limit $\ell \to \infty$, $G(\ell)$ diverges in proportion to $e^{\ell(2-8K_\rho)}$ [see Eq. (7)], while $\tilde{G}(\infty)$ remains a finite value and becomes a unique index for characterizing the RG flow.

Here, we determine the nearest-neighbor repulsion V in the reference system with $U=\infty$ so as to fit the RG flow of the reference system to that of the original system with original V for a finite value of U. The reference parameters V corresponding to several original parameters V for $U=10$ are shown in Table I. The reference parameter V is smaller than the corresponding original parameter V. This suggests that the on-site repulsion U causes the renormalization of the nearest-neighbor repulsion V. Figure 2 also shows that the point indicating the initial condition of the reference system is located further downstream than that of the original system on the RG flow. This means that the effective size of the reference system is larger than the original system size.

Substituting the reference V into Eq. (3), we obtain the charge gap Δ_r of the reference system from Eq. (2). Taking into account the difference in the energy scale, i.e., the charge velocity between the original and reference systems, we estimate the charge gap of the original system as $\Delta = v_\rho^o / v_\rho^r \Delta_r$, where v_ρ^o and v_ρ^r are the charge velocities of the original and reference systems, respectively. Both of the charge velocities are calculated from the ED results with the same size systems through the relation $v_\rho = D/2K_\rho$.

TABLE I. The original and reference parameters V for $U=10$ (see text).

Original V	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Reference V	0.38	0.85	1.33	1.84	2.38	2.92	3.43

In Fig. 3, we plot the charge gap Δ as a function of $V-V_c$ at $U=10$ for $L_2=8$, 12, and 16, together with the result of an extrapolation with $L_2 \to \infty$. Here, V_c is the critical value of the MIT, which is determined by the condition $K_\rho(\ell \to \infty)=1/4$. The V_c values are 2.684, 2.583, and 2.567 for the finite-size systems with $L_2=8$, 12, and 16, respectively, which yield an $L_2 \to \infty$ extrapolated value $V_c=2.55$. We note that detailed analyses of V_c and the MIT have already been discussed in previous works.[6–8,15–17] The L_2 dependence of Δ is assumed to be proportional to $1/L_2$, resulting in an extrapolated value of Δ with $L_2 \to \infty$ as shown in Fig. 3. The obtained result for Δ is in good agreement with the recent DMRG result of Δ at $V-V_c \simeq 1.45$.[18] The inset in Fig. 3 shows the semilogarithmic plot of Δ near the MIT. The system size dependence of Δ is very small even in the critical regime of the MIT near V_c. These results show that the combined approach is especially efficient for analyzing the very small charge gap near the MIT.

In Fig. 4, we show the detailed results of contour lines for the extrapolated value of the charge gap Δ near the MIT on the $U-V$ plane. An approximate estimation of Δ has already been reported in our previous paper.[9] However, the previous

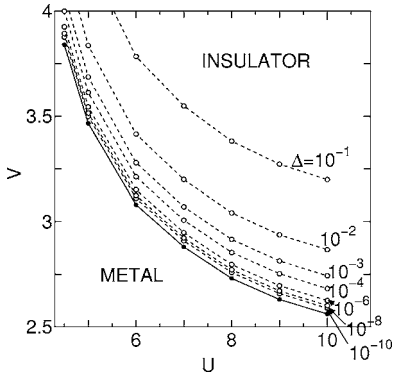

FIG. 4. The contour lines of the charge gap Δ near the MIT on the $U-V$ plane. The solid line represents the phase boundary of the MIT.

result was limited to the case with large gap ($\Delta > 0.25$) region, since finite-size scaling is normally used for the ED result. We stress that our approach has the ability to estimate very small charge gaps down to the order of 10^{-10}, far outweighing the limitations of the numerical estimation methods.

In summary, we have examined a different combined approach using the ED, RG, and BA methods to clarify the charge gap Δ of the 1D extended Hubbard model with both on-site and nearest-neighbor interactions U and V at quarter filling. After analyzing the solution of the RG equations, we connected the original system with a finite U to the reference system with $U=\infty$, whereby the charge gap was obtained as a function of V by the exact BA method. By adjusting the parameter V of the reference system, so as to fit the RG flow of the reference system to that of the original system, we can estimate the absolute value of Δ of the original system, including the prefactor. This approach is able to supply us with unambiguous and accurate results for Δ that are well beyond the usual RG method and/or the ED method, even if the energy scale becomes exponentially small. Detailed analysis of Δ is shown as contour lines on the $U-V$ plane in the critical regime near the MIT with a very small gap.

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