Metal-Insulator Transition of the One-Dimensional U-V Model at Quarter Filling

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Abstract

The metal-insulator transition of the one-dimensional extended Hubbard model with both on-site U and nearest neighbor V interactions is studied by a combination of the numerical diagonalization and the renormalization group (RG) method. We diagonalize finite size systems numerically and calculate the Luttinger-liquid parameter K_ρ. Substituting the numerical result to the RG equations as the initial condition, we explicitly calculate the renormalized K_ρ and the renormalized umklapp scattering parameter G. This approach gives the critical properties of the K_ρ and the charge gap near the metal-insulator transition beyond the usual finite-size scaling for the numerical diagonalization result. We also obtain a contour map of the charge gap by the numerical diagonalization method on the U-V plain.

keywords
D. electrical properties; D.phase transitions

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The extended Hubbard model with on-site repulsive interaction U and nearest neighbor repulsive interaction V has been extensively studied as a simple model of quasi-1D materials[1, 2, 3]. In particular, the insulator transition caused interactions not only U but V at quarter filling, is interesting for the physics of one-dimensional(1D) strongly correlated electron systems[4, 5, 6]. The weak coupling renormalization group method (known as g-ology) and the numerical methods have clarified the nature of the metal-insulator (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, 2, 4, 5]. On the other hand, the numerical approach is useful method to investigate the properties in the strong coupling region[3, 6]. In particular, the numerical diagonalization of a finite-size system has supplied us with reliable and important information of the M-I transition[7, 8, 9]. However, it is difficult for the numerical approach to analyze the critical properties near the M-I transition because the characteristic energy scale of the system becomes exponentially small. To overcome this difficulty, we combine the numerical diagonalization method with the renormalization group (RG) method [10, 11, 12]. It will provide us an approach which gives high accuracy beyond usual finite size scaling of the numerical diagonalization method.

We consider the Hamiltonian of the 1D extended Hubbard model

$$\begin{aligned} H &= t\sum_{i,\sigma}(c^{\dagger}_{i\sigma}c_{i+1\sigma} + h.c.) \\ &+ U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{i,\sigma\sigma'} n_{i\sigma}n_{di+1\sigma'}, \end{aligned}$$

where $c^{\dagger}_{i\sigma}$ stands for creation operators of an 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. In the low energy limit, an effective Hamiltonian of a charge part is given by

$$H = \frac{v_\rho}{2\pi}\int_0^L \mathrm{d}x \left[K_\rho(\partial_x\theta_\rho)^2 + K_\rho^{-1}(\partial_x\phi_\rho)^2\right]$$

$$+ \quad \frac{2g_{3\perp}}{(2\pi\alpha)^2}\int_0^L \mathrm{d}x\cos[\sqrt{8}\phi_\rho(x)] \tag{1}$$

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. 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 and do not consider the effective Hamiltonian of spin 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

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

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

where $G(0) = g_{3\perp}/2\pi v_\rho$ and the scaling quantity l is related to the cutoff α[4, 5]. 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 $K_\rho(l) < 0.25$. In the previous work[12], we have shown that the numerical diagonalization method provides a good initial condition and the one-loop order RG equations yield correct results of the renormalized K_ρ even for large U and/or V.

In this work, we also consider the RG equations introduced by Kehrein[13, 14],

$$\frac{\mathrm{d}K_\rho(l)}{\mathrm{d}l} = -8\frac{G^2(l)K_\rho^2(l)}{\Gamma(8K_\rho(l)-1)}, \tag{4}$$

$$\frac{\mathrm{d}G(l)}{\mathrm{d}l} = [2-8K_\rho(l)]G(l), \tag{5}$$

where $\Gamma(x)$ is Γ-function. This formulation is an extension of the perturbative RG equations and allows us to analyze properties of the system in the strong coupling region. At first, we examine the Kehrein's RG equations by comparison with the one-loop RG equations. 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[5]. Here, v_F is given by $2t\sin k_F$. We substitute the above initial condition to the one-loop RG and Kehrein's RG equations and compare these solutions. We expect that there are few differences for the solutions between the one-loop RG and the Kehrein's RG equations in the weak coupling region.

In Figs.1, we show the RG flows obtained by the both RG equations with the analytical initial condition on the $K_\rho(l)$-$G(l)$ plane. In the weak coupling region($U \lesssim 3$), these RG flows almost agree with each other and the values of the renormalized $K_\rho(\infty)$ consist with the Bethe ansatz results. However, $K_\rho(\infty)$ is not consistent with the exact results away from the weak coupling region. Furthermore, we find that the insulator region appears for $U \gtrsim 7$ at $V = 0$ in the strong coupling region($U \gtrsim 7$). This wrong result suggests that if the initial condition is far away from the fixed point or improper, the solution of the RG equations would be meaningless and the above analytical initial condition is not applicable in the strong coupling region.

Next, we examine the initial condition obtained by the numerical diagonalization method. We numerically calculate $K_\rho(L)$ of the L-sites system[17]. Using a relation $l \simeq \ln L$, we substitute $K_\rho(L)$ to $K_\rho(l)$ in the RG equations and numerically solve them. 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 value $G(l)$ is determined by the solution of the RG equations. In Fig.2, we show the RG flows obtained by the one-loop RG equations and the Kehrein's RG equations with the numerical initial condition on the $K_\rho(l)$-$G(l)$ plane. Here, we set $L_1 = 8$ and $L_2 = 12$.

Figure 2 indicates that the RG flows of both RG equations are very close each other for various U. It also shows that $K_\rho(\infty)$ well agrees with the exact result even in the limit of $U \to \infty$. This result suggests that our approach gives good initial conditions for both RG equations far away from the weak coupling region.

In Fig.3, we show $K_\rho(\infty)$ as a function of V at $U = 5$ and ∞. 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 $\cos(\frac{\pi}{4K_\rho}) = -V/2$[15]. The difference of $K_\rho(\infty)$ for both RG equations is very small and cannot be distinguished in the figure. Figure 3 also indicates that our result is consistent with the exact result at $U = \infty$. When the initial condition is given in the proximity of the fixed point, even the one-loop RG equations can lead accurate $K_\rho(\infty)$ for large U and/or V. It suggests that our approach gives high accurate value of $K_\rho(\infty)$ beyond usual finite size scaling near the M-I transition. On the other hand, the analytical initial condition seems to be applicable to the case of $U = 5$, but it is not correct for $U \gtrsim 8$ even if qualitatively.

Next, we consider the phase boundary of the M-I transition and the charge gap in the insulator region. In the numerical diagonalization method, the charge gap is defined by $\Delta_\rho(L) = E(L/2+1) + E(L/2-1) - 2E(L/2)$, where $E(L/2)$ is the total ground state energy of the system with $L/2$ electrons. We assume that the size dependence of $\Delta_\rho(L)$ is $\Delta_\rho(L) = \Delta_\rho(\infty) + c_1/L + c_2/L^2$, where c_1 and c_2 are constants and $\Delta_\rho(L)$ is calculated up to 16 sites systems[16]. It is difficult to estimate the charge gap numerically near the M-I transition. However, it is easy for the RG method to determine the phase boundary. At the critical point, $K_\rho(\infty)$ is renormalized to 1/4.

In Fig.4, we show contour lines of the charge gap and the phase boundary of the M-I transition on the U-V plain. The charge gap increases with V and/or U. When $V >> 1$, U-dependence of $\Delta_\rho(\infty)$ seems to be saturated and close to $U-4$. This result is interpreted as follows[7, 8, 9, 11]. 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 M-I transition point

$U_c = 4$ at $L \to \infty$.

The boundary of the M-I transition obtained by the analytical initial condition roughly consists with the result of numerical one except the wrong insulator region on the U-axis. In order to check the size dependence, we calculate the phase boundary by using the three different initial conditions $(L_1 = 4, L_2 = 8)$,$(L_1 = 8, L_2 = 12)$ and $(L_1 = 12, L_2 = 16)$. It suggests that the finite size effect is sufficiently small except the $(L_1 = 4, L_2 = 8)$ case. The result is consistent with the result of the level crossing method[11].

Finally, we discuss the charge gap obtained by the combination of the numerical diagonalization and the Kehrein's RG method near the M-I transition. When only the renormalized K_ρ is considered, there are few advantages of the Kehrein's RG method. However, the Kehrein's RG approach can lead the excitation gap in the strong coupling region such as insulator region. The perturbative RG approach leads to divergence in the running coupling constants $G(l)$ and/or $K_\rho(l)$ and becomes invalid in the strong coupling region. The Kehrein's RG method introduces a renormalized coupling constant $\tilde{G}(l)$ constructed by the product of $G(l)$ and the effective energy scale $\exp(-l(2-8K_\rho))$. Although $G(l)$ diverges in the strong coupling limit, $\tilde{G}(l)$ remains a finite value and leads to the charge gap. The value of $G(l)$ is calculated in the same way of the weak coupling problem. Roughly speaking, $G(l)$ diverges as $\exp(l)$ with an increase in l, but the effective energy scale $\exp(-l(2-8K_\rho))$ is renormalized to $\exp(-l)$. Therefore, $\tilde{G}(l)$ converges in the limit of $l \to \infty$. The charge gap is given as $\Delta = c\tilde{G}(\infty)$, where c is a factor of the charge gap and the order of the charge velocity v_ρ. Unfortunately, the RG method can not give c directly. It may be determined to fit the extrapolated value from the charge gap of the finite systems.

In Fig.5, we show the charge gap Δ as a function of V at $U = \infty$ obtained by the combination of the numerical diagonalization and the Kehrein's RG method. Here, c is determined to fit the exact result. It indicates that the V dependence of Δ shows

good agreement with the exact result near the M-I transition[18]. Then our approach can estimate the charge gap which has very small energy scale precisely near the M-I transition. Detail analysis is now in progress and it will be reported elsewhere.

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 RG 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 and the estimation of the charge gap beyond usual finite-size scaling of the numerical diagonalization near the M-I transition. In the insulator region, the contour map of the charge gap is also calculated by the numerical diagonalization method.

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Figurecaptions

Figure 1;

The RG flows by the analytical initial condition on the $K_\rho(l)$-$G(l)$ plane. The solid lines stand the flows from the Kehrein's RG equations and the dashed lines stand the flows from the one-loop RG equations. Open squares represent the exact result of $K_\rho(\infty)$ at $U = \infty$,8,6.5,5,3 respectively.

Figure 2;

The RG flows by the initial condition based on the numerical diagonalization method on the $K_\rho(l)$-$G(l)$ plane. The solid lines stand the flows from the Kehrein's RG equations and the broken lines stand the flows from the one-loop RG equations. Sold circles and open circles denote the initial values calculated by the RG equations. Open squares represent the exact results of $K_\rho(\infty)$ at $U = \infty$,8,7.5,6.5,5,3 respectively.

Figure 3;

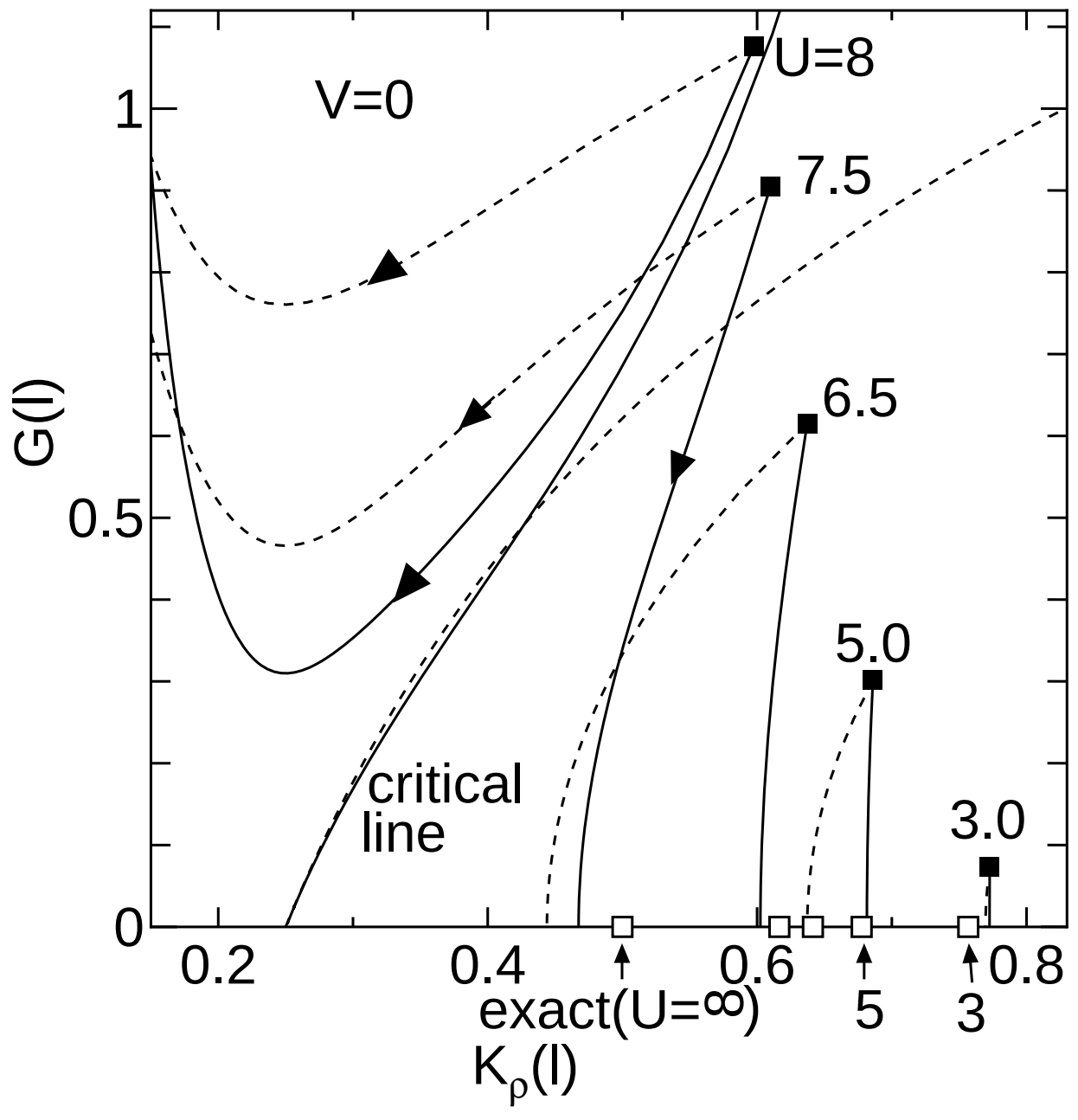
$K_\rho(\infty)$ as a function of V at $U = 5$ and ∞ based on the numerical diagonalization method with the exact result (the solid line). The sold circles and open circles represent the results of the Kehrein's RG and the one-loop RG equations respectively. The dashed and broken lines stand the results of the analytic initial condition from the Kehrein's RG equation and from the one-loop RG equations respectively.

Figure 4;

The contour lines of the charge gap with the phase boundary of the M-I transition on the U-V plain. The values of the charge gap represented by each contour line are 0.25,0.5,1,1.5,2,2.5,3,3.5,4,4.5,5, and 5.5 respectively. The sold circles, the crosses and

open squares represent the phase boundary from the initial condition of the numerical diagonalization method. The dashed lines and broken lines stand the results of the analytic initial condition from the Kehrein's RG equations and from the one-loop RG equations respectively.

Figure 5;
The charge gap Δ as a function of $V - V_c$ at $U = \infty$ by the combination of the numerical diagonalization and the Kehrein's RG method with the exact result (the solid line).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U=8
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6.5
5.0
3.0
critical
line
G(l)
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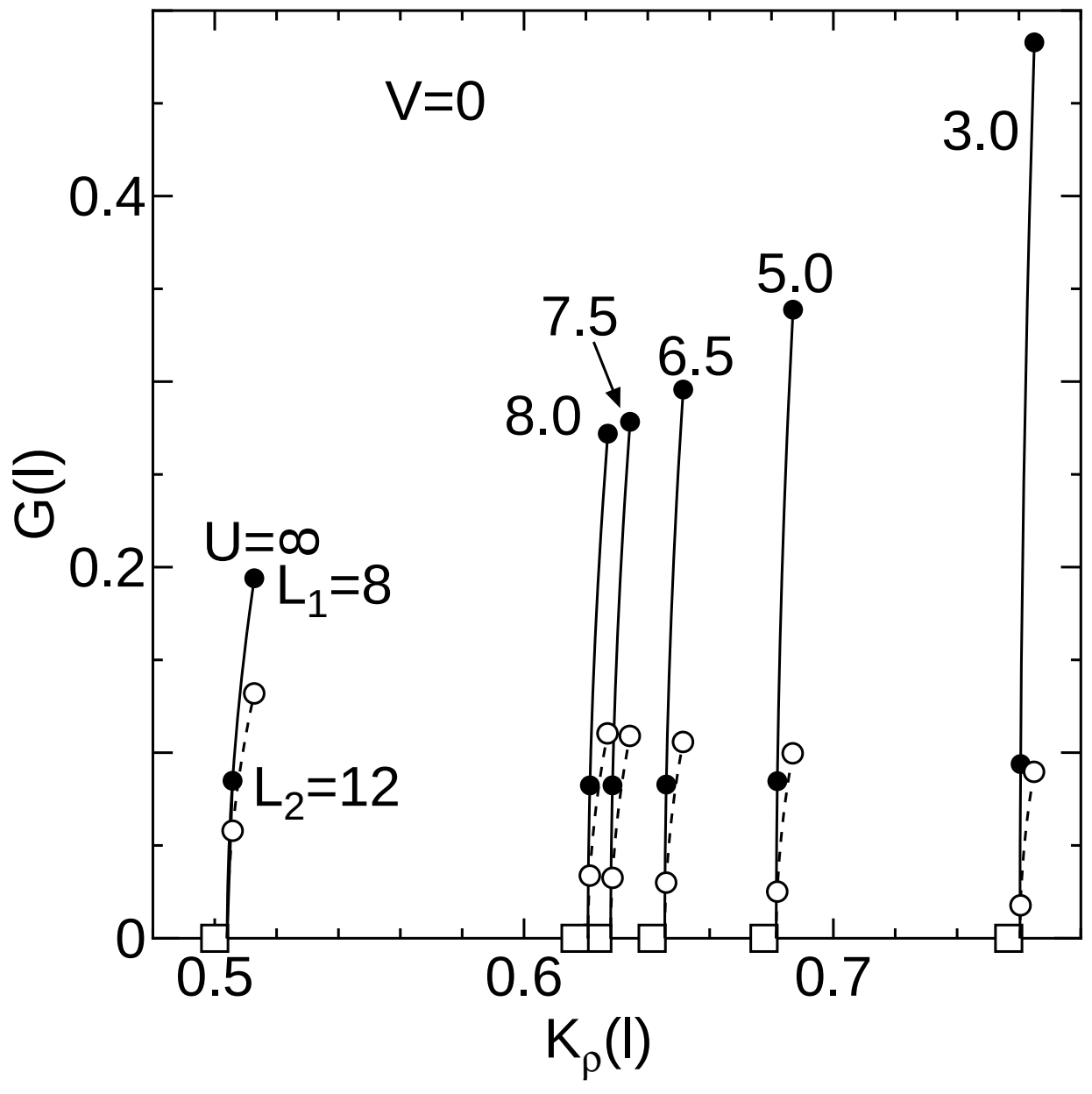
0
0.2
0.4
0.6
0.8
exact(U=∞)
5
3
$K_\rho(l)$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3.0
5.0
7.5
6.5
8.0
U=∞
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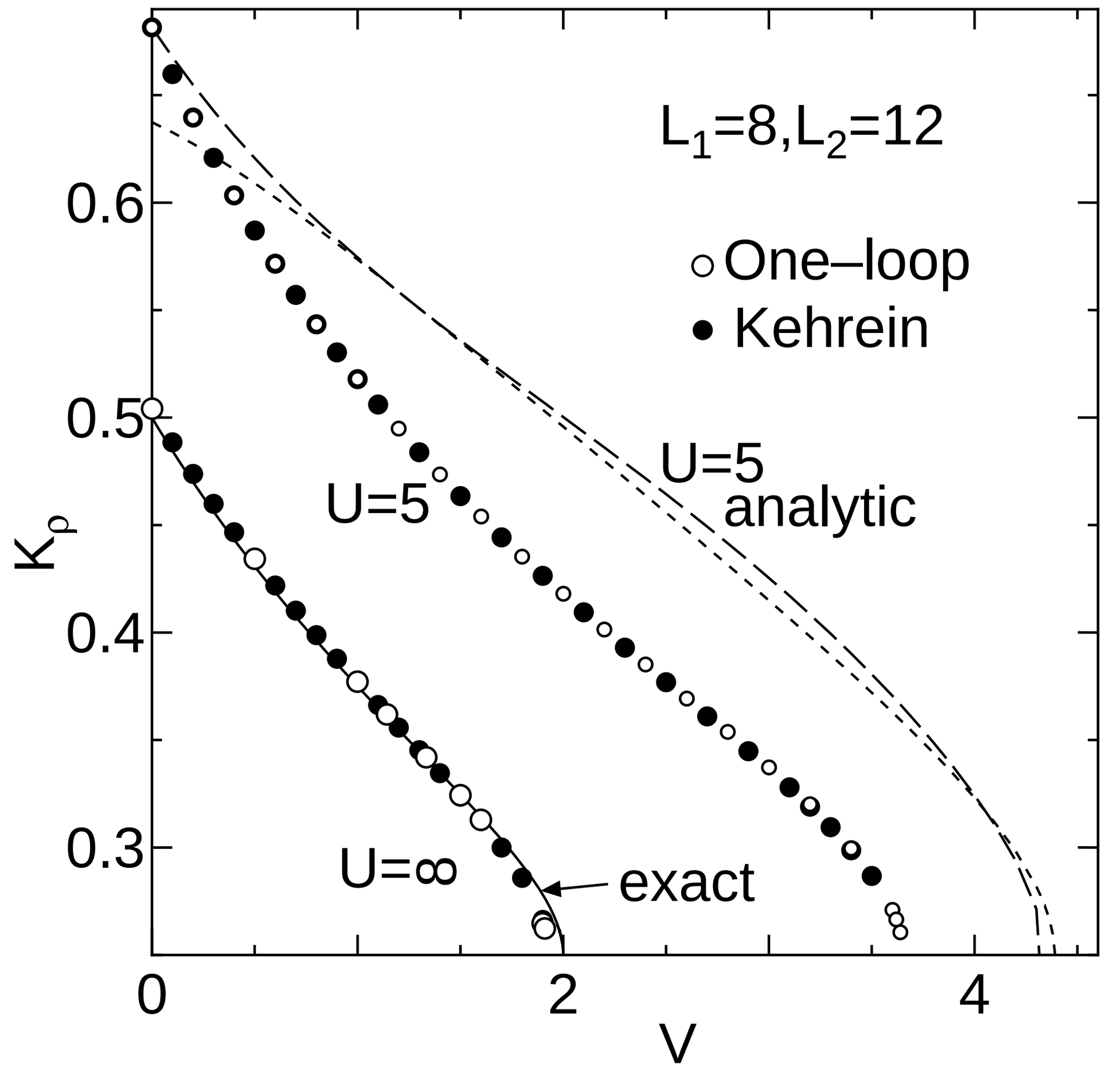
0.2
0
G(l)
0.5
0.6
0.7
K_ρ(l)


L_1=8,L_2=12
One–loop
Kehrein
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U=5
U=∞
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0.4
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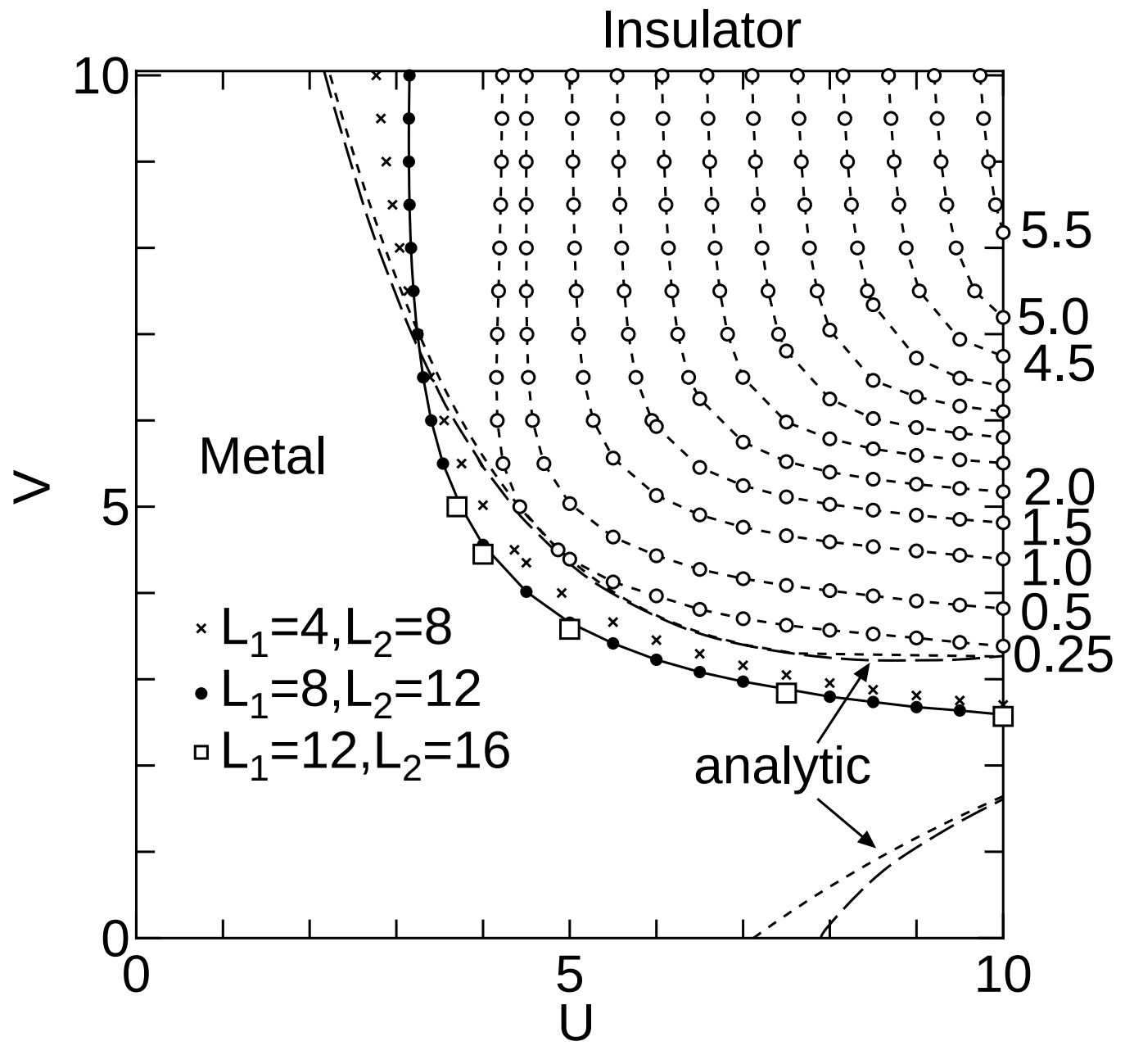
2
4
V


Insulator
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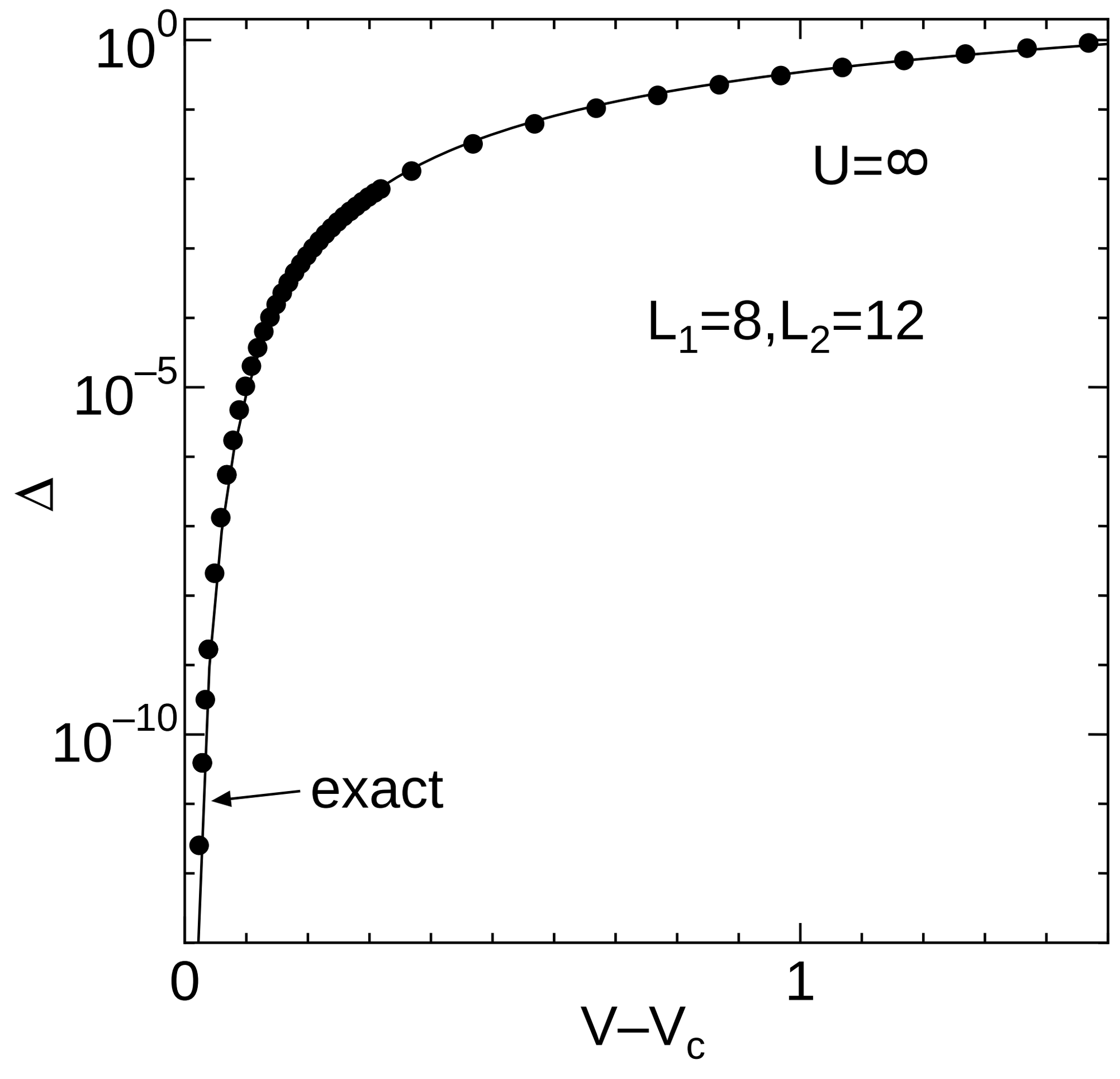
analytic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