Journal of the Korean Physical Society, Vol. 39, No. 2, August 2001, pp. 203∼208

Bethe Ansatz Solutions and Excitation Gap of the Attractive Bose-Hubbard Model

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(Received 12 March 2001, in final form 24 July 2001)

The energy gap between the ground state and the first excited state of the one-dimensional attractive Bose-Hubbard Hamiltonian is investigated in connection with directed polymers in random media. The excitation gap Δ is obtained by exact diagonalization of the Hamiltonian in the two- and three-particle sectors and also by an exact Bethe Ansatz solution in the two-particle sector. The dynamic exponent z is found to be 2. However, in the intermediate range of the size L where $UL \sim \mathcal{O}(1)$, U being the attractive interaction, the effective dynamic exponent shows an anomalous peak reaching high values of 2.4 and 2.7 for the two- and the three-particle sectors, respectively. The anomalous behavior is related to a change in the sign of the first excited-state energy. In the two-particle sector, we use the Bethe Ansatz solution to obtain the effective dynamic exponent as a function of the scaling variable UL/π. The continuum version, the attractive delta-function Bose-gas Hamiltonian, is integrable by the Bethe Ansatz with suitable quantum numbers, the distributions of which are not known in general. Quantum numbers are proposed for the first excited state and are confirmed numerically for an arbitrary number of particles.

I. INTRODUCTION

The dynamics of many simple non-equilibrium systems are often studied through corresponding quantum Hamiltonians. Examples are the asymmetric XXZ chain Hamiltonian and the attractive Bose-Hubbard Hamiltonian for the single-step growth model [1] and the directed polymers in random media (DPRM) [2], respectively. The single-step growth model is a Kardar-Parisi-Zhang (KPZ) universality class growth model where the interface height $h(x,t)$ grows in a stochastic manner under the condition that $h(x\pm 1,t)-h(x,t)=\pm 1$. The process is also called the asymmetric exclusion process (ASEP) in a different context. The evolution of the probability distribution for $h(x,t)$ is generated by the asymmetric XXZ chain Hamiltonian [3]. The entire information about the dynamics is coded in the generating function $e^{\alpha h(x,t)}$. Its time evolution, in turn, is given by the modified asymmetric XXZ chain Hamiltonian [4–6],

$$H_{\mathrm{XXZ}}(\alpha) = -\sum_{i=1}^{L}\left\{e^{2\alpha/L}\sigma_i^-\sigma_{i+1}^+ + \frac{1}{4}(\sigma_i^z\sigma_{i+1}^z-1)\right\}, \qquad (1)$$

with the σ's being the Pauli matrices and L the size of the system. (We consider only the periodic boundary condition in this work.) On the other hand, in the DPRM problem, the partition function $Z(x,t)$, the partition sum over directed polymer configurations with fixed ends at $(0,0)$ and (x,t), is the quantity of main interest. Its generating function $Z(x,t)^n$ then evolves by the one-dimensional attractive Bose-Hubbard Hamiltonian [2],

$$H_{\mathrm{BH}}(n) = -\frac{1}{2}\sum_{i=1}^{L}(b_i b_{i+1}^\dagger + b_i^\dagger b_{i+1} - 2) - U\sum_{i=1}^{L}\frac{b_i^\dagger b_i(b_i^\dagger b_i - 1)}{2}. \qquad (2)$$

Here, the $b^\dagger$'s(b's) are the boson creation (annihilation) operators, $\sum_{i=1}^{L} b_i^\dagger b_i = n$ is the conserved particle number, and $U(>0)$ is the attractive interaction. The two systems are closely related, at the level of continuum stochastic differential equations, through the Cole-Hopf transformation, $Z(x,t)=e^{-h(x,t)}$ [7]. In particular, U in Eq. (2) is related to the particle density, $\rho=\sum_{i=1}^{L}(\sigma_i^z+1)/2$ of Eq. (1), by $U=4\rho(1-\rho)$ [8,9]. Recently, the universal probability distribution function (PDF) at the stationary state was found for both models mentioned above [4–6,10]. Their common structure of the ground-state energies as functions of the scaling variables $\alpha\sqrt{4L\rho(1-\rho)}$ and $-n\sqrt{LU}$, for the single-step growth model and the DPRM problem, respectively, gives the universal PDF at the stationary state.

While the ground-state energy of each Hamiltonian gives information about the stationary state of the cor-

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responding process, the first excited-state energy, combined with the ground-state energy, is related to the characteristic behavior of the process as it approaches the stationary state. For example, in the single-step growth model, as $t \to \infty$, the generating function takes the form

$$\log e^{\alpha h(x,t)} \sim \left\{-E_0(\alpha)t + e^{-\Delta(\alpha)t}\right\}, \tag{3}$$

and similarly for $\log Z(x,t)^n$. Here, $E_0(\alpha)$ is the ground-state energy of Eq. (1), $\Delta(\alpha)$ is the inverse of the relaxation time, as well as the gap between the ground-state energy and the first excited-state energy, $E_1(\alpha)$, such that $\Delta(\alpha) = E_1(\alpha) - E_0(\alpha)$. The size dependence of $\Delta(\alpha)$, $\Delta(\alpha) \sim L^{-z}$, defines the dynamic exponent z.

Because the asymmetric XXZ chain Hamiltonian, $H_{\mathrm{XXZ}}(\alpha)$, is integrable by the Bethe Ansatz, the low-lying state energies, as well as the size dependence of the excitation gap, are well understood. When $\alpha\sqrt{4L\rho(1-\rho)} \gg 1$ and the density of particles is finite in the limit $L \to \infty$, $\Delta(\alpha)$ behaves as $\Delta(\alpha) \sim L^{-1}$. However, when $\alpha\sqrt{4L\rho(1-\rho)} \sim \mathcal{O}(1)$, $\Delta(\alpha)$ behaves as $\Delta(\alpha) \sim L^{-3/2}$ [3,11]. The dynamic exponent $z = 3/2$ is a characteristic of the dynamic universality class of the KPZ-type surface growth. When the number of particles is finite and the density of particles is very low, it is known that $\Delta(\alpha) \sim L^{-2}$ [12]. However, when $\alpha < 0$, which corresponds to the ferromagnetic phase, most Bethe Ansatz solutions are not available although the Bethe Ansatz equations continue to hold. As α becomes negative, the quasi-particle momenta appearing in the Bethe Ansatz equations become complex, so solutions are difficult to obtain analytically.

The attractive Bose-Hubbard Hamiltonian is expected to have some resemblance to the ferromagnetic phase of the asymmetric XXZ chain Hamiltonian considering the equivalence of α and $-n$. The equivalence is identified indirectly by comparing the two scaling variables $\alpha\sqrt{4L\rho(1-\rho)}$ and $-n\sqrt{LU}$ under the relation $U = 4\rho(1-\rho)$ or the two generating functions $\exp(\alpha h(x,t)$ and $Z(x,t)^n$ under the relation $Z(x,t) = e^{-h(x,t)}$. In contrast to the asymmetric XXZ chain Hamiltonian, the Bose-Hubbard Hamiltonian does not satisfy the Bethe Ansatz except in the two-particle sector [13]. Instead, the attractive delta-function Bose-gas Hamiltonian,

$$H_{\mathrm{D}}(n) = -\frac{1}{2}\sum_{i=1}^{n}\frac{\partial^2}{\partial x_i^2} - U\sum_{i<j}\delta(x_i - x_j), \tag{4}$$

which is the continuum version of the attractive Bose-Hubbard Hamiltonian, is known to be integrable by the Bethe Ansatz. The attractive delta-function Bose gas has been studied in [14] and [15]. The ground-state energy is obtained from the Bethe Ansatz solution by using the symmetric distribution of the purely imaginary quasi-particle momenta. However, the structure of the energy spectra is not well known for the same reason as in the asymmetric XXZ chain Hamiltonian with $\alpha < 0$. The unknown energy spectra itself prevents one from understanding the dynamics of DPRM near the stationary state.

In this paper, we discuss in Section II the distribution of the quantum numbers appearing in the Bethe Ansatz equation for the first excited state of the attractive delta-function Bose-gas Hamiltonian, the knowledge of which is essential for solving the Bethe Ansatz equation. In Section III, the excitation gap of the attractive Bose-Hubbard Hamiltonian with a small number of particles is investigated through the exact diagonalization method. We show that the gap decays as $\Delta \sim L^{-2}$, *i.e.*, $z = 2$, but that the exponent becomes anomalous when $U \sim L^{-1}$. The emergence of the anomalous exponent is explained in connection with the transition of the first excited state from a positive energy state to a negative energy state. The Bethe Ansatz solutions in the two-particle sector show how the behavior of the gap varies with the interaction. We give a summary and discussion in Section IV.

II. QUANTUM NUMBER DISTRIBUTION FOR THE FIRST EXCITED STATE

In this section, we study the Bethe Ansatz solutions for the ground state and the first excited state of the attractive delta-function Bose-gas Hamiltonian. The eigenstate of $H_{\mathrm{D}}(n)$, Eq. (4), is of the form

$$\phi(x_1, x_2, \ldots, x_n) = \sum_P A(P)\exp(ik_{P1}x_1 + ik_{P2}x_2 + \cdots + ik_{Pn}x_n), \tag{5}$$

where P is a permutation of $1, 2, \ldots, n$ and $x_1 \le x_2 \le \ldots \le x_n$ with no three x's being equal. The quasi-particle momenta k_j's are determined by solving the Bethe Ansatz equations,

$$k_j L = 2\pi I_j + \sum_{l\neq j}\theta\left(\frac{k_j - k_l}{-U}\right) \quad (j = 1, 2, \ldots, n),$$
$$\theta(x) = -2\tan^{-1}(x). \tag{6}$$

If the distribution of quantum numbers $\{I\}$ is given, the set of quasi-particle momenta $\{k\}$ is uniquely determined. With such k_j's, the energy eigenvalue is simply given by $E = \sum_{j=1}^{n}(k_j^2/2)$.

For the ground state, the set of quantum numbers $\{I\}$ is

$$I_j = -\frac{n+1}{2} + j, \quad (j = 1, 2, \ldots, n), \tag{7}$$

and the quasi-particle momenta are distributed symmetrically on the imaginary axis in the complex-k plane. Care should be taken when dealing with the first excited state. For the repulsive delta-function Bose-gas Hamiltonian, where U is replaced by $-U$ in Eq. (4), the quantum numbers for one of the first excited states are

$$I_j = -\frac{n+1}{2} + j \quad (j = 1, 2, \ldots, n-1),$$

$$I_n = \frac{n+1}{2}. \tag{8}$$

However, for the attractive case, by following the movement of the momenta as U changes sign, we find that the quantum numbers for the first excited state should be given by

$$\begin{aligned} I_j &= -\frac{n-1}{2} + j \quad (j = 1, 2, \ldots, n-1), \\ I_n &= -\frac{n-3}{2} \; (= I_1). \end{aligned} \tag{9}$$

That is, the two quantum numbers I_1 and I_n become the same. Such a peculiar distribution of I_j's does not appear in other Bethe Ansatz solutions such as those for the XXZ chain Hamiltonian or the repulsive delta-function Bose-gas Hamiltonian. We remark that even though the two I_j's are the same, all k_j's are distinct; otherwise, the wavefunction vanishes. Such a distribution of quantum numbers is confirmed by the consistency between the energies obtained by diagonalizing the Bose-Hubbard Hamiltonian exactly and those obtained by solving the Bethe Ansatz equations with the above quantum numbers for very weak interactions, for which the two Hamiltonians possess almost the same energy spectra.

When there is no interaction ($U = 0$), all quasi-particle momenta, k_j's, are zero for the ground state while for the first excited state, all the k_j's are zero except the last one, $k_n = 2\pi/L$. In the complex-k plane, as the very weak repulsive interaction is turned on, the $n-1$ momenta are shifted infinitesimally from $k = 0$ with $k_1 < k_2 < \cdots < k_{n-1}$, and the nth momentum is shifted infinitesimally to the left from $k = 2\pi/L$. All the momenta remain on the real axis. When the interaction is weakly attractive, the $n-1$ momenta become complex with Im $k_1 <$ Im $k_2 < \cdots <$ Im k_{n-1} and Re $k_j \simeq 0$ for $j = 1, 2, \ldots, n-1$, and the nth momentum remains on the real axis, but is shifted to the left. Figure 1 shows the distribution of the quantum numbers and the quasi-particle momenta in the presence of a very weak attractive interaction. The quasi-particle momenta are obtained by solving Eq. (6).

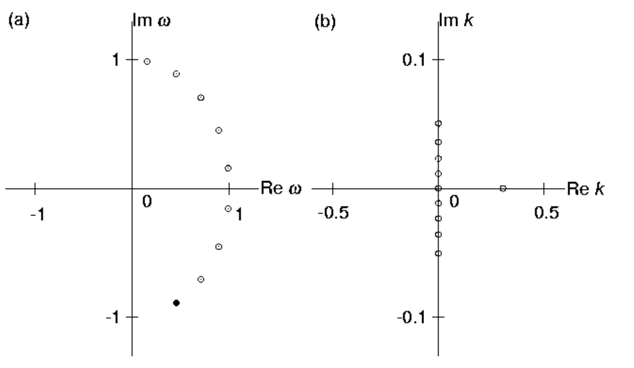

Fig. 1. For the first excited state, (a) the quantum numbers I_j's are depicted in the complex-ω plane with $\omega = e^{2\pi i I/L}$ and (b) the quasi-particle momenta k_j's are shown in the complex-k plane. Here, the size of the system L is 20, the number of particles n is 10, and the attractive interaction U is 0.0025. The filled circle in (a) is where the two quantum numbers overlap.

Knowledge of the distribution of the quantum numbers is essential for solving the Bethe Ansatz equations of the attractive delta-function Bose-gas Hamiltonian. For the original attractive Bose-Hubbard Hamiltonian, the Bethe Ansatz solutions are the exact solutions for the two-particle sector only, but are good approximate solutions in other sectors provided the density is very low and the interaction is very weak. This is because the Bethe Ansatz for the Bose-Hubbard Hamiltonian fails once states with sites occupied by more than three particles are included. Thus, for the sectors with three or more particles, the Bethe Ansatz solutions may be regarded as approximate eigenstates provided states with more than three particles at a site do not play an important role in the eigenfunctions. In [13], it is shown that the error in the Bethe Ansatz due to multiply-occupied sites (occupied by more than three particles) is proportional to U^2, where $U(>0)$ in [13] corresponds to $-U$ in Eq. (2). This applies to the attractive interaction case also. For the repulsive Bose-Hubbard Hamiltonian, the Bethe Ansatz is a good approximation when the density is low and the interaction is strong because the strong repulsion prevents many particles from occupying the same site [16]. For the attractive Bose-Hubbard Hamiltonian, the Bethe Ansatz is good when the density is low and the interaction is weak because a weak attraction is better

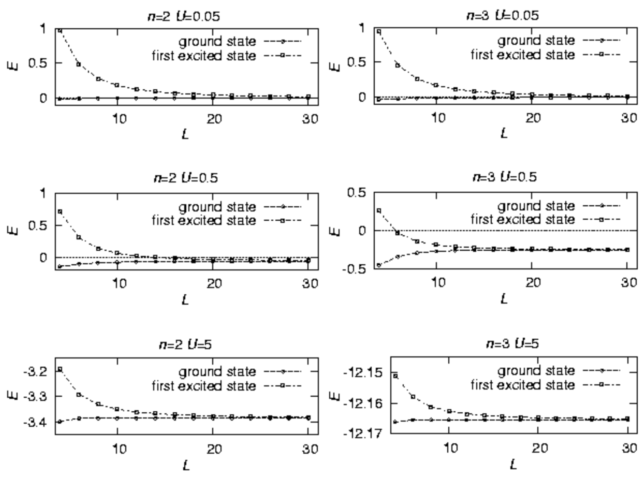

Fig. 2. Ground-state energies and first excited-state energies are plotted versus the size of the system L ($4 \le L \le 30$) for $U = 0.05$, 0.5, and 5 in the two- and the three-particle sectors. The dotted line represents $E = 0$. For all values of U and L, the ground-state energy is negative. On the other hand, when $U = 0.5$, the excited-state energy becomes negative near $L \simeq 14$ in the two-particle sector and $L \simeq 6$ in the three-particle sector. The signs of the excited-state energies for $U = 0.05$ and 5 do not change in the range of L shown here.

for preventing many particles from occupying the same site and because the error is proportional to U^2.

III. POWER-LAW DEPENDENCE AND ANOMALOUS EXPONENT

We are interested in the scaling limit $L \to \infty$ with the scaling variable $n\sqrt{UL}$ fixed because the common structure of the ground-state energies of the asymmetric XXZ chain Hamiltonian and of the attractive Bose-Hubbard Hamiltonian is found in this scaling limit. In this section, we investigate the size dependence of the excitation gap by using exact diagonalization of the attractive Bose-Hubbard Hamiltonian in the two- and the three-particle sectors for L up to 30. Also, for the two-particle sector, we solve the Bethe Ansatz equation using the result of the previous section for larger L.

Figure 2 shows the ground-state energies and the first excited-state energies versus the size of the system in the two- and the three-particle sectors for three values of U. Note that for some value of U, the sign of the first excited-state energy changes as the size of the system increases while for other values of U, no such crossover is seen in the range of L investigated here.

The excitation gaps versus the size of the system are shown in Fig. 3 and Fig. 4 on a logarithmic scale. For $U = 0.05$ and 5, the nearly straight lines indicate the power-law behavior of the gap, $\Delta \sim L^{-z}$, and the slopes of the fitted lines indicate $z \simeq 2.0$. However, for $U = 0.5$, the asymptotic behavior shows up only after a large crossover region where the effective z, $z_{\rm eff}$, is anomalously large. For the two-particle sector with $U = 0.5$, $z_{\rm eff}$ is about 2.4 in the range $14 \le L \le 18$. For the three-particle sector with $U = 0.5$, $z_{\rm eff}$ is about 2.7 in the corresponding range $8 \le L \le 12$.

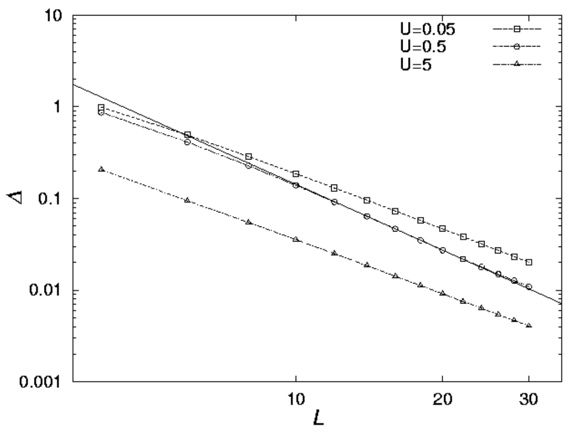

Fig. 3. Log-log plot of the excitation gaps (Δ) versus the size of the system (L) in the two-particle sector. Data for $U = 0.05$ and 5 approach straight lines with slope $z = 2.0$, but those for $U = 0.5$ show a strong crossover before approaching the asymptotic behavior. The solid line for $U = 0.5$ is that fitted in the range $14 \le L \le 18$, and shows an effective $z \simeq 2.4$.

Looking into the first excited-state energy in Fig. 2, one can see that the anomalous value of $z_{\rm eff}$ appears in the range of L where the first excited-state energies change their signs. We conjecture that the wavefunction has a transition as the sign of the energy changes. In order to confirm the connection between the anomalous exponent and the transition of the first excited state, we solved the Bethe Ansatz equation to evaluate the effective exponent $z_{\rm eff}$ near the transition point in the two-particle sector.

In the two-particle sector, the quantum numbers for the ground state and the first excited state are $\{-1/2, 1/2\}$ and $\{1/2, 1/2\}$ (or $\{-1/2, -1/2\}$), respectively. The quasi-particle momenta are purely imaginary, *i.e.*, $k_1 = -i\kappa$ and $k_2 = i\kappa$ for the ground state. For the first excited state, as noted already in [14], when $U < (4/L)\cos(\pi/L)$, the two quasi-particle momenta are real, *i.e.*, $k_1 = \pi/L - k$ and $k_2 = \pi/L + k$, while when $U > (4/L)\cos(\pi/L)$, k is replaced by iq such that $k_1 = \pi/L - iq$ and $k_2 = \pi/L + iq$. The examples of these distributions are shown in Figs. 5(a) and (b) with $L = 100$ for the two values of $U = 0.001$ and 0.1, respectively. The transition of the first excited state occurs when the quasi-particle momenta are imaginary. When $U > (4/L)\cos(\pi/L)$, the ground-state energy(E_0) and the first excited-state energy(E_1) are, respectively, given by

$$E_0 = -4\sinh^2\left(\frac{\kappa}{2}\right), \tag{10}$$

and

$$E_1 = 4\sin^2\left(\frac{\pi}{2L}\right)\cosh^2\left(\frac{q}{2}\right) - 4\cos^2\left(\frac{\pi}{2L}\right)\sinh^2\left(\frac{q}{2}\right), \tag{11}$$

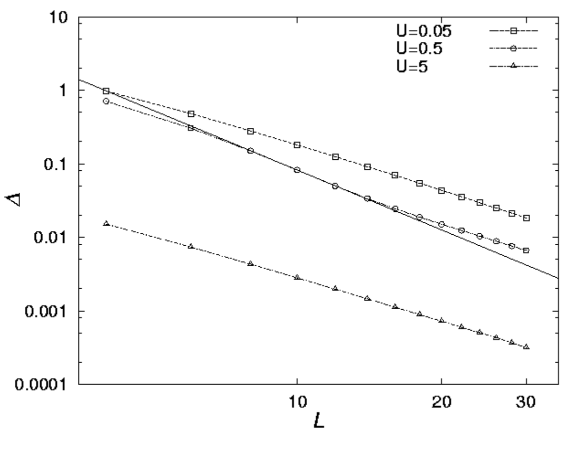

Fig. 4. Same as in Fig. 3, but for the three-particle sector. The fitted solid line used the data for $8 \le L \le 12$, and has a slope of approximately 2.7.

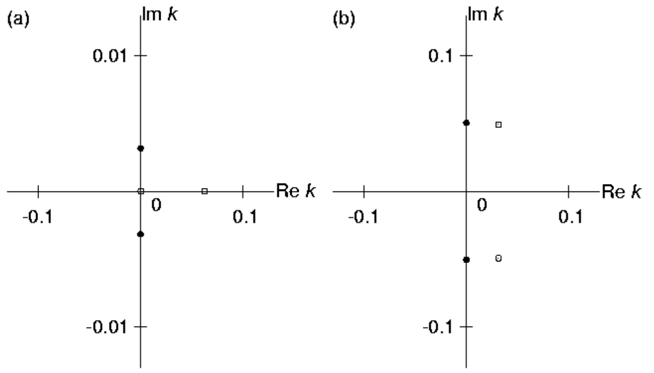

Fig. 5. Distributions of the quasi-particle momenta, k_j's, for the ground state (filled circles) and the first excited state (open circles) are shown in the complex-k plane for $n = 2$. The size of the system L is 100 and the interaction U is (a) 0.001 and (b) 0.1.

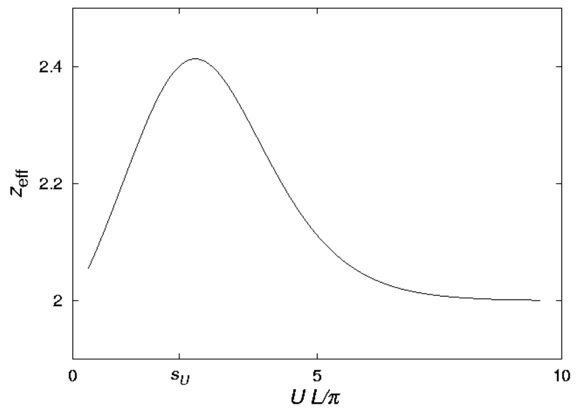

Fig. 6. Effective exponent $z_{\rm eff}$ in the two-particle sector versus the scaling variable UL/π at $L = 10000$. The interaction U varies from 0.0001 to 0.001. At $UL/\pi = s_U \simeq 2.181$, $z_{\rm eff} \simeq 2.401$.

where κ and q are real and satisfy

$$\kappa L = \log\left(\frac{2\sinh\kappa + U}{2\sinh\kappa - U}\right), \tag{12}$$

and

$$qL = \log\left(\frac{U + 2\cos(\frac{\pi}{L})\sinh q}{U - 2\cos(\frac{\pi}{L})\sinh q}\right), \tag{13}$$

respectively. We now consider the scaling limit $L \to \infty$ with UL finite. Let $U = U^* \equiv (\pi/L)s_U$ with $s_U \equiv 2\coth(\pi/2) \simeq 2.181$. At this value of U, the first excited-state energy, E_1, is 0, $\kappa^* \equiv \kappa(U^*) = (\pi/L)s_\kappa$, and $q^* \equiv q(U^*) = \pi/L$. Here, s_κ satisfies

$$\pi s_\kappa = \log\left(\frac{2s_\kappa + s_U}{2s_\kappa - s_U}\right), \tag{14}$$

which gives $s_\kappa \simeq 1.151$. When the size of the system L is increased by δL with $U = U^*$, the changes of κ and q, $\delta\kappa$ and δq, are, from Eqs. (12) and (13),

$$\begin{aligned} \delta\kappa &= -\frac{\pi s_\kappa(4{s_\kappa}^2 - {s_U}^2)}{4{s_\kappa}^2 - {s_U}^2 + (4/\pi)s_U}\ \frac{\delta L}{L^2} \equiv -\pi\Gamma\ \frac{\delta L}{L^2}, \\ \delta q &= \frac{\pi({s_U}^2 - 4)}{(4/\pi)s_U - {s_U}^2 + 4}\ \frac{\delta L}{L^2} \equiv \pi\Sigma\ \frac{\delta L}{L^2}. \end{aligned} \tag{15}$$

The perturbative expansion $\Delta(L + \delta L) \simeq \Delta(L)(1 - z(\delta L/L))$, under the assumption that $\Delta(L) \sim L^{-z}$, gives the value of $z_{\rm eff}$ at U^*:

$$z_{\rm eff} = 2\frac{1 + s_\kappa\Gamma + \Sigma}{s_\kappa^2}. \tag{16}$$

Numerical solutions of Eq. (14) give $z_{\rm eff} \simeq 2.401$.

On the other hand, when $U \ll U^*$, the ground-state energy, E_0, is $\mathcal{O}(U/L)$, and the first excited-state energy, E_1, is $\mathcal{O}(1/L^2)$, which are easily obtained from Eqs. (10) and (11). Therefore, the excitation gap behaves as $\Delta \sim L^{-2}$. Also, when $U^* \ll U \ll 1$, the quasi-particle momenta of the ground state are $\pm i\sinh^{-1}(U/2) - \mathcal{O}(e^{-L})$, and those of the first excited state are $\pi/L \pm i\sinh^{-1}(U/2) + \mathcal{O}(e^{-L})$, which lead to $z_{\rm eff} = 2$.

For arbitrary U, the effective value of $z_{\rm eff}$ is evaluated from the relation

$$z_{\rm eff} = \frac{\log(\Delta(L+1)/\Delta(L-1))}{\log((L-1)/(L+1))} \tag{17}$$

by using the solutions of Eqs. (12) and (13) for sufficiently large L. As discussed above, the exponent $z_{\rm eff}$ shows an anomalous peak near $U = U^*$ or $UL/\pi = s_U$ and approaches 2.0 as $UL/\pi \to 0$ or ∞. Figure 6 shows a plot of $z_{\rm eff}$ versus the scaling variable UL/π at $L = 10000$.

IV. SUMMARY AND DISCUSSION

As the asymmetric XXZ chain generates the dynamics of the single-step growth model, the attractive Bose-Hubbard Hamiltonian governs the dynamics of the DPRM. We studied the attractive Bose-Hubbard Hamiltonian and its continuum version, the attractive delta-function Bose-gas Hamiltonian concentrating on the behavior of the excitation gap, which is related to the characteristics of DPRM relaxing into the stationary state. For the attractive delta-function Bose gas Hamiltonian, The quantum numbers for the first excited state in the Bethe Ansatz equation are found for the attractive delta-function Bose gas Hamiltonian, and the distribution of the quasi-particle momenta is discussed in the presence of a very weak attractive interaction. Our result is the starting point for a further elucidation of the Bethe Ansatz solutions. We show that the excitation gap depends on the size of the system as a power law, $\Delta \sim L^{-z}$, and that the exponent z can be calculated by using an exact diagonalization of the attractive Bose-Hubbard Hamiltonian in the two- and the three-particle sectors and by using the Bethe Ansatz solution in the two-particle sector. The exponent z is 2.0. However, for the intermediate region where $UL \sim \mathcal{O}(1)$, the effective exponent $z_{\rm eff}$ shows a peak.

The equivalence of the differential equations governing the single-step growth model and DPRM implies some inherent equivalence in the corresponding Hamiltonians. The power-law behavior of the excitation gap, $\Delta \sim L^{-2}$, for the attractive Bose-Hubbard Hamiltonian with a very weak interaction is the same as that for the asymmetric XXZ chain Hamiltonian with a small number of particles, which is expected considering the relation $U = 4\rho(1-\rho)$. The fact that the excitation gap behaves anomalously for $U \sim L^{-1}$ implies the possibility of an anomalous dynamic exponent z for a finite scaling variable $n\sqrt{UL}$. If that is the case, one may expect the existence of some singularity at $n \sim L^{-1/2}$ with finite U, where the dynamic exponent z takes an anomalous value, which is similar to the singularity at $\alpha \sim L^{-1/2}$ for the asymmetric XXZ chain Hamiltonian.

ACKNOWLEDGMENTS

This work was supported by the Korea Research Foundation (2000- 015-DP0138).

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