Momentum distribution of the hard-core extended boson Hubbard model in one dimension

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We investigate the momentum distribution associated with quantum phase transitions between a superfluid and a charge-density-wave state in the one-dimensional hard-core extended boson Hubbard model at half filling by using the Lanczos exact diagonalization method. The momentum distribution shows distinct features in different regions. At the Heisenberg point, it shows a universal behavior. In the superfluid phase, the Luttinger-liquid parameters are easily obtained from the finite-size scaling behaviors of the zero-momentum occupancy. Also the signature of a charge-density wave can be identified in the insulating phase.

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I. INTRODUCTION

Interacting bosons hopping around on a lattice show quantum phase transitions in the ground state. Typically, strong on-site repulsions lead to a commensurate Mott-insulating phase while, in the opposite limit, a superfluid (SF) phase is stable.[1] In dilute bosonic gases at an incommensurate density, however, the increase in on-site repulsion does not destabilize the SF phase; it rather suppresses the Bose-Einstein condensation (BEC) onto the lowest-energy single-particle state. In one dimension, the extreme of this situation is described by the impenetrable Tonks-Girardeau gas.[2] Residual longer-range repulsive interactions then play a crucial role in bringing a quantum phase transition into the system. Strong repulsive interactions drive the ground state into a charge-density-wave (CDW) phase.

In experiments, momentum distributions have been used to identify the ground-state phase. For example, in a ballistic expansion measurement of ultracold atoms in an optical lattice,[3–5] where a reversible transition between a Mott-insulating and a SF phase are controlled by just tuning the intensity of an imposing laser, the appearance of a sharp peak at the zero-momentum state is regarded as the advent of the SF phase.[6] A crossover to the Tonks-Giradeu regime in a one-dimensional boson gas by increasing the ratio of the interaction energy to the kinetic energy is also investigated through momentum distributions.[7] In bosonic gases with longer-range interactions, such as ultracold gases of ^{52}Cr atoms with a dipole moment,[8] momentum distributions will also be useful to investigate the transitions between a SF and a CDW state.

The hard-core extended boson Hubbard model with near-neighbor repulsion is a minimal model to investigate the longer-range interaction effects. At half filling, strong near-neighbor repulsions stabilize a CDW ground state. The ground state turns into a SF phase as the interaction decreases. It is well known that this model is equivalent to the spin-1/2 *XXZ* model. The absence of the supersolid phase in the hard-core model can be readily understood in the language of the spin model; either the planar spin order (SF phase) or the antiferromagnetic order (CDW phase) is allowed, separated by the SU(2) symmetry point (Heisenberg point). Thus the phase space of the model is divided into three different regions: the SF phase, the CDW phase, and the Heisenberg point. Identifying traces of different symmetries in the momentum distributions will be very useful to figure out these different regions.

In this work, we study the momentum distributions of the one-dimensional hard-core extended bosonic Hubbard model at half filling via exact diagonalizions of the model Hamiltonian. Even though the analytic Bethe-ansatz solution is available,[9] derivation of the ground-state wave function is too complicated to perform in practice. We calculate the ground-state wave functions and then their momentum distributions by the Lanczos method on lattices up to 32 sites with a periodic boundary condition. Exact results free from statistical errors and the boundary conditions fixed allow us to do finite-size scaling analysis even in small-size systems. We find that the Luttinger-liquid parameter, which governs the power-law decay of the correlation, can be easily obtained from the finite-size scaling of the zero-momentum occupancy in the SF phase. At the Heisenberg point, the momentum distribution has a universal form $n(k) \approx -(1/2)\ln(|k|/\pi)$, where k is the momentum in the unit of the inverse lattice constant. The formation of the CDW in the insulating phase can also be identified.

II. MODEL

The hard-core extended bosonic Hubbard model is given by the Hamiltonian,

$$H = -t\sum_i (b_i^\dagger b_{i+1} + \mathrm{H.c.}) + V\sum_i n_i n_{i+1}, \quad (1)$$

where $b_i^\dagger(b_i)$ denotes the creation (destruction) operator, and n_i (n_i=0 or 1) is the number of bosons at site i, t is the hopping matrix element, and V is the near-neighbor interaction strength. Here we study the systems consisting of N bosons on L sites at half filling (N/L=1/2).

By mapping $S_i^+ = (-1)^i b_i^\dagger$ and $S_i^z = n_i - 1/2$, it is easy to show that this model is equivalent to the spin-1/2 *XXZ* chain,

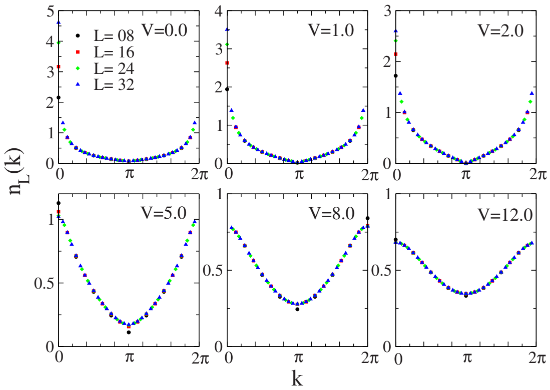

FIG. 1. (Color online) The momentum distributions for different V.

$$H_{\mathrm{spin}} = 2t\sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + V\sum_i S_i^z S_{i+1}^z. \tag{2}$$

Thus the Heisenberg point is defined by the condition $V=2t$, where the isotropic antiferromagnetic spin chain has the SU(2) symmetry. For $V<2t$, the easy-plane phase (SF phase) is stable while, for $V>2t$, the easy-axis phase (CDW phase) occurs.

Momentum distributions are defined by the formula

$$n_L(k) = \frac{1}{L}\sum_{i,j=0}^{L-1} \langle b_i^\dagger b_j\rangle e^{ik(i-j)} \tag{3}$$

for momentum $k=(2\pi/L)l$ $(l=0,1,\ldots,L-1)$, where the average $\langle\cdots\rangle$ is taken over the ground-state wave function. Here we set the lattice constant $a=1$. $n_L(k)$ is equivalent to the spin-correlation function of the spin chain with a shift of the momentum by π. At the SU(2) symmetry point, $n_L(k)$ is associated with the spin structure factor, $S_L(k)$, of the spin chain by the relation

$$S_L(k) = \frac{1}{L}\sum_{i,j=0}^{L-1} \langle S_i^z S_j^z\rangle e^{ik(i-j)} = \frac{1}{2}n_L(k+\pi). \tag{4}$$

Hence, throughout the momentum distributions of the extended hard-core boson model, we are also able to investigate the correlation functions of the spin chain.

III. RESULTS

Figure 1 shows the momentum distributions, $n_L(k)$, for different V on lattices of size L. We set $t=1$ as an energy unit. They show distinct features in different regions. In the SF phase for $V<2$, they have peaks at the zero-momentum state whose height strongly depends on L. However, $n_L(0)$ is not proportional to L. We find that, from the size dependence of $n_L(0)$, the Luttinger-liquid parameter can be obtained easily. At the Heisenberg point ($V=2$), $n_L(\pi)$ vanishes due to the SU(2) symmetry, and $n_L(k)$ for $|k|\gg 1/L$ has a universal behavior independent of L. In addition, the size dependence of $n_L(0)$ is consistent with the asymptotic long-range behavior of the spin-1/2 Heisenberg chain. In the deep CDW phase for $V\gg 2$, we have $n_L(k)\sim 0.5+A\cos(k)$ with a parameter $A\sim 1/V$. This means that the ground state consists of a perfect CDW and small fluctuations due to hoppings. More details are discussed below.

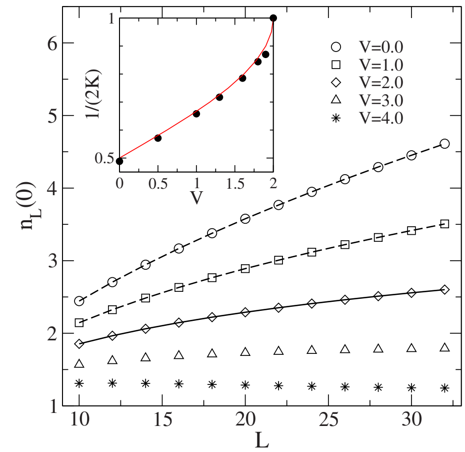

FIG. 2. (Color online) $n_L(0)$ as a function of L for different interaction strengths. In the critical region for $V<2$, the behavior of $n_L(0)$ supports that the long-range correlations characterized by K, which varies continuously as a function of V (see Inset) so that we expect $n_L(0)=C_1+C_2L^{1-1/2K}$. Dotted lines are fitting curves of this form. At $V=2$, the logarithmic corrections with $K=1/2$ strongly supports a scaling form $n_L(0)=B\ln^{1+\lambda}(L/\ell_0)$, which well fits the data with $\lambda=0.45$, as denoted by the solid line. Those fittings fail for $V>2$.

In the SF phase, the momentum distributions have peaks at $k=0$, reminiscence of the BEC of free bosons. How interactions alter this singularity at the origin is an intriguing question. The dependence of $n_L(0)$ on L has been discussed in relation with the existence of the BEC. Figure 2 shows $n_L(0)$ as a function of the size L for different V. Even for $V=0$, it increases more slowly than the linear dependence on L. This implies that the BEC is suppresed in the sense that the condensation fraction $n_L(0)/L$ vanishes in the thermodynamic limit. For $V=0$ in the presence of hard-core repulsions, Girardeau suggested[2] $n_L(0)\sim L/\ln L$ based on an approximation, which was later proved to be incorrect through more rigorous analytic derivations.[10] Our exact calculations also do not support the Girardeau's form.

The dependence of $n_L(0)$ on L can be understood within the Luttinger-liquid picture. Interacting SF bosonic gases in one dimension are Luttinger liquids[9,11,12] whose low-energy properties are governed by an effective Hamiltonian composed of the density and phase fluctuations characterized by the sound velocity and the Luttinger-liquid parameter. The Luttinger-liquid parameter K, then, determines the asymptotic behavior of the correlation function

$$\langle b_i^\dagger b_j\rangle \sim |i-j|^{-1/2K}. \tag{5}$$

By combining Eqs. (3) and (5), we expect

$$n_L(0) = C_1 + C_2 L^{1-1/2K} \tag{6}$$

with fitting parameters C_1 and C_2. Figure 2 shows that this expression fits well the data for $V<2$. Dotted lines are fitting curves of this form. The inset shows the value of K obtained by fitting as a function of V. The Luttinger-liquid parameter has $K=1.02$ at $V=0$, consistent with the analytically expected result $K=1$ for noninteracting fermions. The value approaches $K=1/2$ for the spin-1/2 Heisenberg chain as V comes closer to 2. K's obtained from fitting are consistent with the analytical solution,[9] $V=-2\cos(\pi/2K)$, which is shown by the solid line in the inset, though there are small deviations due to subleading finite-size corrections to Eq. (6), especially near the Heisenberg point where marginally irrelevant operators bring logarithmic corrections.

By using this finite-size scaling properties of the zero-momentum occupancy $n_L(0)$, we can therefore find out the value of K more easily even in small-size systems. It has been calculated[9] so far by computing the compressibility and the spin stiffness via the Bethe ansatz or the numerical exact diagonalization. This process needs changing number of particles and twisting the boundary condition, which are unnecessary in our calculations. The value of K can be obtained[11] more directly from the correlation function in Eq. (5). This method, however, requires a quite large system, for example, $L \gtrsim 100$, to achieve the asymptotic form in a log-log plot.

For $V \geq 2$, Eq. (6) does not fit the data. For $V=2$, $n_L(0)$ is closely related with the asymptotic behavior of the spin-correlation function in the spin-1/2 Heisenberg chain. In the spin model of Eq. (2) at the Heisenberg point, it has been proposed that the asymptotic spin-correlation functions behave as

$$\langle S_0^z S_r^z \rangle \sim (-1)^r \frac{\ln^{\lambda}(r)}{r} \tag{7}$$

with the logarithmic correction, characterized by the exponent λ, due to marginally irrelevant operators. This implies[13] that $S_L(\pi) \sim \ln^{1+\lambda}(L)$. Whether $\lambda=0$ (Refs. 13 and 14) or λ has a finite value[15–17] has been a controversial issue. In general, however, Eq. (7) should carry a nonuniversal constant[9,18] so that we expect $S_L(\pi) \sim \ln^{1+\lambda}(L/\ell_0)$, where ℓ_0 defines the distance over which the correlation reaches the asymptotic form. We use this scaling expression to fit $n_L(0)$, which is equivalent $S_L(\pi)$ as shown in Eq. (4), and find that it fits the data well as denoted by the solid line in Fig. 2 with $\lambda=0.45$. This result is consistent with the analytical[9,19] value $\lambda=1/2$ within our accuracy neglecting subleading corrections.[19,20]

Figure 3 shows $n_L(k)$ as a function of $\ln k$ for finite k. They show distinct features in different regions. For $V<2$, $R(k) \equiv d^2 n_L(k)/d(\ln k)^2 > 0$ in the interval $0<|k|<\pi$ whereas, for $V>2$, $R(k)$ becomes negative for small k. $R(k)$ vanishes at $V=2$. At this point, $n_L(\pi)=0$ because of the SU(2) symmetry. Therefore we expect $n_L(\pi) \propto \ln(|k|/\pi)$ at the Heisenberg point. By fitting the data, we find that the slope is very close to 1/2 (the solid line in the inset), independent of L. This strongly suggests that the momentum distribution has a universal form $n(k)=-(1/2)\ln(|k|/\pi)$ at the Heisenberg point for $1/L \ll |k| \leq \pi$. Actually this form was found[21] in the exactly solvable hard-core boson model with the long-range interaction $v(r)=2/r^2$. This means that our linear fitting is only approximately correct. The slight deviations from the straight fitting line shown in Fig. 3 indicate the difference between two models. On the whole, these above properties will be very useful to distinguish different phases by measuring the momentum distributions.

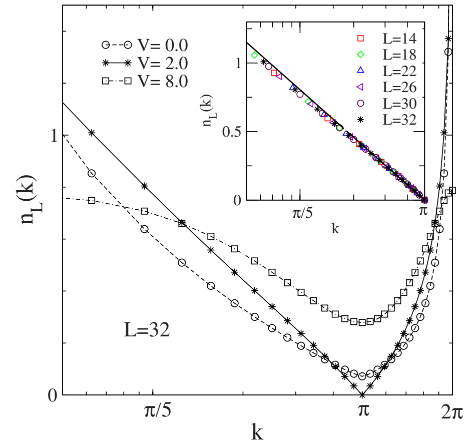

FIG. 3. (Color online) The distinct features of $n_L(k)$ in different regions. Inset: at the Heisenberg point, it shows a universal behavior $n(k) \approx -\frac{1}{2}\ln(|k|/\pi)$ for finite k.

In the deep CDW phase for $V \gg 2$, the ground state is the superposition of the CDW state and the perturbation due to hopping up to the first order in t: $|\psi_0\rangle = |\psi_{\mathrm{CDW}}\rangle + (t/V)|\psi_1\rangle$. The correlation sustains in a single hopping distance so that $|\psi_1\rangle \sim \Sigma_i (b_i^\dagger b_{i+1} + \mathrm{H.c.})|\psi_0\rangle$. One can then easily find, by inserting the wave function in Eq. (3), that the momentum distribution of this ground state has a sinusoidal form $n_L(k)=1/2+A\cos k$, where a parameter $A \propto (1/V)$ in the unit of t. This property can be observed by measuring the visibility[22] v, which is defined by $v=(n_{\max}-n_{\min})/(n_{\max}+n_{\min})$, where $n_{\max}$ and $n_{\min}$ are the maximum and the minimum value of the momentum distribution. For $V \gg 2$, we expect $v \sim 2A$, vanishing linearly in $1/V$. Figure 4 shows this behavior. The visibility has its maximum value $v=1$ for $V=2$ and diminishes in the CDW phase. For $V \gg 2$, it vanishes linearly in $1/V$ as V increases where the momentum distribution has the sinusoidal form.

IV. SUMMARY

The momentum distribution of the one-dimensional hard-core boson Hubbard model with near-neighbor repulsive in-

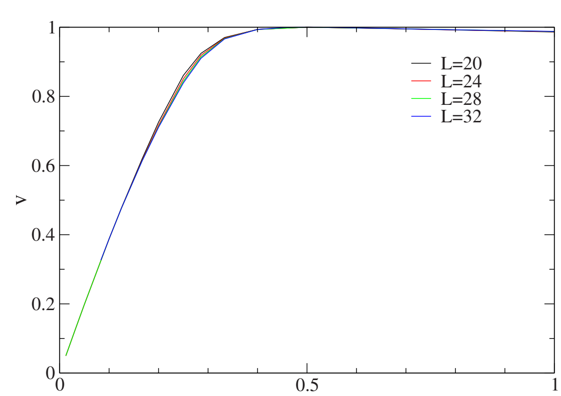

FIG. 4. (Color online) The visibility has its maximum $v=1$ at $V=2$ and vanishes linearly for small $1/V$ in the deep CDW phase where the momentum distribution has a sinusoidal form $n_L(k)=1/2+A\cos k$.

teraction is investigated. We find that it is a convenient tool to identify the ground-state phases and their properties. Especially, in the SF phase, the Luttinger-liquid parameter can be obtained from the finite-size scaling behaviors of $n_L(0)$ even in rather small-size systems. A similar analysis at the Heisenberg point allows us to find the exponent for logarithmic corrections, which is consistent with the analytic solution. At this point, our numerical investigation strongly suggest that the momentum distribution has a universal form for finite k. The momentum distributions also provide a mark for the CDW state: the sinusoidal form of the distribution and the associated visibility $v \sim 1/V$. We believe that these properties of the momentum distributions will be useful to identify the phases of dipolar atoms in an optical lattice whose system size may be characterized by the oscillator length in the presence of the shallow trapping potential.[23]

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