Phase diagram of a bosonic ladder with two coupled chains

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We study a bosonic ladder with two coupled chains using the finite-size density-matrix renormalization group method. We show that in a commensurate bosonic ladder the critical on-site interaction (U_C) for the superfluid to Mott insulator transition gets larger as the interchain hopping ($t_\perp$) increases. We analyze this quantum phase transition and obtain the phase diagram in the $t_\perp - U$ plane. We also consider the asymmetric case where the on-site interactions are different in the two chains and have shown that the system as a whole will not be in the Mott insulator phase unless both the chains have on-site interactions greater than the critical value.

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I. INTRODUCTION

Quantum phase transitions in ultracold atoms provide important insights into the behavior of matter at very low temperatures.[1–3] An important example of this class of transitions is the transition from a superfluid (SF) to a Mott insulator (MI) which has been studied theoretically in details by a variety of methods[4–13] and has been observed in cold bosonic atoms in three-dimensional (3D) optical lattices[14] as predicted by Jaksch *et al.*[15] Subsequently, this transition has been observed in a one-dimensional (1D) optical lattice.[16] An important question to address is, how do the characteristics of this transition alter in going from one to two dimensions? In coupled bosonic chains, competition exists between the ratio of on-site interactions to the intrachain hopping and the interchain hopping. A large value of the former favors a Mott insulator state overcoming the effect of the interchain hopping while if the latter dominates it would tend to delocalize the bosons and drive the system to a superfluid state. Recently coupled chains[17,18] and tubes[19] for bosons in optical lattices have been studied analytically using bosonization techniques. It is desirable to investigate these systems by using a rigorous many-body approach. However, it is not practical to perform numerical studies using such an approach for the above mentioned transitions in a very large number of coupled chains, so one must restrict to a finite number of such chains. The aim of the present work is to study the effect of the interchain hopping on the SF-MI transition for a bosonic ladder consisting of two coupled chains. Although a substantial amount of theoretical and numerical works has been done in this direction for the case of spinless fermionic ladders and spin ladders,[20–22] no work has been reported to our knowledge for the bosonic ladders except the recent work using the bosonization method.[17,18]

The Hamiltonian of the bosonic ladder (as shown in Fig. 1) is given by

$$\mathcal{H} = -t\sum_{i,\alpha}(a^\dagger_{i,\alpha}a_{i+1,\alpha} + \text{H.c.}) + \sum_{i,\alpha}\frac{U_\alpha}{2}n_{i,\alpha}(n_{i,\alpha}-1) - t_\perp\sum_i (a^\dagger_{i,1}a_{i,2} + \text{H.c.}). \quad (1)$$

In this model (1) $a^\dagger_{i,\alpha}$ ($a_{i,\alpha}$) represents bosonic creation (annihilation) operator for the site i of the chain with the index $\alpha=1,2$. t and U_α, respectively, are the intrachain hopping amplitude between the nearest neighboring sites and the on-

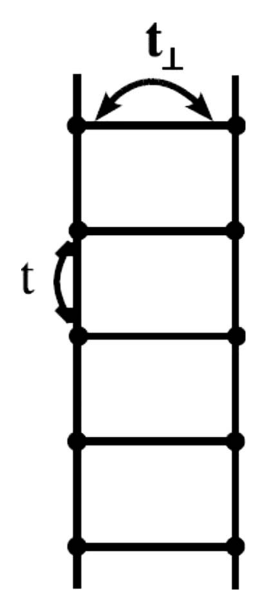

FIG. 1. Schematic picture of a two-leg bosonic ladder. t and $t_\perp$ are, respectively, interchain and intrachain hopping amplitudes.

site interaction between the bosons of chain α. The last term in this model (1) represents interchain hopping with an amplitude $t_\perp$ between corresponding sites on the two chains. We set our energy scale by taking $t=1$.

This model has been studied using the bosonization technique[17,18] at or close to commensurate filling of one boson per site. This study predicts a transition from a Mott insulator to a superfluid phase when the interchain hopping is increased and it is in the Beresenskii-Kosterlitz-Thouless (BKT) universality class at commensurate filling. In the present work we put these predictions to test and in addition consider the various cases when the on-site interactions of the two chains are different and thus complement the earlier analytical results. For these purposes, we study the variation of the critical on-site interaction U_C for the superfluid to the Mott insulator transition by changing the interchain hopping amplitude $t_\perp$ in the framework of finite-size density-matrix renormalization group (FSDMRG) method[8,9,23–25] and obtain the phase diagram in the $(t_\perp - U)$ plane. To the best of our knowledge, the present work is the first application of FSDMRG method to bosonic ladders.

The remaining part of the paper is organized in the following manner. The FSDMRG method in the context of bosonic ladders is briefly described in Sec. II. Our results are described and discussed in Sec. III and our conclusions are stated in Sec. IV.

II. FSDMRG METHOD

We use the FSDMRG technique to obtain the energies and the correlation functions of the ground state. This method is very efficient and has proven to give accurate results for 1D quantum lattice systems and has been applied to low-dimensional strongly correlated fermionic and bosonic systems.[8,9,23–25] To get accurate energies and correlation functions one needs to use FSDMRG rather than infinite-size DMRG. In the conventional FSDMRG, the lattice is built first to the desired length using infinite-size DMRG and then the sweeping is done. We have used a slightly modified version of FSDMRG where we sweep at every length and not just the final length.[9] The calculated length dependence of gap [see Eq. (2) below] for a typical value of parameters $(U_1=U_2=3.5,\ t_\perp=0.4)$ is given in Fig. 2 to demonstrate the improvement of gap using FSDMRG, where sweep is done at every length, over the infinite-size DMRG. We give below some pertinent details of this method adapted to the system of two coupled chains that we have considered.

We begin with a superblock configuration $B^l_{(L/2)-1}\cdot\cdot B^r_{(L/2)-1}$ of L rungs as shown in Fig. 3. The left $B^l_{(L/2)-1}$ and the right block $B^r_{(L/2)-1}$ have $(L/2)-1$ rungs each and the $\cdot$ represents one rung of two sites, one from each chain. Thus in every iteration, the new left and right blocks are $B^l_{(L/2)}=B^l_{(L/2)-1}\cdot$ and $B^r_{(L/2)}=\cdot B^r_{(L/2)-1}$, respectively. For each length sweeping is done till we get the converged value of the energy. The system size is then increased by adding two rungs which increases the number of lattice sites by 4. To keep the density $\rho=1$ fixed, we also increase the number of bosons in the system by 4. The truncation of states of left (right) block in each iterations corresponds to choosing M highest weighted states out of $2\times n_{\max}\times M$ of the left (right) density matrix. Here $n_{\max}$ is the number of states kept at each site, which is in general infinity, but we truncate it for a feasible numerical calculation. We keep $n_{\max}=4$ in this calculation which is found to be sufficient for the values of U considered here.[9] The value of M is chosen such that the truncation error in our calculation is always less than 10^{-5}.

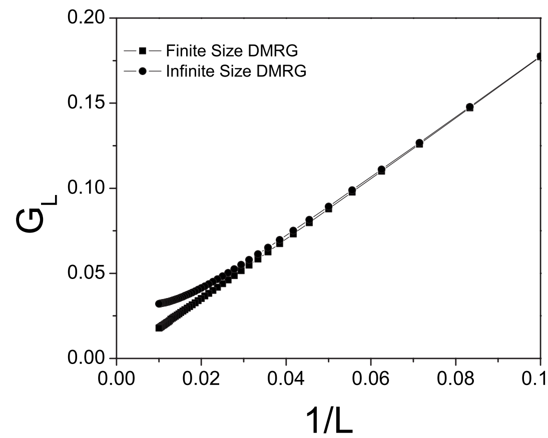

FIG. 2. Comparison of gap obtained using infinite size DMRG and FSDMRG methods for $U_1=U_2=3.5$ and $t_\perp=0.4$.

III. RESULTS AND DISCUSSION

First we discuss the symmetric two-leg ladder where $U_1=U_2=U$. The Mott insulator phase has a finite gap in its energy spectrum. The single-particle gap is defined as

$$G_L = E_L(N+1) - E_L(N) - [E_L(N) - E_L(N-1)], \qquad (2)$$

where $E_L(N)$ is the ground-state energy of two-leg bosonic ladder with length L having N bosons. The MI phase is signaled by the opening up of the gap $G_{L\to\infty}$. However, G_L is finite for finite systems and we must extrapolate to the $L\to\infty$ limit, which is best done by using finite-size scaling.[9] In the critical region, i.e., SF region, the gap

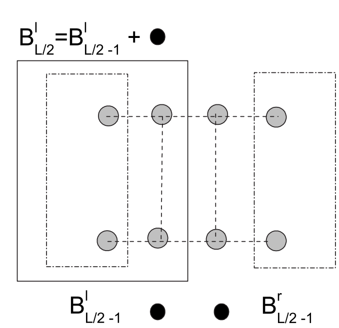

FIG. 3. A scheme of superblock configuration for the FSDMRG algorithm.

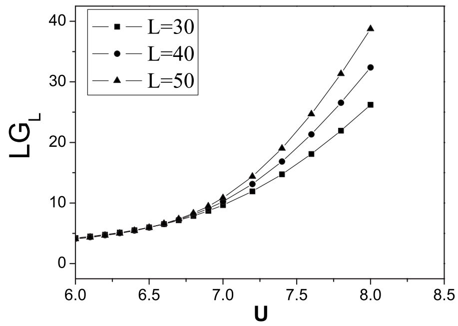

FIG. 4. Scaling of gap LG_L as a function of U for $t_\perp=0.4$ and different lengths. The coalescence of curves for different lengths for $U<U_C\sim 6.6$ shows a superfluid phase and a Mott insulator with finite gap for $U>U_C$.

$$G_L \approx L^{-1} f(L/\xi), \tag{3}$$

where the scaling function $f(x)\sim x,\ \ x\to 0$ and ξ is the correlation length. $\xi\to\infty$ in the SF region. Thus plots of LG_L versus U, for different system sizes L, consist of curves that intersect at the critical point at which the correlation length for $L=\infty$ diverges and gap G_∞ vanishes. In the SF phase we expect the gap $G_{L\to\infty}=0$ so LG_L=constant for all lengths. Numerically we have a certain tolerance limit for the permissible error and if we assume the allowed error in the value $G_{L\to\infty}$ is 0.05 (instead of 0), i.e., our zero is scaled to 0.05, the difference in the LG_L value between two lengths differing by 10 would be 0.5. Similarly if the zero is scaled to 0.01 then this difference should be 0.1. We determined the critical values of U for the SF to MI transition when the values of LG_L for two lengths, L and $L+10$, differ by 0.1. The error in the U_C is obtained when we relax the tolerance in the value of LG_L to 0.5. The phase diagram, as discussed below, is obtained from these critical values of U.

It is now well known that the single chain Bose-Hubbard model with density $\rho=1$ shows a SF-MI transition with the critical on-site interaction $U_C\sim 3.4$.[8,9] In order to understand the effect of the interchain hopping on this transition, we varied $t_\perp$ from 0 to 20 and obtained the corresponding critical on-site interaction $U_C(t_\perp)$ for the SF-MI transition. We

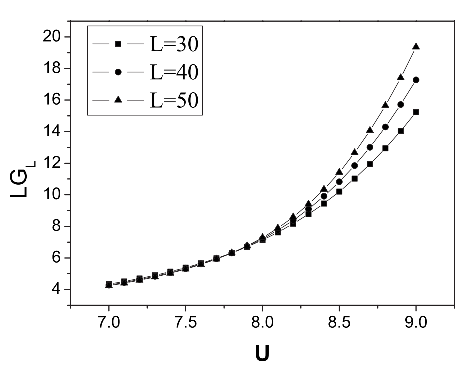

FIG. 5. Scaling of gap LG_L as a function of U for $t_\perp=t=1.0$ and different lengths. The coalescence of curves for different lengths for $U<U_C\sim 7.9$ shows a superfluid phase and a Mott insulator with finite gap for $U>U_C$. Comparing this figure with Fig. 4, we observe that the critical U_C increases with $t_\perp$.

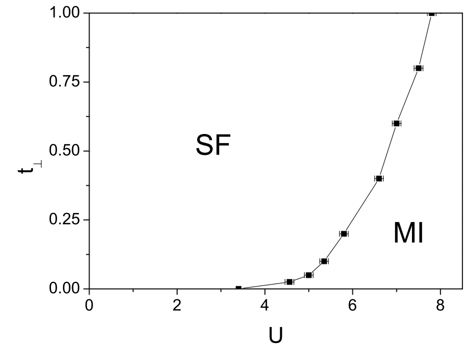

FIG. 6. Phase diagram of model (1) as a function of interchain hopping $t_\perp$ and on-site interaction U for density $\rho=1$. Note that we have set intrachain hopping $t=1$.

found that U_C increases with $t_\perp$ and saturates in the limit $t_\perp\to\infty$. These results are highlighted by the plots of scaling of gap LG_L versus U for different values of $t_\perp$ and lengths L. For example, in the Fig. 4 we plot LG_L versus U for $t_\perp=0.4$. The coalescence of LG_L curves for different values of L below $U<6.6$ demonstrates the SF-MI transition with $U_C(t_\perp=0.4)\sim 6.6$ which is much larger than the corresponding value for the single chain $U_C(t_\perp=0)\sim 3.4$. Figure 5 represents similar plots for $t_\perp=1$. For this case the critical on-site interaction increases further to $U_C(t_\perp=1)\sim 7.9$.

From similar plots of LG_L versus U, we obtain the phase diagram for model (1) in the $t_\perp-U$ plane and it can be seen in Fig. 6. U_C for the SF-MI transition initially increases sharply as the interchain hopping $t_\perp$ increases. This phase diagram verifies the prediction of MI-SF transition with respect to increase in the interchain hopping $t_\perp$.[17] For higher values of $t_\perp$, U_C tends to saturate. For $t_\perp \gg t, U$, each rung has two one-particle states: corresponding to bonding or antibonding. As predicted in the bosonization[17] study, this problem then maps onto a single chain Bose Hubbard model with commensurate density $\rho=2$ and on-site interaction $U/2$. To confirm this prediction we plot the variation of U_C with respect to $t_\perp$ in Fig. 7. Critical on-site interaction U_C for large $t_\perp$ converges to a value equal to 12.5 ± 0.3. Plotting LG_L versus U for single chain Bose-Hubbard model for $\rho=2$ in Fig. 8 we find that $U_C\sim 6.3$, which is one half the converged value of $U_C(t_\perp=\infty)\sim 12.5$ for the bosonic ladder

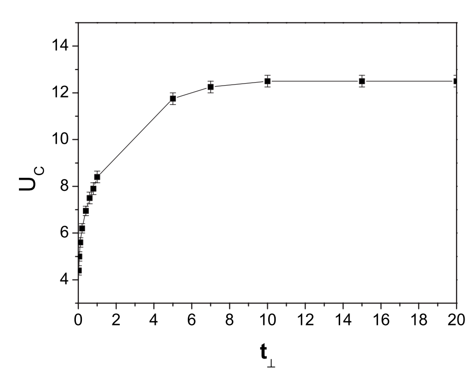

FIG. 7. Variation of critical on-site interaction U_C with respect to interchain hopping $t_\perp$. U_C increases sharply for small values of $t_\perp$ and saturates to 12.5 ± 0.3 as $t_\perp\to\infty$.

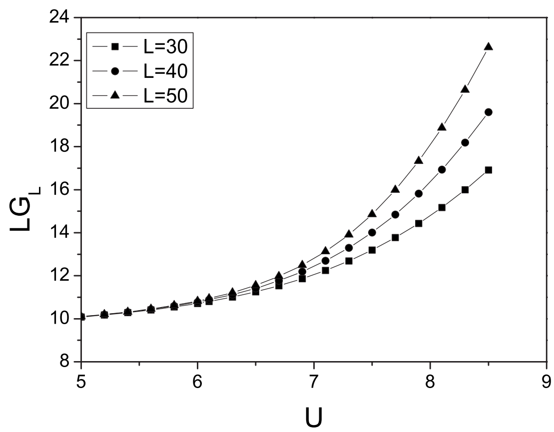

FIG. 8. Scaling of gap LG_L as a function of U for the single chain Bose-Hubbard model with density $\rho=2$. The coalescence of curves for different lengths for $U<U_C\sim 6.3$ shows a superfluid to a Mott insulator transition.

confirming the prediction made in bosonization study.[17]

The Mott insulator to superfluid transition is found to be Beresinskii-Kosterlitz-Thouless universality class at commensurate filling.[17] The correlation function that characterizes the superfluid phase is given by $\Gamma_\alpha(r)=\langle a^\dagger_{i,\alpha}a_{i+r,\alpha}\rangle$ which decays as a power law in the limit $r\to\infty$. Here the expectation value is taken with respect to the ground state. However, in the Mott insulator phase it has an exponential decay due to the finite gap in the energy spectrum. The power-law decay of this correlation function has been obtained using the bosonization method[17] and it is predicted to go as

$$\Gamma_\alpha(r) \propto \frac{1}{r^{1/4K_s}}, \tag{4}$$

with the Luttinger liquid parameter K_s stated to be 1 at the superfluid to Mott insulator transition point.

In order to obtain the Luttinger liquid parameter K_s we have taken three values of U, $U=5,6,7$ and have varied the interchain hopping $t_\perp$ and obtained the Mott insulator to superfluid transition. The scaling of gap LG_L as a function of $t_\perp$ is given in Fig. 9. The critical interchain hopping

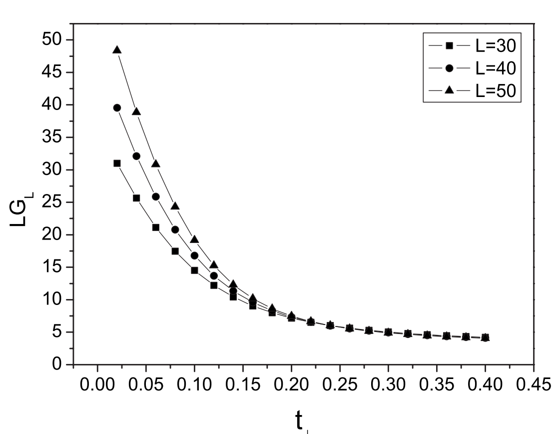

FIG. 9. Scaling of LG_L as a function of $t_\perp$ for $U=6$.

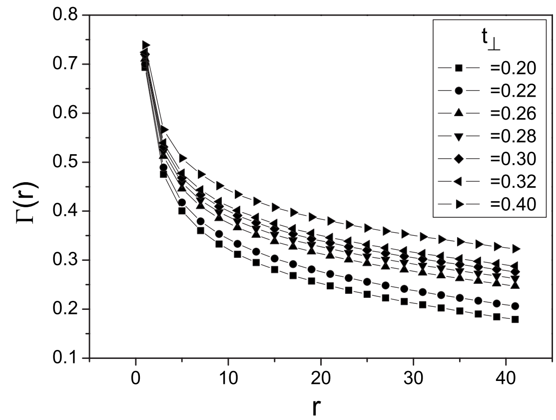

FIG. 10. Power-law decay of $\Gamma(r)$ for various values of $t_\perp$ for $U=6$.

$t^C_\perp=0.24\pm 0.05$ for the MI to SF transition for $U=6$. Similar calculation for $U=5$ and $U=7$ yields $t^C_\perp=0.07\pm 0.05$ and $t^C_\perp=0.6\pm 0.05$, respectively. The correlation functions $\Gamma(r)$ [$=\Gamma_1(r)=\Gamma_2(r)$, for symmetric two-leg ladder] for different values of $t_\perp$ keeping $U=6$ are given in Fig. 10. The Luttinger liquid parameter K_s which is obtained by fitting $\Gamma_\alpha(r)$ with the expression given in Eq. (4) is plotted as a function of $t_\perp$ in Fig. 11 for $U=5$, 6, and 7. From these values the critical $t^C_\perp$ for which $K_s=1$ is given by 0.3 ± 0.03 for $U=6$, 0.1 ± 0.02 for $U=5$, and 0.68 ± 0.02 for $U=7$ which are consistent with values obtained from the scaling of the gap.

The results we have obtained could have experimental implications. It is now possible to prepare bosonic ladders by growing optical superlattices in the form of double-well potential along one direction.[26] The tunneling between the double-well potential will control the interchain hopping.[26,27] By changing dynamically the optical lattice parameters one can control all the interactions and hopping parameters of the model (1). In view of these recent developments, we have generalized our analysis and considered cases where the on-site interactions are different on the two chains. There are three possibilities: in the first both the chains have on-site interactions which are less than the critical value, i.e., $U_1,U_2<U_C$. In this case it is obvious that the system of two chains is in the superfluid phase. Similarly when $U_1>U_C$ and $U_2>U_C$ then the system is in the Mott phase. Most

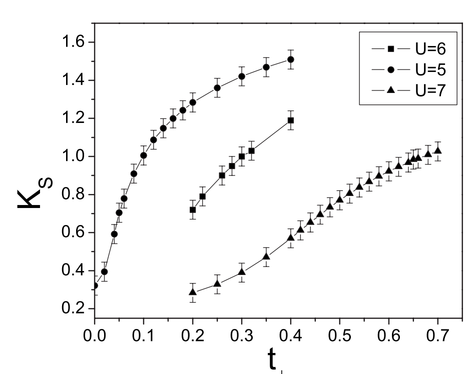

FIG. 11. Variation of Luttinger liquid parameter K_s as a function of $t_\perp$ near MI to SF transition for $U=5,6,7$.

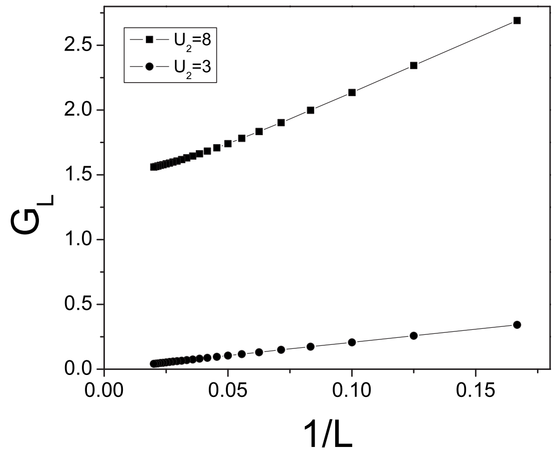

FIG. 12. Gap G_L as a function of $1/L$ for $U_2=3,8$ keeping $U_1=8$, $t_\perp=0.2$ showing the system is in MI phase for $U_2=8$ and in the superfluid phase for $U_2=3$.

interesting case will be the third one when say, $U_1>U_C$ and $U_2<U_C$. A natural question that arises is whether the chain with larger on-site interaction will be in the Mott insulator phase and the other in the superfluid phase. We have answered this question by calculating the gaps and the correlation functions taking $U_1=8$, $U_2=3$ and 8 keeping $t_\perp=0.2$. It may be noted that the critical value for the SF to MI transition when $U_1=U_2$ and $t_\perp=0.2$ is 5.5. In Fig. 12 we plot the G_L as a function of $1/L$ which shows that for the case $U_2=8$ the system of two chain is in the Mott insulator phase. However, when $U_2=3$, which is less than $U_C=5.5$, the gap vanishes in the limit $L\to\infty$ and the system is in the SF phase. The gap yields the nature of the phase of the system as a whole. In order to check the phase of each chain separately, we use the correlation function and the correlation length defined by[9]

$$\xi_L^\alpha = \sqrt{\frac{\sum_r r^2\Gamma_L^\alpha(r)}{\sum_r \Gamma_L^\alpha(r)}}. \tag{5}$$

$\Gamma_L^\alpha(r)=\langle a_{i,\alpha}^\dagger a_{i+r,\alpha}\rangle$ was calculated using the wave function of the system with length L. The correlation length diverges in the superfluid phase. In Fig. 13 we have plotted the correlation length calculated for each individual chain separately keeping $U_1=8$, $U_2=3$, and $t_\perp=0.2$. It is obvious from this figure that both the chains have correlation lengths which diverge in the limit $L\to\infty$, i.e., both the chains are in the superfluid phase. Though $U_1>U_C=5.5$, the chain 1 is in the superfluid phase. From the calculation of the local density of bosons $\rho_\alpha=\langle n_i^\alpha\rangle$, we found that the average densities of the bosons, ρ_1 and ρ_2 for chains 1 and 2, respectively, differ from the average density of the bosons in the whole system, i.e., $\rho=1$ in our case, to minimize the effect of the on-site interactions. If $U_1>U_2$ then $\rho_1<\rho_2$. The bosons migrate from the chain with the larger on-site interaction to that with smaller on-site interaction. We find that the number of bosons which migrate increases as the difference between the on-site interactions gets larger [see Fig. 13 (inset)]. From these studies we conclude that, for an asymmetric chain, whenever one of the chains has on-site interaction less that the critical value, the system as a whole and each chain is in the superfluid phase. The Mott insulator is possible only if both the chains have on-site interactions greater than the critical value, such a phase can have $\rho_1\neq\rho_2$ if $U_1\neq U_2$. Whenever we have coupled chains, a situation where one of the chains is a Mott insulator and the other a superfluid will never arise.

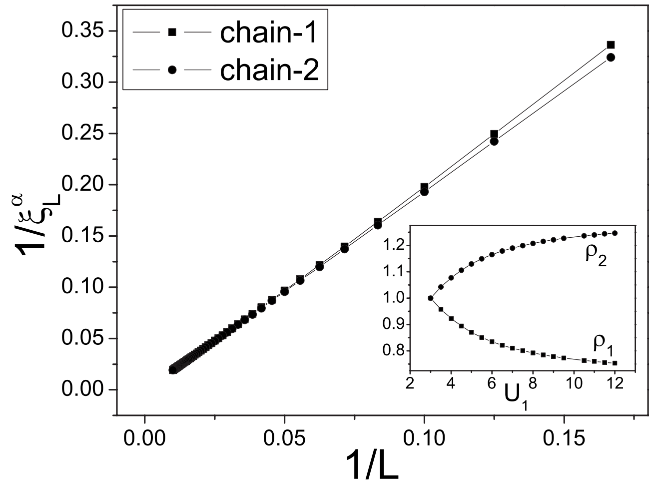

FIG. 13. The inverse correlation lengths $1/\xi_L^1$ and $1/\xi_L^2$ for chains 1 and 2, respectively, as a function of $1/L$ for $U_2=3$ keeping $U_1=8$, $t_\perp=0.2$. In the limit $L\to\infty$ both ξ_L^1 and ξ_L^2 diverge which show both the chains are in the superfluid phase. (inset) Variation of average density of bosons ρ_1 and ρ_2 as function of U_1 keeping $U_2=3$ fixed.

IV. CONCLUSIONS

We have studied the ground-state properties of a two chain bosonic ladder with commensurate filling of one boson per site using the finite-size density-matrix renormalization group method. The critical on-site interaction for the SF-MI phase transition increases sharply for small values of interchain hoping amplitude $t_\perp$. However, it saturates for large values of $t_\perp$. Thus in the presence of large interchain hopping, the system continues to be in the superfluid state even though the individual chains (in the absence of interchain hopping) are Mott insulators. We therefore rigorously establish the dependence of the superfluid to Mott insulator transition on $t_\perp$. We have obtained the Luttinger liquid parameter and it is in good agreement with the bosonization results. In addition to verifying and complementing the predictions made by the bosonization technique, we have extended our study by considering asymmetric ladder case in our model.

The best experimental system to observe the quantum phase transitions reported in this work is the double-well optical lattices.[26] Such a system can be described by the model (1) with the inclusion of trap potential, which introduces inhomogeneity in the system and as a result the average local density of bosons is no more uniform across the lattice. The detailed description of the model (1) in the presence of trap potential is outside the scope of the present study and will be reported elsewhere. However, studies[28,29] in 3D optical lattices by treating this trap potential as an effective local chemical potential have shown the existence of alternative superfluid and Mott insulator shells in the system and these predictions have been verified by recent experiments.[30,31] We hope that our analysis of the SF-MI transition in the bosonic ladder will stimulate similar experimental studies in this direction.

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