

# Mott-insulator phases of nonlocally coupled one-dimensional dipolar Bose gases

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We analyze the Mott-insulator phases of dipolar bosonic gases placed in neighboring but unconnected one-dimensional (1D) traps. Whereas for short-range interactions the 1D systems are independent, the non-local dipole-dipole interaction induces a direct Mott-insulator to pair-superfluid transition which significantly modifies the boundaries of the lowest Mott-insulator phases. The lowest boundary of the lowest Mott regions becomes progressively constant as a function of the hopping rate, eventually inverting its slope, leading to a reentrant configuration which is retained in two dimensions. We discuss the consequences of this effect on the spatial Mott-insulator plateaux in experiments with additional harmonic confinement, showing that counterintuitively the plateaux may become wider for increasing hopping. Our results are also applicable to nondipolar boson-boson mixtures.

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## I. INTRODUCTION

Strongly correlated atomic gases have recently attracted rapidly growing attention, mainly motivated by impressive developments on the manipulation of atoms in optical lattices. When loaded in these lattices, ultracold atoms experience a periodic potential that resembles that of electrons in solids, opening fascinating links between the physics of cold atoms and solid-state physics. In particular, cold bosons restricted to the lowest lattice band can be described by the Bose-Hubbard model [1], which presents two different phases at zero temperature [2], namely a superfluid phase, and a gapped incompressible insulator phase known as Mott-insulator (MI), characterized by a commensurate occupation per lattice site. The superfluid to MI transition in cold bosons in optical lattices was recently observed in a remarkable experiment [3], in which the gapped nature of the MI excitation spectrum was clearly demonstrated. The realization of the MI was indeed possible due to an additional harmonic potential overimposed to the lattice that guaranteed locally the (otherwise practically impossible) commensurability condition necessary for the MI. Such inhomogeneous potential leads to the formation of spatial MI and superfluid shells [1,4], which have been observed very recently [5,6].

Among the various research lines related with optical lattices, the physics of mixtures has attracted a considerable attention. Bose-Fermi mixtures may lead to a wealth of phases of fermion composites [7], and may allow for the generation and engineering of disorder [8–11]. Bose-Bose mixtures have also attracted a major interest [12–16]. In particular, it has been shown [13] that the interspecies interaction may lead to the formation of a pair superfluid (PSF), i.e., a superfluid of boson-boson (or hole-hole) composites, which occurs in addition to MI phases for both components, as well as uncorrelated superfluid phases in each one of the components (2SF).

Dipolar gases also attract currently a major interest, motivated by recent experiments on atoms with large magnetic moment [17], polar molecules [18], and Rydberg atoms [19]. In these gases the long-range and anisotropic dipole-dipole interactions become significant or even dominant when com-

pared to the short-range isotropic interactions [20]. The dipole-dipole interactions can play an important role in the physics of lattice bosons, leading to additional phases, as checkerboard or supersolid, which may be easily controllable by manipulating the atomic confinement [21]. In addition, contrary to short-range interacting gases for which disconnected sites (i.e., without hopping between them) are fully independent, the long-range character of the dipole-dipole interactions induces a coupling even for unconnected sites. The latter leads to fundamentally new physics, as e.g., a condensate of filaments [22], quantum phase transitions in bilayer systems of polar molecules [23], or inelastic interlayer scattering for dipolar solitons [24].

In this paper, we show that the nonlocal dipole-dipole interaction induces a direct MI-to-PSF transition for neighboring unconnected one-dimensional (1D) dipolar gases, which significantly modifies the boundaries of the lowest 1D MI phases. The same effect is also expected under appropriate conditions for nondipolar boson-boson mixtures. Remarkably, the lowest boundary of the first MI lobes eventually inverts its slope as a function of the hopping rate, leading to a reentrant scenario, which is maintained in two dimensions (2D). We show that this effect has direct consequences on the spatial extension of the MI plateaux for the case of an overimposed harmonic confinement. Counterintuitively, we show that the plateaux extension may become constant or even wider for increasing hopping.

The structure of the paper is as follows. In Sec. II we describe the physical system under consideration, and the model and numerical techniques employed. In Sec. III we present our numerical and analytical results concerning the phase boundaries of nonlocally coupled one-dimensional bosons. Section IV is devoted to the analysis of the consequences of the direct MI-to-PSF transition in the spatial extension of the Mott regions in the presence of an additional harmonic confinement. Finally, in Sec. V we summarize our conclusions.

## II. MODEL

In the following, we consider dipolar bosons placed at two neighboring, but disconnected, 1D traps (wires), which

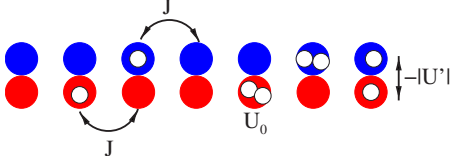


FIG. 1. (Color online) Scheme of the system considered in this paper. Hopping ( $J$ ) is possible between sites at the same wire. On-site interactions are described by the coupling constant  $U_0$ . Interaction between atoms at opposite sites of a rung of the ladder interact attractively via a coupling constant  $-|U'|$ .

can be created using micromagnetic confinement [25] or sufficiently strong 2D optical lattices. In the latter case, the required two-site configuration may be generated by superlattice techniques or by selectively emptying 1D sites neighboring the desired pair. Along the 1D systems we assume an additional lattice equal for both 1D traps, which leads to the ladder configuration shown in Fig. 1. In this paper, we are mostly concerned about interlayer effects, and hence we consider a configuration for which only the (attractive) dipole-dipole interaction between sites at the same rung plays a significant role. This is the case, when the dipoles are oriented forming an angle  $\varphi$  with the axis of the wires, such that  $\cos^2 \varphi = 1/3$ . Under such conditions, the dipole-dipole interaction between neighbors at the same wire vanishes, whereas the dipole-dipole interaction between sites in the same rung is attractive. There is in principle an additional nonzero diagonal dipole-dipole interaction between sites in neighboring rungs belonging to different wires. These terms can be made negligible by considering the spacing between rungs,  $\gamma > 1$  times larger than the separation between the two wires. In that case the spurious diagonal interaction is a factor  $(1 + 2\sqrt{2}\gamma)/(1 + \gamma^2)^{5/2}$  ( $\approx 0.03$  for  $\gamma = 3$ ) smaller than that between sites in the same rung. Of course, for other dipole and lattice configurations, the dipole-dipole interaction between sites belonging to the same wire cannot be neglected, and interesting physics can be expected [26] and will be studied elsewhere.

Under the previous conditions the system is described by a Bose-Hubbard Hamiltonian (BHH) of the form

$$\hat{H} = -J \sum_{\alpha=1,2} \sum_{\langle i,j \rangle} \{ \hat{b}_i^{(\alpha)\dagger} \hat{b}_j^{(\alpha)} + \text{H.c.} \} - \mu \sum_{\alpha=1,2} \hat{n}_i^{(\alpha)} + \frac{U_0}{2} \sum_{\alpha=1,2} \sum_i \hat{n}_i^{(\alpha)} (\hat{n}_i^{(\alpha)} - 1) - |U'| \sum_i \hat{n}_i^{(1)} \hat{n}_i^{(2)}, \quad (1)$$

where  $\hat{b}_i^{(\alpha)}$ ,  $\hat{b}_i^{(\alpha)\dagger}$ , and  $\hat{n}_i^{(\alpha)}$  are, respectively, the annihilation, creation, and number operators for the site  $i$  at the wire  $\alpha$ .  $J$  describes the hopping between neighboring sites  $i$  and  $j$  in each wire,  $U_0$  the on-site interactions (a combination of short-range and dipolar contributions [21]), and we consider the same chemical potential  $\mu$  in both wires. Atoms in sites at the same rung interact attractively by the dipole-dipole interaction, which is characterized by a coupling  $-|U'|$ .

In the following we analyze the effects of the coupling  $U'$  in the physics of the MI phases for the 1D wires. Note that the Hamiltonian (1) is formally equivalent to the case of two

bosonic species in a 1D array, with equal chemical potential  $\mu$  for both, equal hopping  $J$ , equal on-site intraspecies interactions  $U_0$ , and an interspecies interaction  $-|U'|$ . Hence, our results can be equally applied to boson-boson mixtures under these constraints. Indeed, as we show below, the PSF phase introduced in the context of Boson-Boson mixtures [13] is crucial for the understanding of the physics discussed below.

In our analysis of the ground states of  $\hat{H}$ , we have employed matrix-product-state techniques, following closely the method of Ref. [27]. The matrix-product-state represents an optimal Ansatz [28] for problems as that of this paper. Adapted to the two-wire problem, with  $L$  sites per wire, this Ansatz for the many-body wave function is

$$|\Psi\rangle = \sum_{\{n_i^{(\alpha)}=0\}}^{n_{\max}} A_{[1]}^{[n_j^{(1)}, n_j^{(2)}]} \dots A_{[L]}^{[n_j^{(1)}, n_j^{(2)}]} | \{n_i^{(\alpha)}\} \rangle, \quad (2)$$

where we consider a maximal number of atoms  $n_{\max}$  per site, and  $A_{[j]}^{[n_j^{(1)}, n_j^{(2)}]}$  are  $D \times D$  matrices, associated to the case of  $n_j^{(1)}$  and  $n_j^{(2)}$  atoms at the site  $j$  of both wires. The states  $|\{n_i^{(\alpha)}\}\rangle \equiv |n_1^{(\alpha)} \dots n_L^{(\alpha)}\rangle$  denote a particular product state of Fock states. In the following we focus on the regime of low average occupation per site around the first MI lobe, and hence in our calculations it proves enough  $n_{\max} = 2$ . In addition, we have checked in our calculations that relatively low matrix dimensions  $D = 6$  describe properly the problem under consideration [29]. The matrix-product-state Ansatz enormously simplifies the original problem (which scales exponentially with  $L$ ), since it has a complexity given by  $(n_{\max} + 1)D^2L$ . Using a similar approach as that of Ref. [27], we developed a numerical algorithm that allows us to recursively adapt the variational parameters  $A_{[s]}^{[n_s^{(1)}, n_s^{(2)}]}$  until reaching the ground state. This method resembles in many ways that of finite-size density-matrix-renormalization-group techniques [30].

### III. RESULTS

Figure 2 shows the results of our simulations for the surroundings of the lowest MI lobe (with  $\langle n_i^{1,2} \rangle = 1$ ) for  $|U'|/U_0 = 0$  (a),  $1/4$  (b),  $1/2$  (c), and  $3/4$  (d). Note that in order to avoid collapse in a single site,  $|U'| < U_0$ . For the case of  $U' = 0$ , the usual Mott lobes are recovered [31]. However, the dependence of the lobe boundaries in the  $\mu$ - $J$  phase space changes significantly when  $|U'|$  grows. Note, in particular, that the lowest boundary becomes progressively flatter when  $|U'|$  approaches  $U_0/2$ . Indeed our analytical calculations (see below) show that for  $|U'| > U_0/2$  the slope of the lowest boundary of the MI lobe inverts its sign. This behavior is however difficult to observe in our numerical calculations due to the very narrow region between the MI lobe and the region of zero occupation. In the following we discuss in more detail the physics behind the distortion of the MI lobes, and the implications of this distortion on the spatial extension of the MI lobes in axially trapped gases.

The boundaries of the MI lobes are provided by the energy gap between the MI state and the lowest excited state

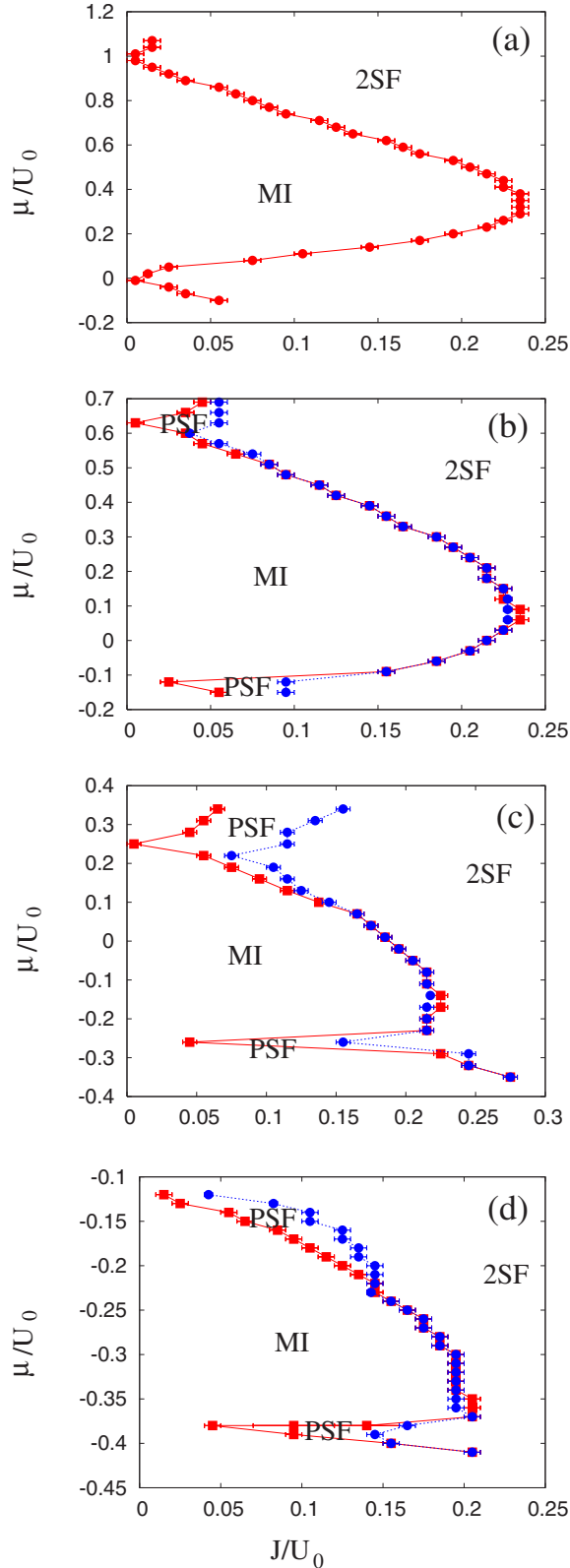


FIG. 2. (Color online) MI lobes as a function of  $J/U_0$  and  $\mu/U_0$ , for  $|U'|/U_0=0$  (a), 0.25 (b), 0.5 (c), and 0.75 (d). The calculations were made for  $L=12$  and  $D=5$ . The error bars indicate the change in the order parameters, (■)  $\Psi_{\text{PSF}}$  and (●)  $\langle b \rangle$ , from  $<10^{-4}$  to  $>10^{-2}$ .

conserving the particle number. In an usual (single-component) Bose-Hubbard Hamiltonian [2] this lowest excitation is provided by particle-hole excitations. The MI boundaries can then be calculated by a strong-coupling expansion (SCE) [32], estimating the energy of a state with an extra particle and a state with an extra hole. This is indeed the case of  $U'=0$ , where the lowest excitations are given by uncorrelated particle-hole excitations in both wires. The situation changes for  $|U'|>0$ , since for sufficiently low tunneling, there is a direct transition between MI and PSF phases, i.e., superfluid phases of composites (or composite holes) [13]. In that case the first excitation of the MI lobe is given by the correlated creation of pairs of particles (or holes) at opposite sites of the two wires, explaining the qualitative change in the shape of the lobe boundaries. In particular, a second-order SCE in  $J/|U'|$  [33], provides the following dependence for sufficiently low tunneling for the lowest boundary of the MI lobe with  $n_0$  particles per site,

$$\frac{\mu}{U_0} = n_0 - 1 + \frac{|U'|}{U_0} \left( \frac{1}{2} - n_0 \right) - 4 \left( \frac{J}{U_0} \right)^2 \left( n_0(n_0 + 1) - \frac{(n_0^2 - 1)/2}{2 - |U'|/U_0} - \frac{n_0^2 U_0}{|U'|} \right). \quad (3)$$

From (3) it becomes clear that for any  $U'>0$  the gap boundaries are quadratic (and not linear) in  $J$  for sufficiently low  $J$ . Interestingly, the lowest boundary of the first MI region ( $n_0=1$ ) inverts its slope at  $J=0$  for  $|U'|>U_0/2$ , in agreement with our numerical results. One may also observe that an inversion of the slope of the lowest boundary is expected also for  $n_0=2$  at  $|U'|/U_0 \approx 0.85$ , but it is not expected for  $n_0>2$ .

Although a detailed 2D analysis is beyond the scope of this paper, and will be the subject of further investigations, we stress here that the SCE for 2D lattices at unconnected layers (or equivalently to two-component bosonic gases in 2D lattices) shows that the lowest boundary of the first MI lobe follows at low  $J$  the relation (3) but substituting  $2(J/U_0)^2$  by  $z(J/U_0)^2$ , where  $z$  is the coordination number. Hence, the change in the sign of the slope occurs exactly as for 1D, and thus a reentrant scenario is also expected in 2D.

In our numerical simulations, we revealed the presence of the pairing phases by monitoring  $\Psi_{\text{PSF}} = |\langle \hat{b}^{(1)} \hat{b}^{(2)} \rangle - \langle \hat{b}^{(1)} \rangle \langle \hat{b}^{(2)} \rangle|$  [34]. A typical dependence of  $\Psi_{\text{PSF}}$  and  $\langle b \rangle = \langle b^{(1,2)} \rangle$  in our simulations is depicted in Fig. 3 for a fixed chemical potential. The MI region is characterized as that in which both  $\Psi_{\text{PSF}} = \langle b \rangle = 0$ . We denote the PSF region as that in which  $\Psi_{\text{PSF}} \neq 0$  but  $\langle b \rangle = 0$ . Finally the 2SF region is that in which  $\langle b \rangle \neq 0$ . Note that there is a finite coexistence region in which both  $\Psi_{\text{PSF}} \neq 0$  and  $\langle b \rangle \neq 0$ . Repeating the calculations for different chemical potentials we obtain the results depicted in Fig. 2. Note that, as we mentioned above, a direct MI-PSF transition can be observed in Fig. 2 at low  $J/U_0$ , which results in a clear distortion of the MI boundaries when compared to the  $U'=0$  case.

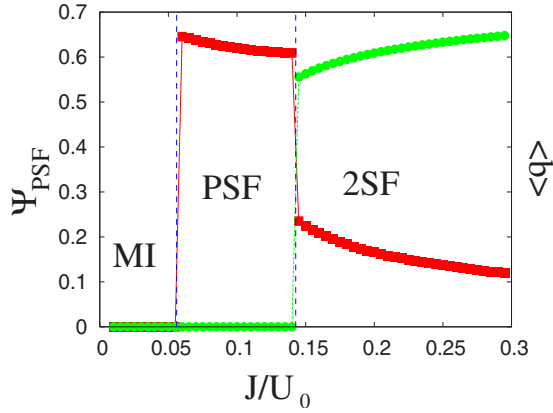


FIG. 3. (Color online) (■)  $\psi_{\text{PSF}}$  and (●)  $\langle n \rangle$  as a function of  $J/U_0$  for  $\mu = -0.15$  and  $|U'|/U_0 = 0.75$  with  $L=24$  and  $D=6$ .

#### IV. SPATIAL MOTT-INSULATOR REGIONS

The qualitative change in the shape of the MI lobe has important consequences on the spatial extension of the MI and superfluid regions in the presence of an overimposed harmonic confinement. In order to analyze this point, we consider a harmonic trap along the wires, such that a term  $\Omega \sum_{i,\alpha} i^2 \hat{n}_i^{(\alpha)}$  is added to the Bose-Hubbard Hamiltonian. This term induces a local chemical potential  $\mu_i = \mu_0 - \Omega i^2$ , where  $\mu_0$  is the local chemical potential at the trap center. Hence,  $\mu_i$  scans values  $\mu < \mu_0$ . If for a given tunneling rate, the system with  $\mu_0$  is inside the first MI lobe, it is hence expected the

appearance of a MI shell at the trap center, characterized by a plateau in the average population per site ( $\langle n \rangle = 1$ ), surrounded by a second superfluid shell (with  $\langle n \rangle < 1$ ) [1,4]. For  $U' = 0$ , for a fixed chemical potential, it is intuitively expected that the MI plateau shrinks when  $J/U_0$  increases, until eventually it disappears. Indeed, this is the case, since the lowest boundary of the MI lobe increases with  $J$ , hence decreasing the spatial MI region [Fig. 4(a)]. However, when  $|U'|$  grows, the change in the slope of the lowest boundary of the first MI lobe leads to a significant modification of the spatial extension of the MI plateau. In particular, as shown in Fig. 4, the basically  $J$ -independent lowest MI boundary for  $|U'| = U_0/2$  leads to a  $J$ -independent MI plateau [Fig. 4(c)]. Moreover, for  $|U'| > U_0/2$ , the reentrant character of the MI lobe leads to the anti-intuitive observation, that for enhanced mobility ( $J$  larger) the MI plateaux become even broader [Fig. 4(d)].

#### V. CONCLUSIONS

In this paper we have analyzed the physics of dipolar gases in unconnected neighboring 1D systems. Whereas without dipolar interactions the 1D systems are independent, the nonlocal dipole-induced interlayer interaction leads to a direct MI to PSF transition, significantly distorting the MI lobes along the wires. In particular, the lowest boundary of the first MI lobes becomes progressively flatter as a function of the hopping, inverting eventually its slope, leading to a reentrant configuration (that remains in 2D). We have shown

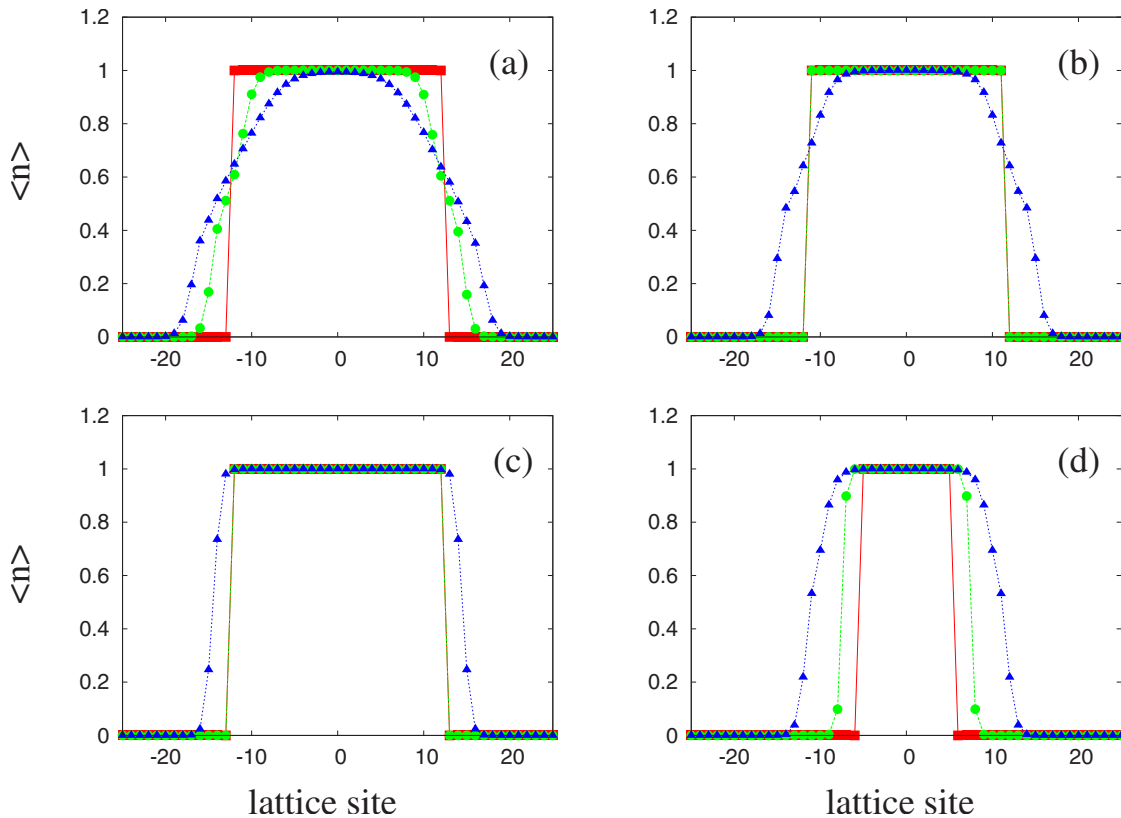


FIG. 4. (Color online) Spatial distribution of  $\langle n \rangle$  for  $U'/U_0 = 0$  (a), 0.25 (b), 0.5 (c), and 0.75 (d), for, respectively,  $10^4 \Omega/U_0 = 12.3, 9.26, 9.26, 4.32$ , with  $\mu_0/U_0 = 0.2, 0, -0.1, -0.36$ , for  $J/U_0 = 0$  (■), 0.05 (●), 0.1 (▲).



that such an effect leads to a nontrivial behavior of the MI plateaux in experiments with an axial harmonic confinement [5,6]. In particular, the MI plateaux may (for low hopping) become insensitive to the hopping, or even counterintuitively grow for larger tunneling. Finally, we would like to stress that our results also apply to two-component Bose gases, predicting exciting phenomenology in on-going experiments in bosonic mixtures in lattices.

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