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Mott insulator and superfluid phases in bosonic superlattices

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Abstract. We study the ground-state phase diagram of boson chains on a 2-period superlattice using the density matrix renormalization group method. New insulators for commensurate densities were found, differentiated by the arrangement of the particles in the unit cell, which was corroborated by analysis of the density versus the potential strength. Also, phase transitions between insulators for $\rho \geq 1$ were seen, and a maximum in the behavior of the von Neumann entropy in the critical region was revealed, which suggests a superfluid phase between the insulators.

1. Introduction

A lot of research in recent years has focused on the ground state of bosonic chains due to the advantage of being able to emulate them in optical lattices. These allow controlling the parameters, such as the kinetic energy, the density, and the particle interactions [1, 2]. Some experiments using optical lattices have established that the phase diagram exhibits a transition from superfluid to Mott insulator [3], which was observed by Greiner et al. in 2002 [4]. An interesting problem is to study the chains of particles in l-period superlattices, whose arrangement is characterized by a unit cell with l sites, where for instance there is an energy difference (λ) between one site and the other $l-1$ sites [5, 6].

Through mean-field approximation, Buonsante and Vezzani [7] described an ultracold system and found that at zero temperature, insulator domains appeared for fractional densities. More recently, Dhar et al. [8] showed new insulators in the 2-period superlattice. They demonstrated insulators at $\rho = 1/2$ and $\rho = 1$, and a phase transition between the Mott insulator and the new insulator phase when λ is near the strength of the local interaction U at $\rho = 1$. However, although the above results describe the behavior for particular densities of one-dimensional boson systems on superlattices, the phases for densities larger than one, the localization of the particles, and the state of the system around the critical point remain unclear.

In the present paper, we show the phases of the ground state of boson chains on 2-period superlattices. Applying the density matrix renormalization group method at the thermodynamic limit, we determined the phase diagram, and new insulators for commensurate densities were obtained. Also, we calculated the local density and identified periodic arrangements of the particles in the superlattice for some values of λ, when the system is in an insulator phase. Finally, we explored the critical region through calculations of the von Neumann entropy, obtaining a maximum at the transition point, which suggests a superfluid phase in that region.

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2. Model and results

One-dimensional systems of bosons in superlattices are described by the modified Bose-Hubbard model, defined as:

$$H = -t\sum_i (a_{i+1}^\dagger a_j + H.c.) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_i \lambda_i \hat{n} i \tag{1}$$

Where t is the hopping parameter, $a_i^\dagger$ (a_i) creates (annihilates) a boson at site i, U represents the local interaction, $\hat{n}_i = a_i^\dagger a_i$ is the number operator, and λ_i denotes the shift in the energy levels of the sites in each unit cell. We set our energy scale taking $t = 1$ and the interaction parameter $U/t = 10$. The 2-period superlattice has two sites per unit cell, which is represented in Figure 1.

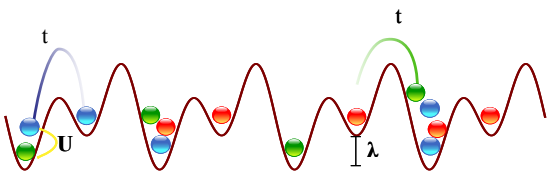

Figure 1. (color online) Schematic representation of the 2-perid superlattice. This is formed by the superposition of two waves, where the first has double frequency than the other. We consider that the difference of the hopping parameter between neighboring states is very small.

In the present paper, $\lambda_i = \lambda$ for even sites, and $\lambda_i = 0$ for odd sites. The current investigation involved calculating the energies $E(N, L)$ for lattices with different lengths L and N, $N + 1$ and $N - 1$ particles such that we obtain the chemical potential for increase (μ_p) and decrease (μ_h) the number of particles by one, where the general expressions for chemical potentials are: $\mu_p = E(N + 1, L) - E(N, L)$ and $\mu_h = E(N, L) - E(N - 1, L)$. To obtain the energies, we used the density matrix renormalization group method for lattices from 24 to 84 sites, obtaining an error of around 10^{-13}. Then we extrapolated our results at the thermodynamic limit and repeated the process for a wide range of values of the parameter λ, as illustrated by Figure 2. In Figure 2(a), we show the chemical potential at the limit $L \longrightarrow \infty$ for $\rho = 1$ and $\lambda/t = 20$, and we observe an insulator phase due to the presence of the finite gap. In Figure 2(b), we obtain a superfluid phase because the gap is zero when $L \longrightarrow \infty$.

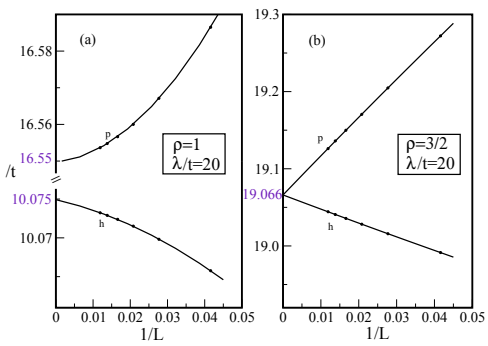

Figure 2. The chemical potential μ/t versus $1/L$, with L the size of the lattice. a) exhibits an insulator state and b) exhibits a superfluid phase at the thermodynamic limit.

Data obtained with the previous methodology allow us to study this system and obtain the following results: Figure 3 illustrates the findings of the density ρ against the chemical potential μ for the 2-period superlattice at values of λ/t between 0 and 24. $U/t = 10$ is taken

for comparison with the previous results. The homogeneous system of bosons is represented in Figure 3(a), where plateaus at densities $\rho = 1$ and $\rho = 2$ are exhibited, indicating the size of the energy gap in the Mott insulator phase. For different values of μ/t that do not imply an insulator phase, a compressible phase is achieved and the system is superfluid. Figure 3(b) for $\lambda/t = 10$ shows plateaus at semi-integer densities, while the plateaus at integer densities are fewer than in the previous case. In fact, when λ is near U, the findings suggest a phase transition from a Mott insulator to a new insulator. In Figure 3(c), we show the density for $\lambda/t = 20$. The plateau at $\rho = 3/2$ is not present, and this happens when $\lambda/t \approx 2U$. Finally, the presence of insulators at all commensurate densities (integer and semi-integer) for $\lambda/t = 24$ are given in Figure 3(d). From the above results, it could be inferred that for $\rho > 1$ there may be phase transitions between two types of insulators, passing through a superfluid phase.

Now, we explore the charge distribution for some insulator states by observing the local density along the superlattice as detailed in Figure 4. It can be observed that the boson configuration $\{2, 1, 2, 1, ...\}$ for $\rho = 3/2$ and $\lambda/t = 10$ is shown in Figure 4(a). Data in Figure 4(b) suggest a configuration $\{3, 0, 3, 0\}$ when λ increases. From Figure 4(c), it can be seen that the configuration of particles is around two when $\rho = 2$ and $\lambda/t = 2$, which is itself in a Mott insulator phase. It can be seen in Figure 4(d), with $\rho = 2$ and $\lambda/t = 24$, that the system is organized as $\{3, 1, 3, 1, ...\}$. Accordingly, the boson organization depends on the competition between the parameter λ and the particle interaction U.

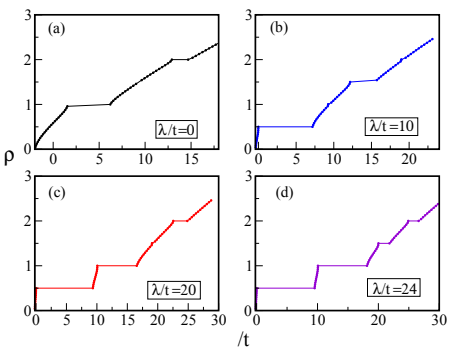

Figure 3. (color online). Density profile ρ versus chemical potential μ for bosons in a 2-period superlattice, with $U = 10$.

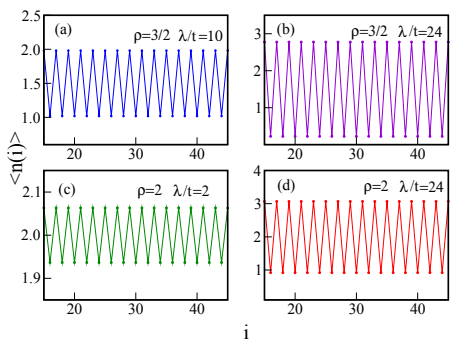

Figure 4. (color online). On-site number density plotted against lattice site index with $L = 50$ sites.

As mentioned earlier, we calculated the phase diagram, and this is shown in Figure 5. In this case, we take the values of λ and μ in U scale. We can observe that the gap size for $\rho = 1/2$ remains constant for large values of λ/U, and the remaining integer and semi-integer densities have insulator regions and transitions between them for values of densities $\rho \geq 1$ with λ values near U (for $\rho = 1$ and $\rho = 2$) and λ near $2U$ (for $\rho = 3/2$).

França and Capelle [9] showed that the average of local von Neumann entropy is able to indicate the critical points in an inhomogeneous system, which is given by: $\epsilon^* = \frac{1}{L}\sum_i \epsilon_{\nu N}(i)$, where $\epsilon_{\nu N}(i) = -Tr\sigma_i \log_2 \sigma_i$ is the local von Neumann entropy, and $\sigma_i = Tr_B\sigma$ is the density matrix of a single site located at i, where B represents the environment with $L - 1$ sites, and σ is the density matrix of the whole system [10]. We can infer a superfluid region between the insulators, as is corroborated by Figure 6. In this plot, the average entropy achieves a maximum for values around the transition region, which implies a significant growth in the degrees of freedom and a superfluid phase. This is shown in Figure 6(a), where the average entropy is calculated for the density $\rho = 1$ with a superlattice of $L = 80$ sites, and it can be observed that

the maximum is near $\lambda \approx U$. In Figure 6(b), the average entropy is shown for $\rho = 3/2$ and the maximum is given for λ near $2U$.

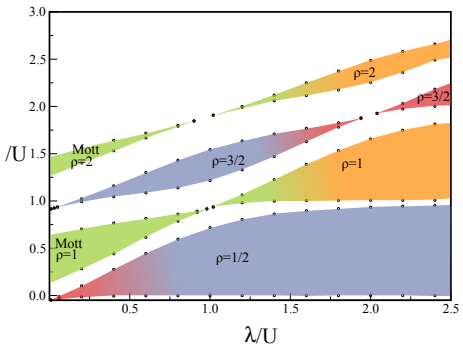

Figure 5. (color online). Phase diagram of the AB chain. The points are DMRG data.

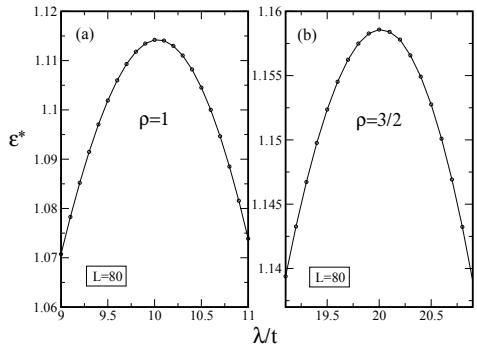

Figure 6. Average von Neumann entropy for a lattice with size $L = 80$ and density (a) $\rho = 1$ and (b) $\rho = 3/2$.

3. Conclusions

Using the density matrix renormalization group method, we determined the chemical potential of the 2-period superlattice at the thermodynamic limit and found the phase diagram. For a small energy difference (λ), we observe that insulator regions with a peculiar charge distribution appear for semi-integer densities, which doesn't occur for integer densities, for which the Mott insulator phase still appears. The size of the new insulator phases for densities less than one increases with λ but then stabilizes, and these phases remain in the phase diagram. On the other hand, for densities $\rho \geq 1$, we always found a superfluid region that separates two insulator phases. For integer densities, the system starts in a Mott insulator phase, but for $\lambda > U$ the system exhibits a new insulator phase. The most surprising result is that the new insulator for $\rho \geq 1$ is unstable with increasing λ, and we obtain an insulator phase for values of $\lambda > U$, which depends on the density. Between the insulator phases, we always have a superfluid phase, a result that was confirmed using von Neumann entropy.

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