

Mott lobes evolution of the spin-1 Bose-Hubbard model

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Abstract. We study spin-1 bosons confined in a one-dimensional optical lattice, taking into consideration both ferromagnetic and antiferromagnetic interaction. Using the density matrix renormalization group, we determine the phase diagram for the two firsts lobes and report the evolution of the first and second Mott lobes with respect to the spin-exchange interaction parameter (U_2). We determine that for the antiferromagnetic case, the first lobe is suppressed while the second grows as $|U_2|$ increases. For the ferromagnetic case, the first and second Mott lobes are suppressed by the spin-exchange interaction parameter. We propose an expresion to describe the evolution of the critical point with the increase in $|U_2|$ for both cases.

1. Introduction

The confining of ultracold atoms in optical lattices has been a very important tool for the study of condensed matter. The precision and the easy control of the various couplings makes of this a natural quantum simulator. Fermionic and bosonic systems have been explored in these experimental setups. The most well-known experiment was carried out in 2002 by Greiner *et al.* [1]. They show the phase transition from a superfluid state to the Mott insulator state, which has been much studied theoretically [2, 3].

In conventional magnetic traps, the spins of atoms are frozen so effectively that they behave like spinless particles. Now, recent progress in cooling techniques has opened the door to new studies of these systems. For instance, using purely optical traps, alkali atoms such as ⁸⁷Rb or ²³Na can be condensed and loaded into an optical lattice, preserving the spin component [4]. The size of the effects of the spin interaction can be irrelevant when the number of atoms is relatively large, so, it's natural to think about the idea of taking these interactions into consideration in optical lattices where the number of atoms is about 3 or 4 per lattice site [1].

The spin-1 Bose-Hubbard model shows the superfluid to Mott insulator phase transition [5,6], and the phase diagram was presented and discussed by Rizzi *et al.* [7] using the density matrix renormalization group (DMRG) method for the antiferromagnetic case, and by Batrouni *et al.* [8] using quantum Monte Carlo for the ferromagnetic case for small lattices. They show the location of the phase boundary, and Rizzi shows the asymmetry present with the odd-even filling discussed in [6]. But evolution of the critical point with the change in the spin-exchange interaction parameter has never been shown. This is the aim of this paper.



2. Model

The Hamiltonian for describing spin-1 bosons in an optical lattices is given by

$$H = -t \sum_{i=1, \sigma}^{L-1} \left(\hat{b}_{i, \sigma}^\dagger \hat{b}_{i+1, \sigma} + \text{h.c.} \right) + \frac{U_0}{2} \sum_{i=1}^L \hat{n}_i (\hat{n}_i - 1) + \frac{U_2}{2} \sum_{i=1}^L (\mathbf{S}_i^2 - 2\hat{n}_i) \quad (1)$$

Where $\hat{b}_{i, \sigma}^\dagger$ creates a boson with spin component σ at site i in a lattice of L sites, h.c denotes the hermitian conjugate, $\hat{n}_i = \sum_{\sigma} \hat{b}_{i, \sigma}^\dagger \hat{b}_{i, \sigma}$ and $\mathbf{S}_i = \sum_{\sigma, \sigma'} \hat{b}_{i, \sigma}^\dagger \mathbf{T}_{\sigma, \sigma'} \hat{b}_{i, \sigma'}$ are the number and spin operators for site i where \mathbf{T} are the spin 1 Pauli matrices [5]. The first term in the Hamiltonian represents the kinetic energy and t is the hopping parameter, and the second and third term represent the on-site interaction (U_0) and spin exchange interaction (U_2), respectively. The local strengths are given by

$$U_0 = \frac{4\pi\hbar^2}{M} \frac{a_0 + 2a_2}{3} \quad \text{and} \quad U_2 = \frac{4\pi\hbar^2}{M} \frac{a_0 - a_2}{3} \quad (2)$$

Where a_n are the scattering lengths and M is the mass of the atoms. These coupling parameters obey the constrain $-1 < U_2/U_0 < 1/2$, U_2 can be positive (antiferromagnetic case) or negative (ferromagnetic case) [4]. We fix our energy scale taking $U_0 = 1$.

3. Results

To study the Hamiltonian (1), we used the finite-size density matrix renormalization group method. The local Hilbert space for the on-site part of the Hamiltonian is fixed, imposing a maximum occupation number $\hat{n}_{max} = 4$. We carried out five iterations, considering $m = 250$ states per block, and the discarded weight was around 10^{-8} or less.

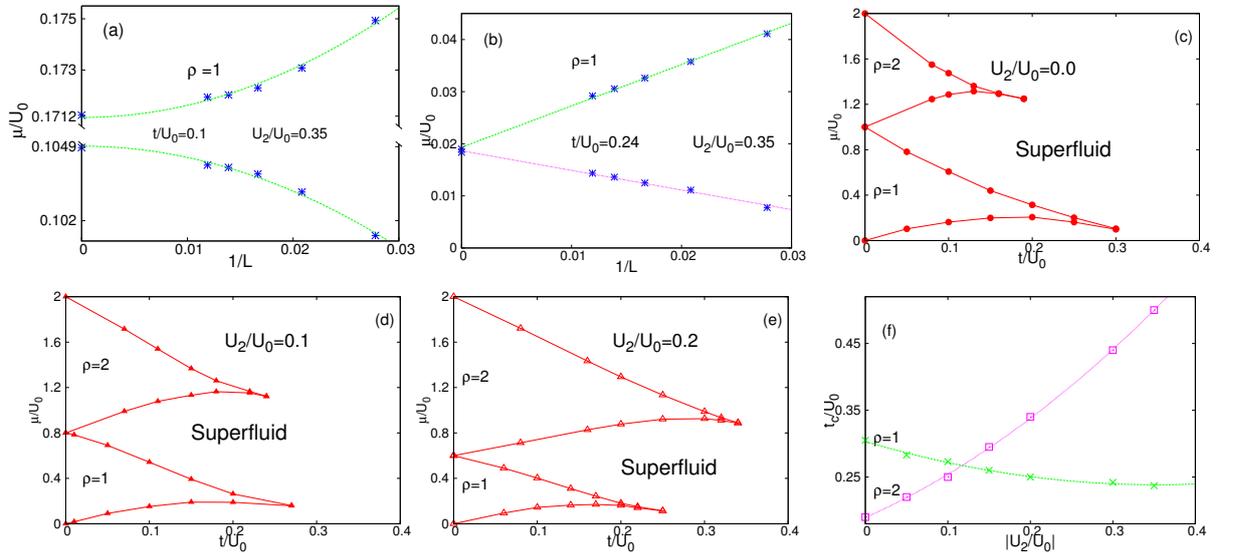


Figure 1. (Color online) Antiferromagnetic case. Chemical potential versus $1/L$ for $U_2/U_0 = 0.1$, density $\rho = 1$ and (a) $t/U_0 = 0.1$ (b) $t/U_0 = 0.24$. (c-e) Phase diagrams for the first two Mott lobes of the model case for $U_2/U_0 = 0, 0.1$ and 0.2 .

For a small kinetic energy, we expected that the bosons would be localized in the lattice and the system would be in a Mott-insulator phase. In order to show this, we calculated the energy for adding or removing a boson, given by $\mu^a(L) = E(L, N + 1, S_z) - E(L, N, S_z)$ and

$\mu^r(L) = E(L, N, S_z) - E(L, N-1, S_z)$ respectively, where $E(L, N, S_z)$ is the ground state energy for L sites, N particles and S_z spin component. Following Katsura, our results are obtained considering $S_z = 0$ for the ground state [10]. The dependence of the size of the system on adding or removing energy is shown in Figure 1(a) for $\rho = 1$, $t/U_0 = 0.1$ and $U_2/U_0 = 0.35$; we can see that the added energy decreases and the removed energy increases as the lattice size increases. It can be seen that the dependence is quadratic, and we can determine its values at the thermodynamic limit. We calculated the gap given by $\Delta = \mu^a(L) - \mu^r(L)$, and obtained a nonzero finite value, showing the existence of a Mott insulator state. In Figure 1(b), we show the addition and removal energies for $\rho = 1$, $t/U_0 = 0.24$ and $U_2/U_0 = 0.35$. It can be seen that the dependence now becomes linear, and at the thermodynamic limit the gap is zero, showing the existence of a superfluid state.

In Figure 1(c), we show the phase diagram for the two first Mott lobes ($\rho = 1$ $\rho = 2$) of the model, taking $U_2/U_0 = 0$. We observe that our results are in accordance with the reported results for the spinless case [11]. On the other hand, if we turn on the spin interaction when considering the antiferromagnetic case, we obtain that the Mott insulator area for $\rho = 1$ decreases and for $\rho = 2$ increases with the spin-exchange interaction parameter, confirming the odd and even asymmetry discussed by Imambekov [5]. This behavior is shown in Figure 1(a) for $U_2/U_0 = 0.1$ and Figure 1(b) $U_2/U_0 = 0.2$. Also, at the no-hopping limit ($t/U_0 = 0$) the spin-1 Bose-Hubbard model exhibits features that are in contrast with the spinless model. In Figure 1(d-e), we show that the antiferromagnetic interaction favors the singlet state, where the total local spin is $S_i = 0$ and the energy is set by $E_n = n_i U_0 - 2U_2$. In Figure 1(f), we report the evolution of the critical point. It can be seen that the critical value increases for $\rho = 2$ and decreases for $\rho = 1$ monotonically, and the best possible fit would be quadratic for both cases. For $\rho = 2$, we see that the spin interaction favors the Mott insulator state, and in order to evolve into superfluid state a large kinetic energy is necessary as the spin-exchange interaction parameter increases.

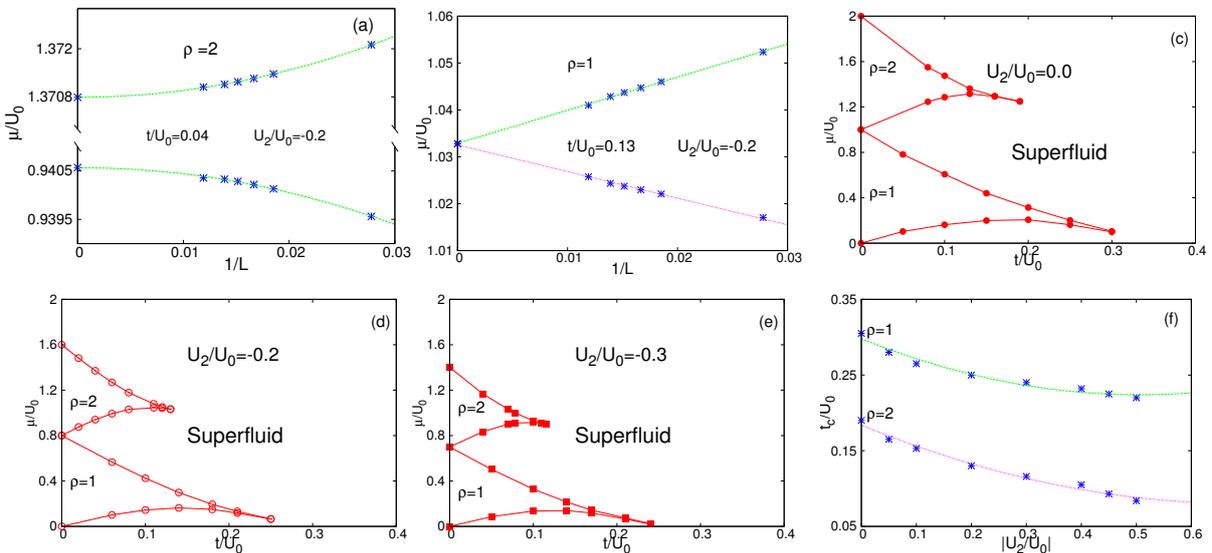


Figure 2. (Color online) Ferromagnetic case. The chemical potential versus $1/L$ for $U_2/U_0 = -0.2$, density $\rho = 2$ and (a) $t/U_0 = 0.04$ (b) $t/U_0 = 0.13$. (c-e) Phase diagrams for the first two Mott lobes of the model for $U_2/U_0 = 0, -0.2$ and -0.3 .

For the ferromagnetic case, which has not been much studied, we performed a numerical study at the thermodynamic limit, in contrast with Batrouni *et al.* [8] who show the phase diagram considering finite small lattices and using quantum Monte Carlo (QMC). Based on the

power of our DMRG code, we extended their calculations to the thermodynamic limit. Then, considering ferromagnetic interaction, we show that for small kinetic energy the system has a nonzero finite value for the gap, as is shown in Figure 2(a), and the system will be in a Mott insulator state, as in the antiferromagnetic case. If the hopping parameter increases, the gap will vanish at a critical value and the system evolves into the superfluid state, as is shown in Figure 2(b). Again it is possible to see that in the insulator region the best fit is quadratic, whereas in the superfluid region it is linear. In Figure 2(c-e) we show the phase diagrams for the ferromagnetic case for the two first Mott lobes ($\rho = 1$ $\rho = 2$) of the model. We show that the area of the Mott lobes decreases with an increase in the spin-exchange interaction, in contrast with the antiferromagnetic case, which accord with Batrouni. Also, at the no-hopping limit, the energy is set as $E_n = n_i(U_0 + U_2)$, implying that the interaction favors on-site ferromagnetic states where the total local spin is $S_i = 2$. In Figure 2(f), we report the evolution of the critical point. It can be seen that the critical value decreases monotonically for $\rho = 1$ and $\rho = 2$, and the best possible fit would be quadratic for both cases. We see in both cases that the spin interaction favors the superfluid state, and to evolve into a Mott insulator state, a small kinetic energy is necessary as the spin-exchange interaction parameter increases. Furthermore, if we compare the behavior of the critical point for the first Mott lobe in each case, ($U_2 < 0$ and $U_2 > 0$) in Figure 2(f) and Figure 1(f), we can see that the evolution is almost the same, and the corresponding fits would be similar.

4. Conclusions

We performed a numerical study of the ground state of the spin-1 bosons confined in a one-dimensional optical lattice. Using the density matrix renormalization group method, we determined the phase diagram for the first lobes ($\rho = N/L = 1$ and 2), reporting the evolution of the critical point of the transition, calculated by means of the chemical potential with respect to the spin-exchange interaction parameter (U_2), for ferromagnetic and antiferromagnetic interactions, and showed that the best fit would be quadratic in both cases. For the antiferromagnetic case, we found that the area of the first lobe decreases while that of the second increases as the $|U_2|$ increases, and for the ferromagnetic case, we calculated the phase diagram at the thermodynamic limit, reporting that the area of the first and second Mott lobes decreases as $|U_2|$ increases. We conclude that the behavior of the critical point for the first Mott lobe is almost the same for both cases considered.

Acknowledgments

The authors are thankful for the support of DIB-Universidad Nacional de Colombia.

References

- [1] Greiner M, Mandel O, Esslinger T, Hänsch T W and Bloch I 2002 *Nature* **415** 39
- [2] Jaksch D, Bruder C, Cirac J I, Gardiner C W and Zoller P 1998 *Phys Rev Lett* **81** 3108
- [3] Fisher M P A, Weichman P B, Grinstein G and Fisher D S 1989 *Phys Rev B* **40** 546
- [4] Stamper-Kurn D M, Andrews M R, Chikkatur A P, Inouye S, Miesner H-J, Stenger J and Ketterle W 1998 *Phys Rev Lett* **80** 2027
- [5] Imambekov A, Lukin M and Demler E 2003 *Phys Rev A* **68** 063602
- [6] Demler E and Zhou F 2002 *Phys Rev Lett* **88** 163001
- [7] Rizzi M, Rossini D, De Chiara G, Montangero S and Fazio R 2005 *Phys Rev Lett* **95** 240404
- [8] Batrouni G G, Rousseau V G and Scalettar R T 2009 *Phys Rev Lett* **102** 140402
- [9] White S R 1992 *Phys Rev Lett* **69** 2863
- [10] Katsura H and Tasaki H 2013 *Phys Rev Lett* **110** 130405
- [11] Kühner T D and Monien H 1998 *Phys Rev B* **58** 14741