Revista Mexicana de Física S **58** (2) 225–228 DICIEMBRE 2012

Entanglement in one-dimensional bosonic chains

C.A. Ávila, J.J. Mendoza-Arenas, R. Franco, and J. Silva-Valencia
Departamento de Física, Universidad Nacional de Colombia, A.A 5997, Bogotá Colombia
e-mail: caavilapa@unal.edu.co

Recibido el 23 de junio de 2010; aceptado el 21 de julio de 2011

We studied the one-dimensional Bose-Hubbard model, by means of the Density Matrix Renormalization Group (DMRG). The U parameter, which contains the Coulombian repulsion information, is fixed to $U = 1$ and it is performed a swept over the hopping parameter t. The entanglement is investigated by implementing the one-site, two-site and block von Neumann entropy looking for which of these measures give account of the quantum phase transition from Mott insulator to superfluid. The one-site and two-site entropy do not give information of the phase transition of the system. In contrast, the block entropy shows, in the Mott insulator phase a behavior that saturates rapidly to a finite value and in the superfluid phase shows a logarithmic behavior that agrees with the mean field theory. From the derivative of the block entropy average as a function of t we found the phase transition takes place at t_c=0.15.

Keywords: Bose-Hubbard model; quantum phase transitions.

Nosotros estudiamos el modelo de Bose-Hubbard unidimensional mediante el grupo de renormalización de la matriz densidad (DMRG), se fija el parámetro U el cual contiene la información de la repulsión Coulombiana en U = 1 y se realiza un barrido sobre el parámetro de hopping t. El entreveramiento es investigado implementando la entropía de Von Neumann de bloque, de un sitio y de dos sitios buscando cuál de estas medidas nos da información de la transición de fase cuántica de ailante de Mott a superfluido. Las entropías de un sitio y de dos sitios no dan información de la transición de fase que sufre el sistema. En cambio la entropía de bloque en la fase de aislante de Mott muestra un comportamiento que satura rápidamente a un valor finito y en la fase superfluida presenta un comportamiento logarítmico que está de acuerdo con la teoría de campo medio. A partir de la derivada del promedio de la entropía de bloque en función de t se encuentra que la transición de fase se da en t_c=0.15.

Descriptores: Modelo de Bose-Hubbard; transiciones de fase cuánticas.

PACS: 03.67.Bg; 03.65.Ud; 71.10.Fd; 71.10.Pm; 71.30.+h

1. Introduction

Recently, it has been discussed that the entanglement can be a relevant quantity in many-body systems which experiment quantum phase transitions. Furthermore, it has been become in a tool for the understanding and characterization of the ground state for many-body quantum systems [1], for this reason the entanglement research has became an active field in the investigation of strongly correlated systems. One rather relevant phenomenon in many-body physics is the occurrence of quantum phase transitions, which consist in critical changes in the properties of the ground state; the quantum phase transitions are associated with level crossings, which usually lead to the presence of nonanalyticities in the energy spectrum [2,3]. On the other hand, the study of bosonic systems has been turned in a great interest field in the latest years due to the growing possibility of perform experiments in optical lattices. The basic physics of bosons interacting strongly in a lattice is contained in the Bose-Hubard model, this is a model of many bosonic particles which can not be reduced to a model of a single particle. The bosons interact due to the Coulombian repulsion between them and this in turn can make that these bosons gain energy to jump to neighbors sites in the lattice [5,6].

For systems at zero temperature, all the thermic fluctuation dissapear, while the quantum fluctuation maintain. These quantum fluctuations can induce a macroscopic phase transition in the ground state of a many-body system when the relative force of the two competing energy terms is varied through a critical value [7]. Motivated by the experimental result of Greiner *et. al.* in Ref. 7, where it was observed the quantum phase transition of the Mott insulator phase to the superfluid phase in a Bose-Einstein condensate with repulsive interactions in a 3D optical lattice, it is investigated how the von Neumann entropy gives account of the phase transition in a one-dimensional boson chain.

The obtaining of the numerical results was implemented in the Density Matrix Renormalization Group (DMRG) algorithm, for a 1024 sites chain with 100 states and open boundary conditions. Each site in the chain has five states with the number occupation n= 0, 1, 2, 3, 4. The biggest numerical error was 5×10^{-7}.

The outline of this paper is a follows: In Sec. 2 the Bose-Hubbard model are discussed. Some aspects of the von Neumann entropy are discussed in Sec. 3. The calculation of the von Neumann entropy is presented in Sec. 4. Conclusions are given in Sec. 5.

2. Bose-Hubbard (BH) model

The Bose-Hubbard Hamiltonian is given by:

$$H_{BH}^{=} - t\sum_i \left(\hat{b}_i^\dagger \hat{b}_{i+1} + \hat{b}_i \hat{b}_{i+1}^\dagger\right) + \frac{U}{2}\sum_i \hat{n}_i\left(\hat{n}_i - 1\right), \quad (1)$$

where $\hat{b}_i^\dagger$ and $\hat{b}_i$ are the creation and annihilation operators in the i site and $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ gives account of the number of particles in the i site. The first term of the Eq. (1) models the kinetic energy of the atoms and the t parameter indicates the tunneling force or hopping between adjoined sites. The second term represents the short range interaction between the atoms and the U parameter characterizes the Coulombian repulsion between two atoms in one site of the lattice. A scheme of the Bose-Hubbard model is shown in Fig. 1. In equilibrium the Bose-Hubbard model shows a quantum phase transition in a critical value $u_c = (U/J)_c$ between the superfluid phase $(U/t < u_c)$ and the Mott insulator phase $(U/t > u_c)$ [1].

In the limit when the tunneling dominates the Hamiltonian, $(U/t < u_c)$, the ground state energy is minimized and the ground state for a many-body homogeneous system is given by

$$|\Psi_{SF}\rangle \, \alpha \left(\sum_{i=1}^{M} \hat{b}_i^\dagger \right)^N |0\rangle \, . \tag{2}$$

There all the atoms occupy the same Bloch state. The distribution probability for the local occupation n_i of atoms in a lattice site is of Poisson kind, which indicates that the variance is given by $Var\,(n_i) = \langle n_i \rangle$. Furthermore, this is well described by a macroscopic wave function with phase coherence of long range through the lattice [7]. In the superfluid phase, the system has no energy gap and hence the system is compressible [6].

If the Coulombian interactions dominates the Hamiltonian $(U/t > u_c)$, the ground state of the system consists of localized wave functions with a fixed number of atoms per site. The ground state is then the Fock local state product for each site on the lattice. Then, the ground state of a many-body system for a proportional filled of n atoms per site of the lattice in the homogeneous case is given by:

$$|\Psi_{MI}\rangle \, \alpha \prod_{i=1}^{M} \left(b_i^\dagger \right)^n |0\rangle \, . \tag{3}$$

This phase can not be described as a macroscopic wave function. In this state the phase coherence does not dominate in the system, but there exist correlations in the number of atoms between sites in the lattice [7]. In the Mott insulator phase, the system has a finite energy gap and therefore the system is incompressible [6].

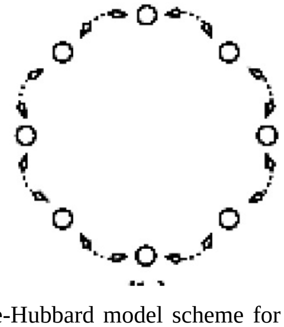

FIGURE 1. Bose-Hubbard model scheme for periodic boundary conditions. [4]

A schematic phase diagram show in a Fig. 2. It show the Mott insulator (MI) phase for several values of ρ surrounded by the superfluid phase.

To determinate the positions of the phase boundaries can be done using the usual Landau theory argument given by

$$E_0 = E_{00} + r \left|\Psi_B\right|^2 + O\left(\left|\Psi_B\right|^4 \right) \tag{4}$$

the phase transition will occur when $r = 0$, and that can be found using second order perturbation theory.

$$lr = \chi_0 \left(\mu/U\right) \left[1 - Z\omega\chi_0 \left(\mu/U\right)\right] \tag{5}$$

where

$$\chi\left(\mu/U\right) = \frac{n_0\left(\mu/U\right) + 1}{Un_0\left(\mu/U\right) - \mu} \frac{n_0\left(\mu/U\right)}{\mu - U\left(n_0\left(\mu/U\right) - 1\right)} \tag{6}$$

where $n_0\left(\mu/U\right)$ is given by

$$n_0\left(\mu/U\right) = \begin{cases} 0 & \text{para} \quad \mu/U < 0 \\ 1 & \text{para} \quad 0 < \mu/U < 1 \\ 2 & \text{para} \quad 1 < \mu/U < 2 \\ . & \\ . & \\ . & \\ n & \text{para} \quad n-1 < \mu/U < n \end{cases} \tag{7}$$

solving 5 for $r = 0$ gives the ohase boundaries of the Fig. 2. [8,9]

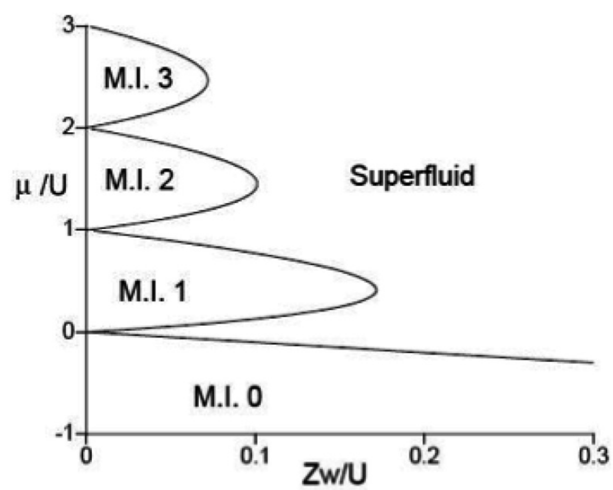

FIGURE 2. Mean field phase diagram of the ground state of the model Bose-Hubbard. Z is the number of nearest neighbors around each lattice point, ω is the hopping term and μ is the chemical potential. [8]

3. Von Neumann entropy

The von Neumann entropy gives account of the existing entanglement between two blocks. If the system is divided in two blocks, then, being A a block of size l and B the block that contains the rest of the system. The von Neumann entropy for block A is defined as

$$S_A\left(l\right) = -Tr\left[\rho_A \ln \rho_A\right], \qquad (8)$$

where the reduced density matrix of block A is defined as $\rho_A = Tr_B \left|\Psi\right\rangle \left\langle\Psi\right|$, [10].

The Mott insulator phase, is characterized as mentioned above, by an energy gap in the ground state and by a finite correlation length. For systems with finite correlation length it is expected that the block entropy saturates to a finite value [1].

The superfluid phase can be described by a Luttinger liquid, which is a conformal field theory whit central charge $c = 1$. For such systems with open boundary conditions the block von Neumann entropy is defined as:

$$S_A\left(l\right) = \frac{c}{6}\log\left[\frac{2L}{\pi}\sin\left(\frac{\pi l}{L}\right)\right] + K, \qquad (9)$$

where K is the frontier entropy of Affleck and Ludwig and L is the size of the system [1].

4. Results and discussion

For all the cases was fixed $U = 1$ and was performed a swept over the t parameter. According to Fig. 2 an increase in t should show a change in the behavior of the system due to there is occurring a quantum phase transition of the Mott insulator phase tho the superfluid phase.

First, it was studied the one-site entropy for the $L/2$ site as a function of l obtaining the following results from Fig. 3, it is observed that the one-site entropy saturates rapidly for all the values of t of the studied range, as t increases the saturation value of the one-site entropy also grows. Due to the behavior of this entropy is the same for all the values of t we conclude this measure does not give information about the point where the phase transition takes place.

It was also studied the two-site entropy, corresponding to the entanglement between the block comprised by the $L/2$ and $L/2 + 1$ sites and the block that contains the rest of the lattice when the symmetric configuration has been reached by means of the DMRG method, as a function of t obtaining the next result in the upper part of Fig. 4 it is observed that the two-site entropy behaves as a growing monotone function when t increases. To determine if this entropy shows a characteristic behavior it is calculated its derivative which is shown in the lower part of Fig. 4. There it is observed that the derivative does not show any anomalous behavior. Therefore, the two-site entropy and its derivative does not give information about where is taking place the quantum phase transition.

Finally, it was studied the block entropy, corresponding to the entanglement present between the $L/2$ size block and the block comprised by the rest of the lattice, as a function of l obtaining the next result from Fig. 5.

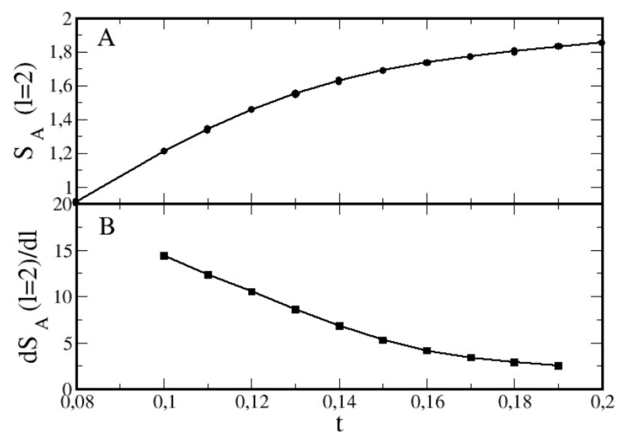

FIGURE 4. Upper. Two-site entropy $(S_A(l = 2))$ as a function of t parameter. Lower. Derivate of the Two-site entropy.

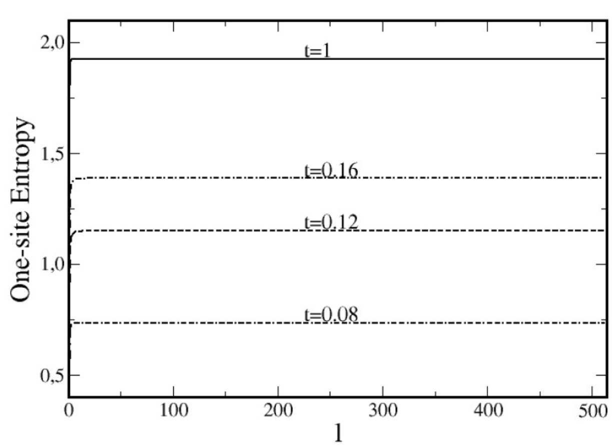

FIGURE 3. One-site entropy as a function of the site number for $L = 1024$.

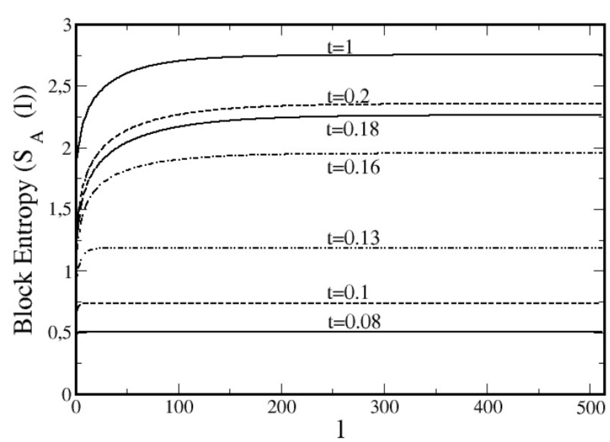

FIGURE 5. Block entropy as a function of the number site for $L = 1024$.

First of all, it is observed that as the t parameter is increased the block entropy increases as well. This, due to the entanglement in the system also grew. Secondly, it is observed that for the range $0.08 \leqslant t \leqslant 0.13$ the block entropy saturates rapidly indicating us that the system has finite correlations, which shows that the system is in the Mott insulator phase. For the range $0.16 \leqslant t \leqslant 1$ the block entropy shows a divergent behavior that indicates that the system is in the superfluid phase, where the fit of the central charge using Eq. (9) for each value of t is shown in Table I.

Lauchli *et. al.* in Ref. 1 performs a study of the block von Neumann entropy for a 1024 boson chain with density ρ=1 where he reported $u_c = (U/t)_c = 3.3$, so that for $u_c < 3.3$, the block entropy also has a logarithmic behavior indicating that the system is in the superfluid phase and which its fit for the central charge is in average $c = 1$. While for $u_c > 3:3$ the block entropy saturates unveiling the finite correlation length existing in the Mott insulator phase.

To determine the t value in which takes place tha phase transition, we plotted the average of the block entropy as a function of the t parameter obtaining the next result it is observed in the upper part of Fig. 6 that the block entropy average, behaves as a rising function which derivative it is shown in the lower part of Fig. 6, the derivative exhibit a maximum at $t = t_c = 0.15$. This t_c value is in the region where the block entropy changes its behavior from a saturated one to a logarithmic one and consequently it represents the point where the quantum phase transition takes place.

TABLE I. Extracted value of c for each curve in the superfluid phase.

t	$c \pm 0.03$
0.19	0.89
0.18	0.89
0.17	0.83
0.16	0.61

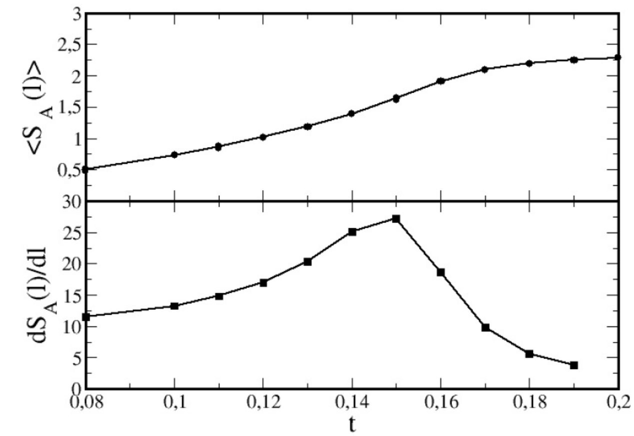

FIGURE 6. Upper. Block entropy average ($\langle S_A(l) \rangle$) as a function of the t parameter. Lower. Derivate of the Block entropy average.

5. Conclusions

We calculated the block von Neumann entropy, the one-site entropy and the two-site entropy by means of the Density Matrix Renormalization Group (DMRG) for the Bose-Hubbard model. We observed that the block von Neumann entropy gave us information about the quantum phase transition this model presents from the Mott insulator phase to the superfluid phase, while the other two measures calculated do not give account of the mentioned transition. For the case studied, a boson chain of $L = 1024$, ρ = *2* and $U = 1$ it was observed that the phase transition takes place for $t_c = 0:15$.

Acknowledgments

This work was partially financed by Universidad Nacional de Colombia (DIB-8003357).

1. A. Lauchli and C. Kollath, *J. Stat. Mech* (2008) P05018.
2. L-A Wu, M.S. Sarandy, and D.A. Lidar, *Phys. Rev. Lett.* **93** (2004) 250404.
3. L-A Wu, M.S. Sarandy, D.A. Lidar, and L.J. Sham, *Phys. Rev. A* **74** (2006) 052335.
4. R.J. Costa and M.C. de Oliveira; arXiv:0812.4381v1 (2008).
5. T.D. Kuhner and H. Monien, *Phys. Rev. B.* **58** (1998) 14741.
6. T.D. Kuhner, S.R. White, and H. Monien, *Phy. Rev. B* **61** (2000) 12474.
7. M. Greiner, O. Mandel, T. Esslinger, T.W. Hansch, and I. Bloch, *Nature* **415** (2002) 39.
8. Subir Shachdev, *Quantum Phase Transitions* (Cambrige University Press 2008)
9. Stanimir Kondov, http://guava.physics.uiuc.edu/nigel/courses/563/Essays_2008/index.html
10. A. Kallin, I. Gonz'alez, M. HAstings, and R. Melko; *Phys. Rev. Lett.* **103** (2009) 117203.