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QUANTUM PHASE TRANSITIONS OF A BOSE-EINSTEIN CONDENSATE

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Quantum phase transitions of a Bose-Einstein condensate

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Abstract. Bose-Einstein condensates display quantum phase transitions that cannot be explained with a mean field theory. Describing each trap as an effective site of a Bose-Hubbard model and using the Schwinger representation the system can be mapped onto a spin model. We show that it is possible to define correlations between bosons in such a way that critical behaviour is associated to the divergence of a correlation length accompanied by a gapless spectrum in the thermodynamic limit. Such description provides critical exponents and encompasses the notion of universality.

Keywords: Bose-Einstein condensation, Quantum phase transitions, Correlation functions, Critical exponents, Finite-size scaling.

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1. Introduction

The Hubbard model, originally proposed as an idealization to study magnetic properties of electrons in transition metals [1], has become a paradigmatic model in condensed matter and a good model to describe quantum simulators with ultracold atoms. Ultracold atoms confined in sufficiently deep optical lattices can be described by a Bose-Hubbard (BH) model [2]. This model predicts the Superfluid (SF) - Mott Insulator (MI) phases [3], experimentally observed for the first time by the Bloch-Hansch group [4]. It was the begining of the studies of strongly correlated systems with ultracold atoms [5], a field that has broadened enormously [6, 7, 8].

We focus our studies in ultracold bosons in a double well potential. In weakly interacting systems, the relevant properties of the system can be analyzed within the Gross-Pitaevsky mean field approach [9] and the model can be further simplified by using the two-mode approximation which describes the system with only two variables [10]. For some values of interactions and tunneling, the strongly correlated regime is also achieved in the double well potential. In this situation, the mean field approximation does not work and phase transitions appear [11, 12]. In general, when approaching a Quantum Phase Transition (QPT) some observables present a behaviour that can be characterised by critical exponents, which in turn define the type of phase transition occurring in the system [13].

The aim of this work is to explain and understand the QPTs produced in a Bose-Einstein condensate (BEC) trapped in a double well potential. My main contribution has been to solve the BH Hamiltonian of the system using the exact diagonalization technique and analyse some important properties such as the Ground State (GS), the energies or the population imbalance of the system, which show us the different phases of the system and where the phase transition occurs. The second part of the work consists in mapping our model onto a spin model using the Schwinger representation to study the QPTs. We propose a definition of two body quantum correlations which incorporates the concept of length and 'traslation invariance' which allows us to associate the QPT with the divergence of the correlation length. Finally, using finite size scaling techniques we have obtained the correspondent critical exponents.

2. The system: Bose-Hubbard approach

Our system is composed of N spinless bosons trapped in a potential $V(x)$. At zero temperature, the Hamiltonian can be expressed as:

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla^2 + V(x) + \sum_{i,j=1}^{N} V(x_i, x_j). \tag{1}$$

We are interested in working with a localized basis that we denote as Left (L) and Right (R) instead of the eigenenergy basis that corresponds to the delocalized wavefunction. The relation between the basis is $|\varphi_L\rangle = (|\varphi_+\rangle + |\varphi_-\rangle)/\sqrt{2}$ and $|\varphi_R\rangle = (|\varphi_+\rangle - |\varphi_-\rangle)/\sqrt{2}$.

In second quantization, the Hamiltonian is expressed as:

$$\hat{H} = \hat{H}_0 + \hat{H}_I, \tag{2}$$

$$\hat{H}_0 = \int \hat{\psi}^\dagger(x)\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\hat{\psi}(x)dx, \tag{3}$$

$$\hat{H}_I = \int\int \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')V(x,x')\hat{\psi}(x)\hat{\psi}(x')dxdx', \tag{4}$$

where $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$ are the bosonic field operators that annihilate and create a boson at a point x. These operators are defined as $\hat{\psi}(x) = \sum_i \varphi_i(x)\hat{a}_i$ where $\hat{a}_i$ and $\hat{a}_i^\dagger$ are the bosonic annihilation and creation operators fulfilling the commutation relations $[\hat{a}_i^\dagger, \hat{a}_j] = \delta_{ij}$. The particle number operator $\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i$ counts the number of particles on site i. The total number of bosons is conserved $\hat{N} = \sum_{i=1}^{M}\hat{n}_i$, where M is the number of sites.

Introducing the operators we obtain the BH Hamiltonian:

$$\hat{H} = -\frac{t}{2}\sum_{<i,j>}^{M}(\hat{a}_i^\dagger \hat{a}_j + h.c.) + \frac{U}{2}\sum_i^M \hat{n}_i(\hat{n}_i - 1). \tag{5}$$

The first term corresponds to the kinetic part, characterized by the tunneling t between adjacent sites. The second term corresponds to the particle interaction, characterized by the parameter U which can be either positive (repulsive interaction) or negative (attractive interaction). Our Hamiltonian exhibits different phases depending on the ratio between the tunneling energy and the on-site interactions which can be treated as a single parameter U/t.

First, if the repulsive interaction term dominates ($U/t \to \infty$), our system is in the MI phase if the number of bosons N is even. The ground state is characterized by a well defined number of atoms per site $n = N/M$, finite correlation length and a gapped spectrum. The many-body GS is a product of local Fock states, with a fixed atom number at each lattice site:

$$|\Psi_{MI}\rangle \propto \left(\prod_{i=1}^{M} \hat{a}_i^\dagger\right)^n |0\rangle \quad \overset{M=2}{\rightarrow} \quad |\Psi_{MI}\rangle \propto \left(\hat{a}_1^\dagger \hat{a}_2^\dagger\right)^n |0\rangle = |\frac{N}{2}, \frac{N}{2}\rangle. \tag{6}$$

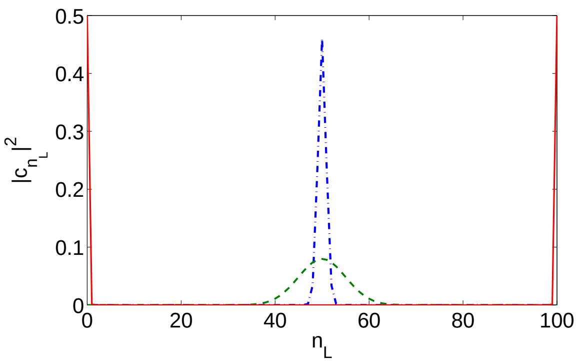
Second, if the tunneling term dominates ($U/t \to 0$) our system is in the SF phase. The ground state is characterized by delocalized atoms, which corresponds to large fluctuations on the one-site number of particles, divergent correlation length and vanishing gap. In the limit $U = 0$, the many-body state on a lattice site is a superposition of different atom numbers, following a Poissonian atom number distribution:

$$|\Psi_{SF}\rangle \propto \left(\sum_{i=1}^{M} \hat{a}_i^\dagger\right)^N |0\rangle \quad \overset{M=2}{\rightarrow} \quad |\Psi_{SF}\rangle \propto \left(\hat{a}_1^\dagger + \hat{a}_2^\dagger\right)^N |0\rangle. \tag{7}$$

Finally, if the attractive interaction term dominates ($U/t \to -\infty$), the ground state is characterized by a superposition of all the atoms being in the left and the right side of the well simultaneously. This state is called a Schrödinger cat-like state:

$$|\Psi_{cat}\rangle = \frac{1}{\sqrt{2}}(|N, 0\rangle \pm |0, N\rangle). \tag{8}$$

To solve the system and observe its properties and QPTs, exact diagonalization [14] takes a unique position because it is not burdened by any appoximation and thus provides unbiased benchmarks for other analytical or numerical approaches. The basic idea is to express the Hamiltonian in a Fock basis, which is characterized by the number of particles at each site $|n_L, n_R\rangle$ and then apply the Lanczos algorithm [15] which diagonalize our matrix and allow us to find the eigenstates and eigenvalues of the system. One important aspect is that we do not need to solve all the eigenvalues and eigenvectors of the Hamiltonian. Physically, the most rellevant eigenstates are the GS and low lying excited states. High excited states, due to Boltzman factor, almost do not contribute to the thermodynamics of the system at low temperatures.



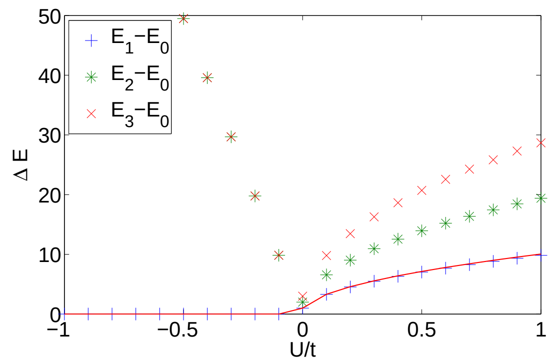


Figure 1. Spectral decomposition in the Fock space of the GS for: $U/t = 10$ (dash-dot line), $U/t = 0$ (dashed line), $U/t = -1$ (solid line).

Figure 2. Energies of the first energy levels respect to the GS for a system with $N = 100$. The solid line corresponds to the semiclassical approach [16].

2.1. Ground state

The ground state, expressed in the Fock space as $|\Psi\rangle = \sum_{n_L=0}^{N} c_{n_L}|n_L, N-n_L\rangle$, depends strongly on the parameter U/t. In Figure 1 we represent the probability $|c_{n_L}|^2$ of our state having n_L particles in the left-side for a system with $N = 100$. We should remark that if we increase the value of $|U|/t$, the curves become thinner, higher and located at the exact points.

When the interactions are large and repulsive ($U/t > 0$) the bosons repeal each other and the most stable state occurs when half of them are on each site. For this reason, the higher probabilities are located around $k = N/2$ which corresponds to a MI ground state $|\Psi_{MI}\rangle$. On the contrary, when the interactions are large and attractive ($U/T < 0$) the bosons tends to be all in the same site and the largest probabilities are located close to $k = 0, N$ which corresponds to a Schrödinger cat-like state $|\Psi_{cat}\rangle$. Finally, when there are no interactions ($U = 0$), we have a Poissonian atom number distribution around $k = N/2$ corresponding to a SF ground state $|\Psi_{SF}\rangle$.

2.2. Energy

When we diagonalize the Hamiltonian, the lower eigenvalues correspond to the first energy levels of the system. In Figure 2 we can observe the energies of the energy levels respect to the GS. When the system is in the MI phase ($U/t > 0$) all the energies tend to separate and we have a gapped energy spectrum as expected. On the contrary, when it is in the SF phase, $U/t \to 0$ the difference between energies vanish and the property of having a gapless spectrum is fulfilled. Finally, when $U/t < 0$, the states are degenerated in pairs, the first with the ground and the third with the second, due to the symmetry of the system.

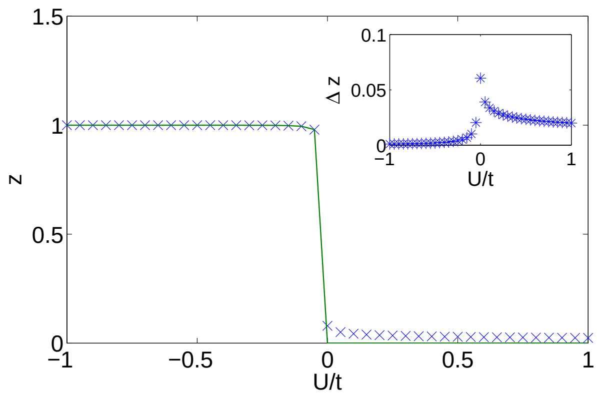


Figure 3. Population imbalance of the GS (x) and its Fluctuations ($*$) for a system with $N = 100$ as a function of U/t. The solid line corresponds to the semiclassical approach [16].

2.3. Population Imbalance

The population imbalance, defined as $\hat{z} = (\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2)/N = (\hat{n}_1 - \hat{n}_2)/N$, is the most natural observable in this system. It indicates the difference on population between the left and right wells. The fluctuations of this quantity, defined as $\Delta z = \sqrt{\langle z^2 \rangle - \langle z \rangle^2}$, give a measure of the quantum effects [11, 12] and have been investigated by several authors [17, 18].

In Figure 3 we can observe how the QPT occurs at $U/t = 0$ as expected. For attractive interactions the population imbalance tends to one because we have a Schrödinger cat-like state and all the particles are in the left or the right side. On the contrary, if the interaction is repulsive it tends to zero because we have a MI ground state and half of the particles are on each site, so the difference of population between left and right is zero. A part of the change in the population imbalance, the fluctuations located around $U/t = 0$ are also a good indicator to find where the QPT occurs.

3. The LMG model

Although Lipkin, Meshkov and Glick (LMG) introduced the model in nuclear physics [19], it has been used in many different fields such as statistical physics of spin systems [20], Bose-Einstein condensates [21] and more recently, in quantum information framework to display interesting entanglement properties [22].

Hubbard models reduce to spin models in certain limits [23]. If bosonic atoms can occupy only $2S+1$ different states in a lattice site, then one can always map these states onto states of pseudo-spin S. Our system can be mapped onto the LMG spin model by using the Schwinger representation $\{\hat{S}^+ = \hat{a}_1^\dagger \hat{a}_2, \hat{S}^- = \hat{a}_2^\dagger \hat{a}_1, \hat{S}_z = \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2)\}$ and the holonomic constraint, $2\hat{S} = \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 = \hat{N}$, which fixes the total number of bosons or equivalently the total spin and cuts in this way the infinite tower of states of the harmonic oscillators.

The BH Hamiltonian simplifies introducing the commutation relations $[\hat{H}, \hat{N}] = [\hat{H}, \hat{S}] = 0$ and $\hat{S}_x = (\hat{S}^+ + \hat{S}^-)/2$ and can be rewritten as:

$$\hat{H} = U(\hat{S}^2 + \hat{S}_z^2 - \hat{S}) - \frac{t}{2}(\hat{S}^+ + \hat{S}^-) = \frac{UN}{N}\hat{S}_z^2 - t\hat{S}_x. \tag{9}$$

The $1/N$ prefactor ensures that the free energy per spin is finite in the TL. The Hamiltonian describes an Ising model (system of spin 1/2 particles mutually interacting embended in a transverse magnetic field in x-direction) where $\hat{S}_\alpha = \sum_{i=1}^{N} \hat{\sigma}_i^\alpha/2$ where $\hat{\sigma}_i^\alpha$ are the Pauli operators. We can observe that the double well Hamiltonian is just a particular case of the general LMG model $\hat{H}_{LMG} = -\frac{\lambda}{N}\sum_{i<j}(\hat{\sigma}_i^z\hat{\sigma}_j^z + \gamma\hat{\sigma}_i^y\hat{\sigma}_j^y) - h\sum_i \hat{\sigma}_i^x$ which has been recently used in many contexts [20, 24, 25, 26]. In our case, $\gamma = 0$, the tunneling is equivalent to an external magnetic field $t = 2h \equiv h'$ along the x-direction and the on-site interactions acts as an effective spin-spin interaction $UN = -4\lambda \equiv -\lambda'$ and rewrites as:

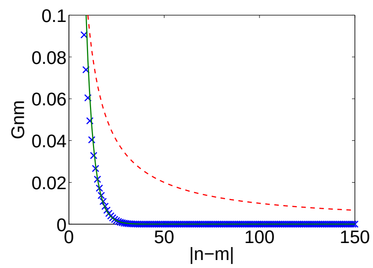
$$\hat{H}_{LMG} = -\frac{\lambda'}{N}\hat{S}_z^2 - h'\hat{S}_x. \tag{10}$$

This model has a QPT whose character depends on if the transition is antiferromagnetic or ferromagnetic. In the latter case and at finite size, some nontrivial scaling behaviour of observables have been found numerically [20]. For $\lambda' > 0$ (ferromagnetic coupling) exists a second order phase transition at $\lambda' = |h'|$. The transition between ferromagnetic and paramagnetic order occurs at $|U|N/t \to 1$, which in the thermodynamic limit ($N \to \infty$) converges to $U/t \to 0$.

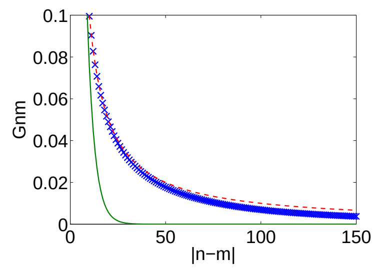
For systems of large but finite size, there are two quasi-degenerate ground states in the ferromagnetic phase ($\lambda' >> h'$), being the combination of all spins up and all down, symmetric and anti-symmetric with respect to the flip of all spins. Moreover, the spectrum is gapped and excitations cost at least energy of order λ'. In the other limit, ($\lambda' << h'$), the ground state is non-degenerated and the spectrum exhibits a gap of order h. The gap vanishes at the criticality as we have just seen when we have observed the energies of the system.

4. Correlations and critical exponents

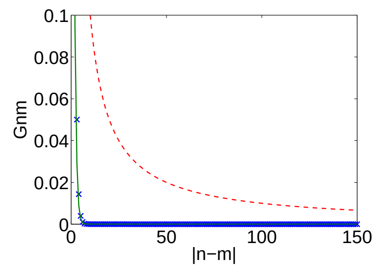
Our aim is to provide a definition of correlations, which naturally embraces the notion of correlation length and allows to link critical behavior to its divergence. With this purpose we first calculate the phase diagram of the double well for different values of N near criticality (where physical quantities exhibit scaling behavior and the exponents of these power laws are called critical exponents). Then, we analyse the scaling behaviour of some operators and performing Finite Size Scaling (FSS), measuring some quantities for different number of bosons, we obtain the corresponding critical exponents. Finally, we check if other models of the restricted Bose-Hubbard family share the same critical exponents and belong to the same universality class.



(a) $UN/t = 100$



(b) $UN/t = -1$



(c) $UN/t = -20$

Figure 4. Two body correlation function G_{nm} versus distance fitted by an exponential decay (solid line) and an algebraic decay (dashed line).

4.1. Correlations

In spin chains, the length is naturally settled by the number of sites L, and the two-body correlations are given by $C_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$. Translational invariance ensures that their behaviour depends on the distance between the two sites $|i - j|$, but not on the specific sites i, j. The latter allows to define the correlation length ξ which fixes the length scale at which all spins are correlated between them. Far from criticality, the decay is exponetial $C_{ij} \propto \exp(-|i-j|/\xi)$ and the correlation lenght diverges as $\xi \propto |U - U_{crit}|^{-\nu}$, where U_{crit} corresponds to the critical point and ν is the mass gap exponent. At criticallity, for continuous second order phase transitions, the decay is algebraic $C_{ij} \propto |i-j|^{-(d-2+\eta)}$.

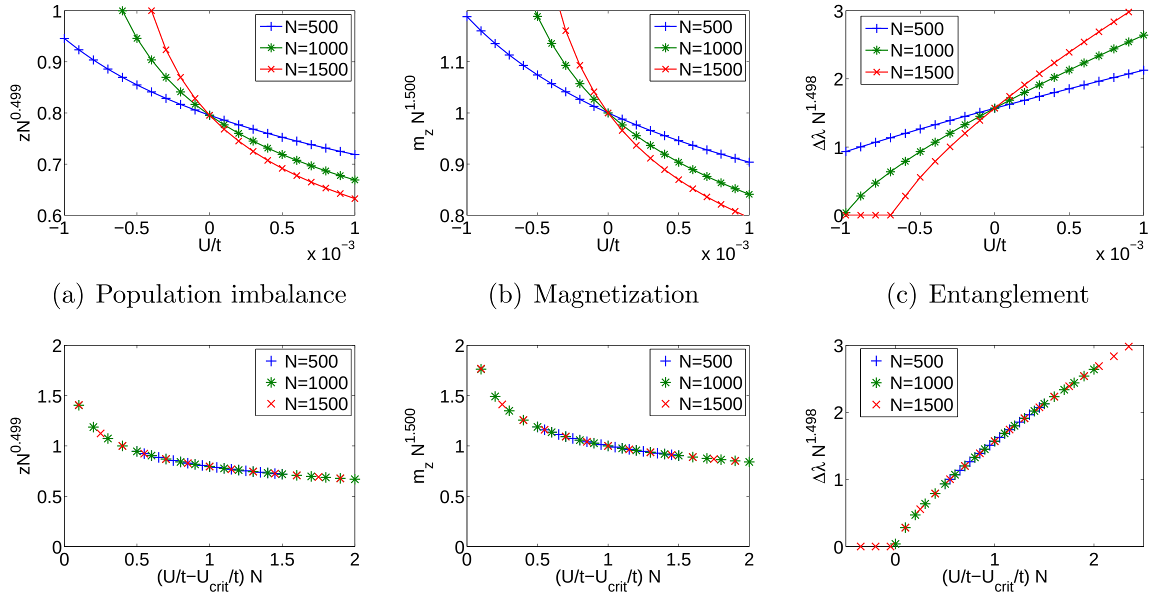
Our system is located in a double well potential and we cannot interpret the correlation lenght as the natural length as it happens in spin chains. We have to associate 'length' to the number of bosons because it settles the dimension of the corresponding Hilbert space. We define the correlation function, which correlates boson occupation numbers within a well, as:

$$C_{nm} = |n\rangle\langle m| \otimes |N-n\rangle\langle N-m|, \tag{11}$$

where the operator $|n\rangle\langle m|$ acts on the first trap and $|N-n\rangle\langle N-m|$ on the second one. In order to recover the 'traslational invariance' concept rooted in spin chains, we weight the correlation function by the 'effective distance' $|n-m|$. This renormalization factor ensures the proper behaviour of correlations as it neglects contributions from any intermediate level between n and m. If we introduce this term, the two body correlations function of our system is defined as:

$$G_{nm} = \sum_{|n-m|} \frac{C_{nm}}{|n-m|} = \sum_{|n-m|} \frac{|n\rangle\langle m| \otimes |N-n\rangle\langle N-m|}{|n-m|} \tag{12}$$

In Figure 4 we can observe how the decay is algebraic where the QPT occurs ($UN/t = -1$) and how the decay is exponential as expected if we go to the other limits $UN/t >> 0$ (repulsive interactions) and $UN/t << 0$ (attractive interactions).



(a) Population imbalance (b) Magnetization (c) Entanglement

(d) Population imbalance (e) Magnetization (f) Entanglement

Figure 5. Scaling behaviour of the population imbalance, the magnetization along the z-axis and the Shcmidt gap for a system with $N = 500, 1000, 1500$. The critical exponents obtained via this method are summarized in Table 1.

4.2. Critical exponents

Since condensed matter systems are typically very complex, theorists make simplified models of the systems. In this simplification, symmetries of the original problem are usually kept intact, and the concept of universality is used. Different Hamiltonians with similar symmetry properties belong to the same universality class, exhibit the same phase transitions and have the same critical exponents [13, 27, 28].

To obtain a deeper understanding of criticality as well as the exact location of the phase transition, we analyse some quantities such as: the population imbalance $\langle\hat{z}\rangle \equiv \langle\hat{S}_z\rangle$, its fluctuations $\Delta\hat{z}$, the magnetization along the z-axis $m_z = \sqrt{\langle\hat{S}_z^2\rangle}/N$ [24] and the entanglement spectrum $\Delta\lambda$.

The entanglement spectrum is defined as the eigenvalues of the reduced density matrix of one mode or trap $\rho_{L(R)} = Tr_{R(L)}(|\Psi\rangle\langle\Psi|) = \sum_i \lambda_i |u_i\rangle\langle u_i|$ where L (R) stand for the left (right) trap in the double well configuration. In spin chains it has been demonstrated that the Schmidt gap, defined as the difference between the two largest non-degenerate eigenvalues of the entanglement spectrum (Schmidt eigenvalues), $\Delta\lambda = \lambda_1 - \lambda_2$, closes at the critical point in the TL [29, 30]. Finite size effects inhibit such behaviour, which can be recovered from FSS [31].

In Figure 5 (a,b,c) we can observe how the phase transtion occurs at $U/t \to 0$ because it is the point where all the curves corresponding to different number of bosons N cross each other. Furthermore, in Figure 5 (d,e,f), performing FSS techniques we can observe the scaling behaviour of our quantities and extract the critical exponents.

The quantites scale near a critical point as $\hat{O} \sim N^{\beta/\nu} \int |U - U_{crit}| N^{-1/\nu}$, where ν is the mass gap exponent (associated to the correlation length divergence) and β is the critical exponent of the operator $\hat{O}$. In infinitely correlated models such as the LMG, critical exponents obtained in the mean-field limit, i.e. assuming a large classical spin, and critical exponents for large but finite N are not equivalent [20, 24, 25]. The clear scaling behaviour of the quantities allows us to find the critical exponents which are summarized in Table 1.

	$\hat{S}_z$	$\Delta\hat{z}$	m_z	$\Delta\lambda$
β	0.499	0.502	1.500	1.498
ν	1	1	1	1

Table 1. Critical exponents associated to the correlation length divergence (ν) and to the scaling operators $\hat{O}$ (β).

From the scaling of population imbalance we obtain the mean field critical values ($\beta = 1/2$) and mass gap ($\nu = 1$) [16, 25, 26]. To further check that our definition of correlations is phisically correct, we compute from the algebraic decay of G_{nm} (Fig. 4) the exponent $(d - 2 + \eta)$, where d is the dimensionality of the system and gives the value $(d - 2 + \eta) = 1$. Critical exponents are not all independent and should verify some algebraic relations [32] valid in the TL such as $2\beta = \nu(d-2+\eta)$, which reduces to $2\beta = \nu$. In our system, this relation if fulfilled for the critical exponents of the quantities $\hat{z}$ and $\Delta\hat{z}$.

Interestengly enough, the critical exponents obtained from the scaling of the magnetization m_z and the entanglement spectrum $\Delta\lambda$ coincide with the finite size critical exponents of the LMG model ($\beta = 3/2$) and ($\nu = 1$) [20, 24].

5. Conclusions

In this work we have presented the Bose-Hubbard model for a Bose-Einstein condensate trapped in a symmetric double well potential. We have analysed some static properties, the phase transition that occurs in the strongly correlated regime and the behaviour around the critical point.

We have shown that Bose-Einstein condensates displaying quantum phase transitions can be mapped onto spin models. We have proposed a definition of two body quantum correlations function for the system, which incorporates the concept of length and 'traslational invariance', and allow us to demonstrate that mean field QPTs can also be associated to the divergence of the correlation length which yields the mass gap exponent. By using Finite Size Scaling techniques we have obtained the critical exponents and checked that those obey the well known algebraic relations.

Finally, we have analysed the meaning of universality in these systems by studying different QPTs we have verified that some of them share the same critical exponents and fall, therefore, in the same universality class.

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