# Phase transition in a model of bosons on a dynamic lattice

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The study of model of bosons on a dynamical lattice revealed presence of a new quantum phases of matter [1]. In this work we present our study of the commensurate Bond Order Wave ($\mathrm{cBOW}_{1/2}$) to super fluid (SF) phase transition. We find the ground states of the system with the use of DMRG method for finite non-periodic systems. We use staggered magnetisation as an order parameter that allows us to find distinct phases of the system. We find critical exponents and location of the phase transition with a use of finite scaling of fidelity susceptibility.

## I. INTRODUCTION

The model proposed in work of González-Cuadra et al. describes a minimal version of a Bose-Hubbard model on a dynamical lattice [1]. It is given by a Hamiltonian

$$\begin{aligned} H = &- t\sum_{\langle ij\rangle}(b_i^\dagger b_j + h.c.) + \frac{U}{2}\sum_i n_i(n_i-1) - \mu\sum_i n_i \\ &- \alpha\sum_i (b_i^\dagger \sigma_i^z b_j + h.c.) + \frac{\Delta}{2}\sum_i \sigma_i^z + \beta\sum_i \sigma_i^x. \end{aligned} \tag{1}$$

The first line of the equation (1) is a Bose-Hubbard Hamiltonian [...]. In the second line of the Hamiltonian there appears Pauli $\sigma$ operators. They corresponds to a two-level systems located in between each neighbouring bosonic systems, we call it a bond. States of bonds represent states of a lattice. The two-level bond system is the minimal model that is proposed to account for the lattice vibrational states.

Each two-level bond system is coupled to the neighbouring bosonic systems. The parameter $\alpha$ gives strength of that coupling, and affects the tunneling constant $t$ of the bosons. The parameter $\beta$ tells weather or not the bond states are inclined towards any orientation. When the $\beta/\alpha$ factor is large, bonds will be in the $|\downarrow\rangle$ state, and the opposite, they will be in the $|\uparrow\rangle$ state when the $(\beta/\alpha)^{-1}$ is large. The last term of the Hamiltonian is smaller in comparison to all the remaining ones, and it generates a quantum dynamics of the bond states.

One of the results of González-Cuadra et al. is that the ground-state phase diagram of such system exhibits phases called commensurate Bond Order Waves (cBOW) [1]. They can be characterised by an average density of boson per each bosonic system. Therefore one can distinguish $\mathrm{cBOW}_{1/2}$, $\mathrm{cBOW}_{1/3}$, and $\mathrm{cBOW}_{2/3}$ where subscript of the name indicates the average bosons density. On the phase diagram the cBOW phases are souronded by super fluid (SF) and solitionic (S) ones. In this work we study a phase transition between $\mathrm{cBOW}_{1/2}$ and SF phases that occurs when the parameter $\Delta$ is changing (is driving the transition).

To study a phase transition one needs to select an order parameter. To select the right one we take advantage of an important characteristic of the $\mathrm{cBOW}_{1/2}$ phase, namely, this phase poses a periodic structure both in bond and in bosonic states. Bond systems are interchangeably in $|\uparrow\rangle$, $|\downarrow\rangle$ states. Consequently as the order parameter we select a staggered magnetisation (sM)

$$sM = \frac{1}{L-1}\sum_i (i)^{-1}\langle\sigma_i^z\rangle, \tag{2}$$

where $L-1$ is a number of bonds in the studied system.

The order parameter is close to $\pm 1$ in the $\mathrm{cBOW}_{1/2}$ phase which indicates presence of the up-down bond pattern. And on contrary, when bonds are uniformly oriented the order parameter reaches 0. Therefore, staggered magnetisation is a desired order parameter that indicates breaking of the translation symmetry that occurs on the phase transition.

### A. Fidelity susceptibility

A zero temperature phase transition occurs when properties of a ground state of a system change drastically under small variation in one of the system parameters. Work of You et al. describes a method which allows to locate a quantum phase transition that is driven by a selected parameter of the system [2]. The cited work proposes fidelity susceptibility $\chi_{\mathrm{F}}$ as a tool to detect that sudden change. Fidelity susceptibility (FS) is defined as a limit

$$\chi_{\mathrm{F}}(\lambda) = \lim_{\delta\lambda\to 0}\frac{-2\ln F_i(\lambda,\delta\lambda)}{\delta\lambda^2}. \tag{3}$$

In this definition $\lambda$ is the parameter of a system that drives the phase transition. $F_i$ is a fidelity between ground states $|\Psi\rangle$ of a model that corresponds to values of the driving parameter $\lambda$ and $\lambda+\delta\lambda$

$$F_i(\lambda,\delta\lambda) = |\langle\Psi(\lambda)|\Psi(\lambda+\delta\lambda)\rangle|. \tag{4}$$

The usefulness of FS was extended in a later work by Gu et al. where it was shown that finite size scaling of that quantity allows to find critical exponent of the phase transition [3]. Gu et al. assumed that FS scales as

$$\chi_F(\Delta, L) = \frac{A}{L^{-\mu} + B(\Delta-\Delta_{\max})^\alpha}, \tag{5}$$

where $A$ and $B$ are constants, and $\Delta_{\max}$ is value of $\Delta$ for which FS reaches the maximum value. Such assumption allowed to find the finite size scaling relations for the peak of FS $\chi_F(\Delta_{\max}) \propto L^\mu$. Additionally, from the same assumption, it follows that a universal function for the

rescaled FS $[\chi_F(\Delta_{\max}) - \chi_F(\Delta)]/\chi_F(\Delta)]$ will be a function of $L^\nu(\Delta - \Delta_{\max})$. The universality become apparent for the value of $\nu$ at which the rescaled FS collapses onto a single curve for all system sizes.

The critical exponent $\alpha$ depends on the the two others as $\alpha = \mu/\nu$. It was also pointed out that the critical exponent $\alpha$ extracted with the use of this method can be greater by 1 from a tabular values as it corresponds to scaling of FS which is second order derivative of the the order parameter as opposed to specific heat (1st order derivative of energy) [3].

## II. METHODS AND COMPUTATIONAL DETAILS

We consider a model (1) composed of $L < \infty$ bosonic states and $L-1$ bond states arranged in a linear one dimensional lattice. With the use of a density matrix renormalisation group (DMRG) and representation of system states as matrix product states (MPS) we find the ground states of a studied model as a function of parameters of the system $|\Psi(t, U, \mu, \alpha, \beta, \Delta)\rangle$. All computations are done with a use of TeNPy library [4].

Throughout this work we use the tunneling constant of the Bose-Hubbard model equal to t = 1.0, and the bond-boson coupling constant equal to $\alpha = 0.5$. The $\text{cBOW}_{1/2}$ phase is present only for relatively small values of the $\beta$ parameter, for this reason we mostly focus on small values of $\beta$ parameter.

We study strong interaction between boson $U/t = 10.0$. In extreme case we study the $U/t \to \infty$ limit in a detail. For such case each bosonic state can be occupied by at most a single boson. Therefore when bosonic operators are replaced with fermionic ones ($a_i$) the Hamiltonian gives exactly the same dynamics

$$H = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + h.c.) - \mu\sum_i n_i - \alpha\sum_i(a_i^\dagger \sigma_i^z a_j + h.c.) + \frac{\Delta}{2}\sum_i \sigma_i^z + \beta\sum_i \sigma_i^x. \quad (6)$$

Most of the effects, that we observe, are driven by changes in the $\Delta$ parameter. The phase transition of interest occurs for values $\Delta \approx 0.9$.

We impose some restrictions on our computational method. First of them is motivated by the periodicity of $\text{cBOW}_{1/2}$ phase in its bosonic degrees of freedom. Throughout the whole phase the density of states remains the same and equal to 1/2. Taking advantage of this fact we restricted our space of possible solutions only to those that satisfy the bosonic density condition ($\rho = 0.5$), also in the neighbourhood of the $\text{cBOW}_{1/2}$ region which is already the SF phase. With this restriction we neglect the $\mu$ term in Hamiltonians, as its role reduces to contributing a constant to the system energy.

Another restriction, which is necessary in all computations that use an MPS representation of a state, is a maximal bond dimension D. This is a parameter that accounts for truncation of the space of possible solution. Luckily, there exists a convenient measure of the quality of our results in the truncated space. It is the entropy of entanglement $S_l$

$$S_l = -\text{tr}(\rho_l \log_2 \rho_l), \quad (7)$$

where $\rho_l = \text{tr}_{L-l}(|\Psi\rangle\langle\Psi|)$, where $L - l$ is a part of the chain that is limited to the $l$-th bosonic system [5]. The entropy of entanglement saturates (does not change when the value of bond dimension is increased) with an increase of bond dimension for gapped system with finite range interactions. We run computations only in the saturation region to assure that the quality of our results is reliable.

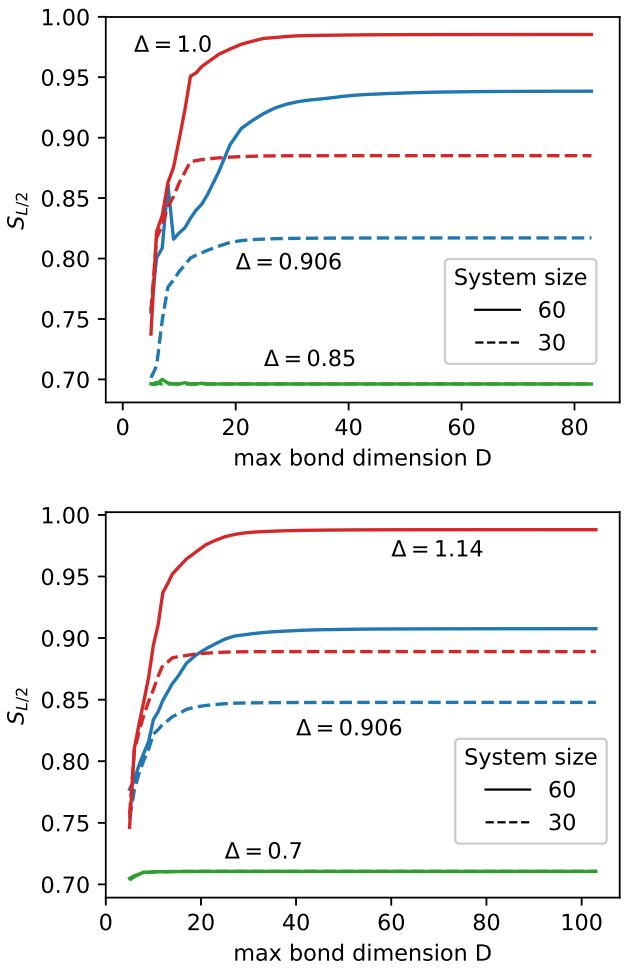



FIG. 1. Entanglement entropy at the middle of the chain as a function of the $\Delta$ parameter. Different colors represent different values of $\Delta$ parameter, different line styles corresponds to different lengths of bosonic chains. The top figure presents results for $U = \infty$ and $\beta = 0.02$ system (small dynamics of bonds). The picture in the middle represent more dynamic $\beta = 0.1$ system. The bottom picture shows results for $U = 10$ and $\beta = 0.02$.

TABLE I. Summary of critical parameter.

| System details | $\Delta_c$ | $\nu$ | $\mu$ | $\alpha = \mu/\nu$ |
|---|---|---|---|---|
| $U \to \infty, \beta = 0.02$ | 0.906(1) | 1.7(5) | 3.5 | 2.0(6) |
| $U \to \infty, \beta = 0.1$ | 0.887(1) | 0.28(5) | 1.2 | 4.0(8) |
| $U = 10, \beta = 0.02$ | 0.913(1) | 0.18(5) | 1.5 | 8(2) |

In order to find the saturation region we select several values of the $\Delta$ parameter that corresponds to both studied phases as well as to the region of a phase transition, then we run the DMRG computations for different values of the bond dimension D and finally we observe the behaviour of the entropy of entanglement at the middle of the chain $S_{L/2}$ as a function of D. Then in our computations we use the values of D for which entropy of entanglement is saturated in all regions, see Fig. 1.

We use the criterion of saturation of entropy of entanglement as our tool to quantify the reliability of the DMRG output. Additionally, we also observe the bond dimension dependence of values of observables (bosonic occupation number $\langle n_i \rangle$, bond state $\langle \sigma_i^z \rangle$) and the staggered magnetisation but these saturate faster than entropy of entanglement.

## III. RESULTS

We discriminate different phases of the studied systems with a use of staggered magnetisation $sM(\Delta)$. The region of $sM \approx 1$ corresponds to $\mathrm{cBOW}_{1/2}$ phase, whereas the region of $sM \approx 0$ is a SF phase. We find that for a wide range of system parameters ($U \geq 10, \beta \leq 0.1$) the ground state of the system undergoes a phase transition at a value of $\Delta$ parameter close to 0.9. We compare the $sM(\Delta)$ dependence for different system sizes ($30 \leq L \leq 60$) in Fig. 2, and we note that the curves do not cross at any point, which would be an early indication of a location of the phase transition. We find that in the $U \to \infty, \beta = 0.1$ system, the curves of staggered magnetisation surprisingly cross at $\Delta = 1.12$, but our later study of fidelity susceptibility rule out this point as a candidate for the location of a phase transition.

In order to find a critical value of the $\Delta_c$ parameter, at which there would occur a phase transition in a thermodynamic limit, we find the values of FS in the studied regions. In all studied system we observe a peak in FS at the region where the values of $sM$ indicate phase change of the ground state order, see Fig. 3.

The scaling of the peak gives an information about values of critical exponents that describe the phase transition. In all studied system the location of the peak moves towards smaller values of $\Delta$ (deeper into $\mathrm{cBOW}_{1/2}$ region) with an increase in a system size, see Fig. 3.

Scaling of the FS allows to find critical exponent $\mu$ for the studied phase transition. For all studied system its values were found and reported on Fig. 3.

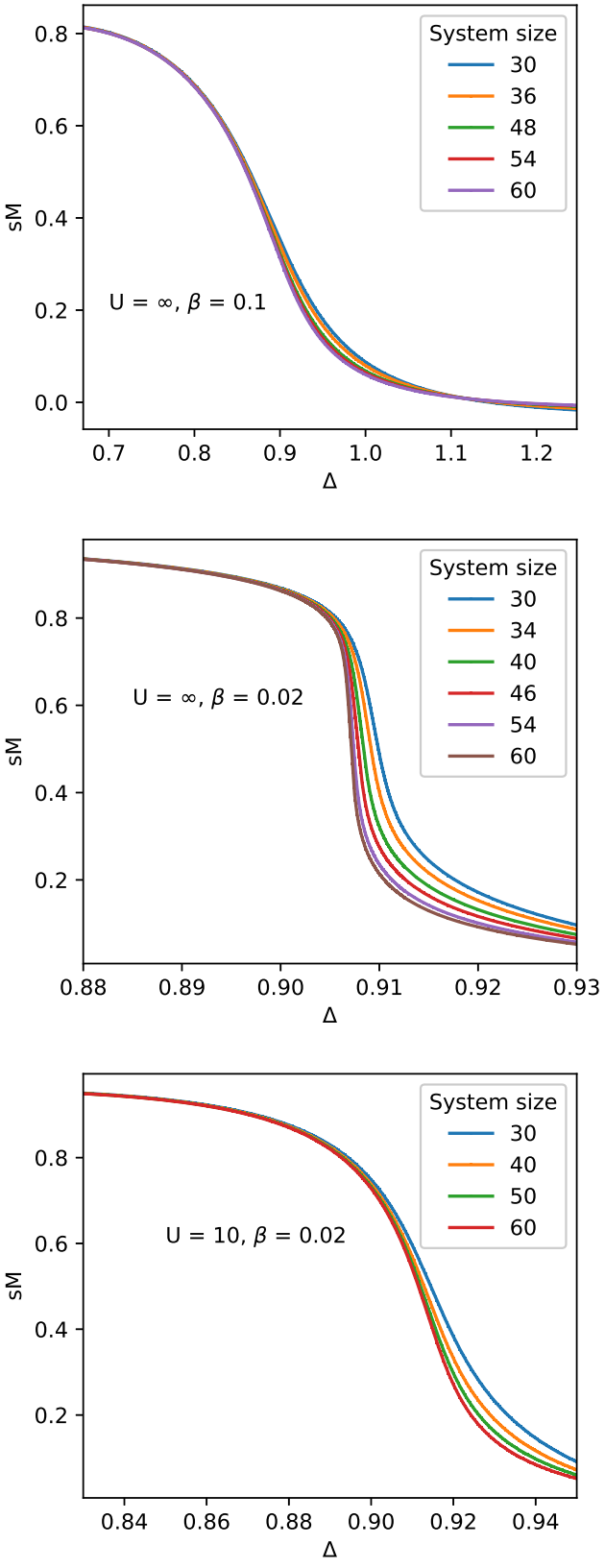
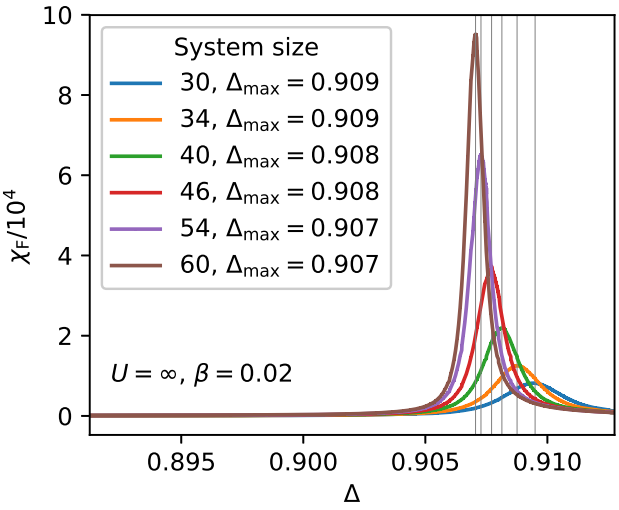
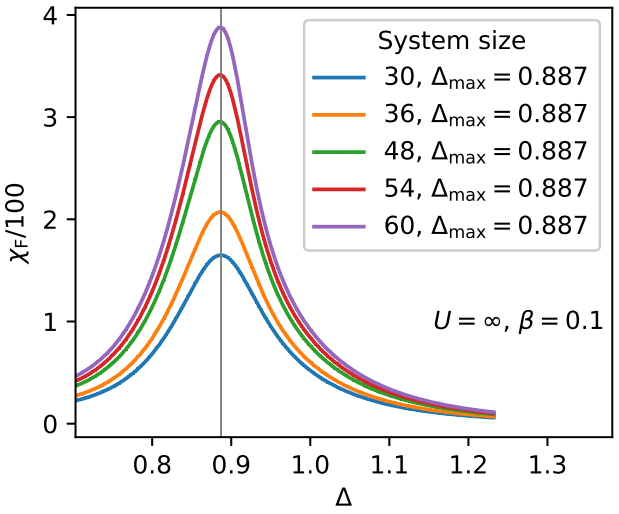



FIG. 2. Staggered magnetisation presentd as a function of the $\Delta$ parameter. Each graphics presents how does this dependence change when the system size increases. All graphics corresponds to systems described by parameters $\alpha = 0.5$, $t = 1.0$. None of the presented systems exhibits a crossing in the order parameter upon a change in the chain length.



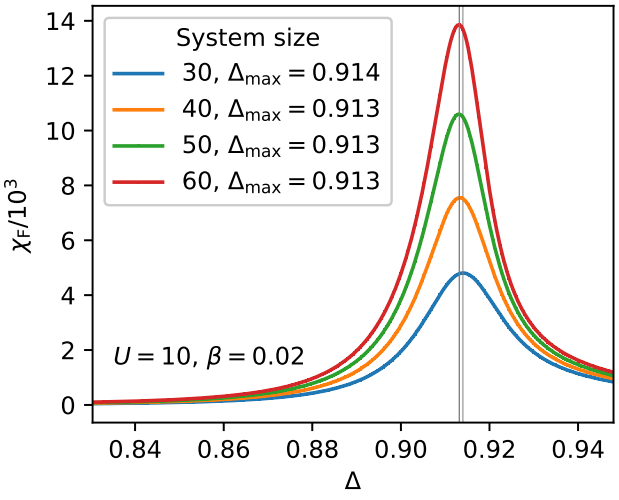
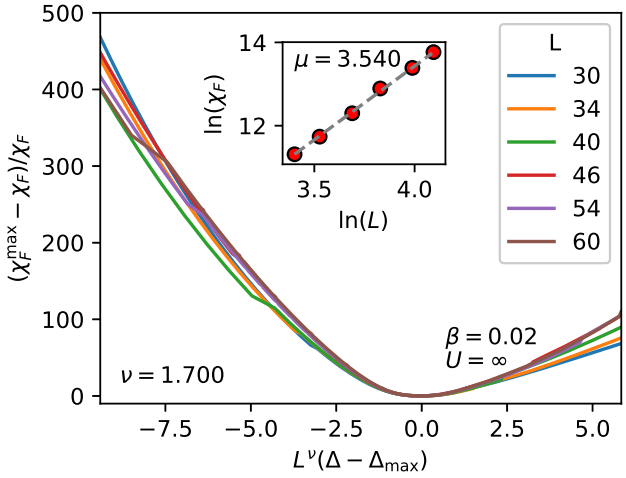
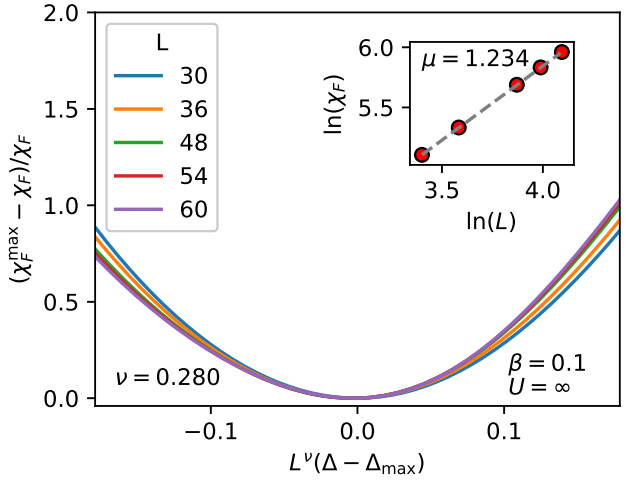




FIG. 3. Fidelity susceptibility $\chi_F$ as a function of the driving parameter $\Delta$. Vertical gray line indicate locations of FS peaks maxima $\Delta_{max}$. Note different scales.



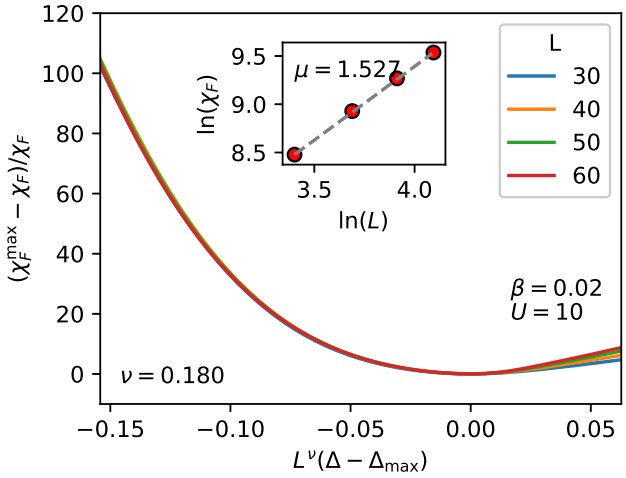




FIG. 4. Finite size scaling of fidelity susceptibility $\chi_F$. Lack of a good measure of the collapse of all curves leads to some significant obstacles with determination of the exact value of the critical exponents $\nu$, ones presented in the above graphics lie in the region were collapse is the most apparent.

We perform $1/L$ finite scaling analysis for the $\Delta_{\max}$ value to find the location of phase transition $\Delta_c$. Summary of the criticality in studied system is presented in Tab. I.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