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Cite as: AIP Conference Proceedings **2115**, 030016 (2019); <https://doi.org/10.1063/1.5112855>  
Published Online: 12 July 2019

Chetana G. F. Gaonker, B. K. Alavani, A. Das, and R. V. Pai



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# Spin-1 Bosons in optical superlattice

Chetana G.F. Gaonker<sup>1,a)</sup>, B. K. Alavani<sup>1</sup>, A. Das<sup>2</sup> and R. V. Pai<sup>1</sup>

<sup>1</sup>Department of Physics, Goa University, Taleigao Plateau, Goa 403206

<sup>2</sup>Department of Physics, Parvatibai Chowgule College of Arts and Science, Gogol, Margao, Goa 403602

a) physics.chetana@unigoa.ac.in

**Abstract.** In this paper, we analyze superfluid, insulator and various magnetic phases of ultracold spin-1 bosonic atoms in two-dimensional optical superlattices. Our studies have been performed using Cluster Mean Field Theory. Calculations have been carried out for a wide range of densities and the energy shifts due to the superlattice potential. We find superlattice potential do not change the symmetry of the polar superfluid phases. Superlattice potentials induce Mott insulator phases with half-integer densities. The phase diagram is obtained using superfluid density, nematic order and singlet density. Second order Rényi entanglement entropy is also calculated in different phases. The results show that Rényi entanglement entropy is large in the nematic Mott insulator phase.

## INTRODUCTION

Ultracold atoms in optical lattices and superlattices provide us with the realization of engineered quantum many-body lattice models [1]. One remarkable development in this context is the realization of Bose gases in the optical lattices. Superfluid (SF) to Mott Insulator (MI) quantum phase transition in cold bosonic atoms has received great scientific attention since its theoretical prediction in the context of Bose Hubbard model (BHM), and followed by its experimental realization [2-4]. When traps are purely optical, Alkali atoms like <sup>87</sup>Rb, <sup>23</sup>Na and <sup>30</sup>K, with hyperfine spin F=1, have spin degrees of freedom and thus, the interaction between bosons is spin-dependent [5]. The interaction is ferromagnetic (e.g. <sup>87</sup>Rb) or anti-ferromagnetic (e.g. <sup>23</sup>Na), depending upon scattering lengths of singlet and quintuplet channels [6]. The spin-dependent interaction in spinor gases exhibits richer quantum effects than their single-component counterparts and it not only modifies the nature of phase diagrams but also allows the study of superfluidity and magnetism.

The optical superlattices are obtained by super-imposition of two monochromatic lattices with slightly different wavelengths [7]. Manipulating the relative phase between the two standing waves and their respective depths independently, a periodic pattern of potential wells with two different depths at two adjacent sites is obtained. This difference in the depth of two adjacent sites is the measure of superlattice potential. In this report, we investigate spin-1 ultracold bosons loaded into 2-dimensional bi-chromatic optical superlattices.

## MODEL AND METHOD

The spin-1 Bose–Hubbard model, which describes spin full bosons in an optical superlattice, is given by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma}) + \frac{U_0}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{U_2}{2} \sum_i (\vec{F}_i^2 - 2\hat{n}_i) - \sum_i \mu_i \hat{n}_i, \quad (1)$$

where first term represents hopping of bosons between nearest neighbour sites  $\langle i, j \rangle$  with an amplitude  $t$ . Here  $a_{i,\sigma}$  ( $a_{i,\sigma}^\dagger$ ) represents annihilation (creation) operator at site  $i$  with spin projection  $\sigma = \{-1, 0, 1\}$ , number operator  $\hat{n}_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma}$  and  $\hat{n}_i = \sum_\sigma \hat{n}_{i,\sigma}$ . Spin operator  $\vec{F}_i = (F_i^x, F_i^y, F_i^z)$  where  $F_i^\alpha = \sum_{\sigma,\sigma'} a_{i,\sigma}^\dagger S_{\sigma,\sigma'}^\alpha a_{i,\sigma}$ , with  $\alpha = x, y, z$  and  $S_{\sigma,\sigma'}^\alpha$  are standard spin-1 matrices. Spin independent (dependent) interaction  $U_0$  ( $U_2$ ) arises due to the difference in the scattering length  $a_0$  and  $a_2$  in the spin S=0 and S=2 channels respectively. The spin dependent interaction  $U_2$  can be positive (anti-ferromagnetic) or negative (ferromagnetic) depending on the values of  $a_0$  and  $a_2$  [5]. The site dependent chemical potential  $\mu_i = \mu + (-1)^i \delta$  where  $\mu$  controls the bosons density and  $\delta$  is the shift in energy due to superlattice potential. Here, we consider a bi-chromatic superlattice and thus, the whole lattice is bipartite into A and B sub-lattices with  $\mu_A = \mu + \delta$  and  $\mu_B = \mu - \delta$ .

In the cluster mean-field theory [8], the entire lattice is divided into clusters with  $N_C$  number of sites. In this calculation we take  $N_C = 2$  and thus, each cluster consists of one site each from A and B sub-lattices. Decoupling each cluster from its nearest neighbor clusters using standard mean-field procedure [6,8,9], the model (1) is given by

$$\begin{aligned} \mathcal{H} &= \sum_{\text{clusters}} \mathcal{H}^C \\ \mathcal{H}^C &= -t \sum_{\sigma} (a_{A,\sigma}^\dagger a_{B,\sigma} + a_{B,\sigma}^\dagger a_{A,\sigma}) - 3t \sum_{\sigma} [(a_{A,\sigma}^\dagger + a_{A,\sigma})\psi_{B,\sigma} + (a_{B,\sigma}^\dagger + a_{B,\sigma})\psi_{A,\sigma} - 2\psi_{A,\sigma}\psi_{B,\sigma}] \\ &\quad + \frac{U_0}{2} \sum_{i=A,B} \hat{n}_i(\hat{n}_i - 1) + \frac{U_2}{2} \sum_{i=A,B} (\hat{F}_i^2 - 2\hat{n}_i) - \sum_{\sigma} (\mu_A \hat{n}_{A,\sigma} + \mu_B \hat{n}_{B,\sigma}). \end{aligned} \quad (2)$$

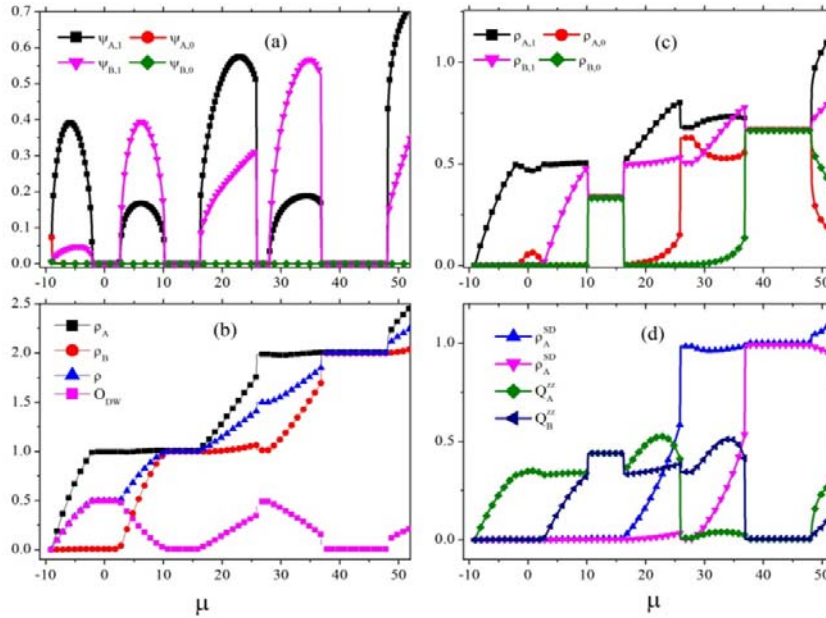
Here  $\psi_{A,\sigma} = \langle a_{A,\sigma} \rangle$  ( $\psi_{B,\sigma} = \langle a_{B,\sigma} \rangle$ ) is the A (B) sub-lattice superfluid order parameter with spin component  $\sigma$ . We determine  $\psi_{A,\sigma}$  and  $\psi_{B,\sigma}$  self-consistently using the method described in Ref. [8]. Sub-lattice superfluid densities  $\rho_{A(B)}^S = \sum_{\sigma} |\psi_{A(B),\sigma}|^2$  and densities of bosons  $\rho_{A(B)} = \langle \hat{n}_{A(B)} \rangle$  are calculated from this self-consistently determined ground state. We also calculate the average density of bosons  $\rho = \frac{1}{2}(\rho_A + \rho_B)$  and the density wave order parameter  $O_{DW} = |\rho_A - \rho_B|$ . We can characterize the ground state of model (1) from these quantities. The ground state is a superfluid (Mott insulator) if  $\rho_{A(B)}^S$  is non-zero (zero). The magnetic properties of the superfluid and Mott insulator phases are determined from Nematic order parameter  $Q_{A(B)}^{\alpha,\alpha} = \langle (F_{A(B)}^\alpha F_{A(B)}^\alpha - \frac{1}{3} \langle \hat{F}_{A(B)}^2 \rangle) \rangle$  [10] and singlet pair density  $\rho_{A(B)}^{SD} = \langle \hat{A}_{A(B)}^\dagger \hat{A}_{A(B)} \rangle$ , where the singlet creation operator  $\hat{A}_{A(B)}^\dagger = (2a_{A(B),1}^\dagger a_{A(B),-1}^\dagger - a_{A(B),0}^\dagger a_{A(B),0}^\dagger)$ . In addition to these quantities, we also investigate entanglement properties [10] of different ground states by calculating Rényi entanglement entropy (EE) [11] given by  $S_2[A(B)] = -\log(\text{Tr}(\rho_{A(B)}^2))$  where  $\rho_{A(B)}$  is the reduced density matrix for sub-lattice A (B).

## RESULTS

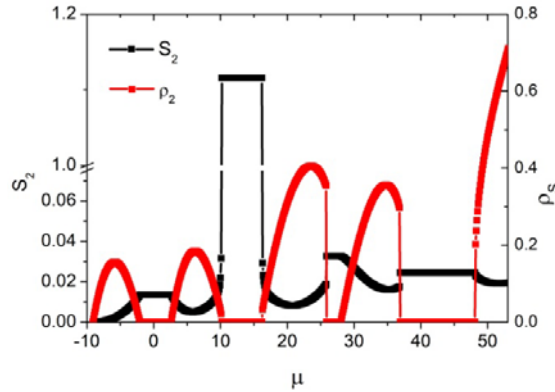
We now present the results of the Cluster Mean Field Theory applied to 2-dimensional spin-1 Bose Hubbard model in bi-chromatic superlattice, with cluster size  $N_C = 2$ . Here we restrict ourselves to the anti-ferromagnetic case  $U_2 > 0$ . We set our energy scale by choosing  $t=1$  and thus all parameters are dimensionless. It is known from the earlier studies that, for the anti-ferromagnetic case ( $U_2 > 0$ ), the symmetry the superfluid phase is polar (PSF) [8] and in the mean-field level symmetry restricts values of the superfluid order parameters such that either  $\psi_{A(B),1} = \psi_{A(B),-1} \neq 0$ ,  $\psi_{A(B),0} = 0$  or  $\psi_{A(B),1} = \psi_{A(B),-1} = 0$  and  $\psi_{A(B),0} \neq 0$  [8]. Superfluid order parameters are plotted in the Fig. 1(a) for  $U_0 = 30$ ,  $U_2 = 0.03U_0$  and superlattice potential  $\delta = 6$ . It is evident from the Fig. 1(a) that the superfluid phases have polar symmetry: we find  $\psi_{A(B),1} = \psi_{A(B),-1} \neq 0$  and  $\psi_{A(B),0} = 0$  and thus, superlattice potential do not change this symmetry. There are four regions in the chemical potentials where  $\psi_{A(B),\sigma} = 0$  thus, correspond to four insulator phases. The sublattice bosons densities  $\rho_A$  and  $\rho_B$ , the average boson density  $\rho = \frac{1}{2}(\rho_A + \rho_B)$  and the density wave order parameter  $O_{DW}$  are plotted in the Fig. 1(b). The four insulator regions have average densities  $\rho = \frac{1}{2}, 1, \frac{3}{2}$  and 2 with sublattice densities  $(\rho_A, \rho_B) = (1, 0), (1, 1), (2, 1)$  and  $(2, 2)$ , respectively. Insulators with the density  $\rho = 1$  and 2 are the normal Mott insulators where the density is uniform across whole lattice and  $O_{DW} = 0$ . However, insulators with  $\rho = \frac{1}{2}$  and  $\frac{3}{2}$  have finite  $O_{DW}$  and are called density wave insulators. Thus, the superlattice potential introduces additional insulator phases with half-integer bosons densities. The sublattice bosons densities with different spin component  $\rho_{A(B),\sigma}$  are plotted in the Fig. 1(c). In general, we find  $\rho_{A(B),\pm 1} > \rho_{A(B),0}$  except in the Mott insulator region, i.e., for  $\rho = 1$  and 2, we find  $\rho_{A,\pm 1} = \rho_{A,0} = \rho_{B,\pm 1} = \rho_{B,0}$ . It should be noted here that the symmetry of the polar superfluid phase is such that  $\psi_{A(B),1} = \psi_{A(B),-1} \neq 0$  and  $\psi_{A(B),0} = 0$ . This imply that the bosons with spin component  $\sigma = 0$ , though present in the system are not in the superfluid phase. Only bosons with spin component  $\sigma = \pm 1$  form superfluid. This leads to a situation where we have a two-fluid model with bosons with  $\sigma = \pm 1$  are in superfluid phase while bosons with  $\sigma = 0$  are in the normal fluid phase. Magnetic properties of the superfluid and the insulating phases are given in the Fig. 1(d) where we plot Nematic order parameter  $Q_{A(B)}^{z,z}$  and singlet pair density  $\rho_{A(B)}^{SD}$ . We find that density  $\rho = 2$  Mott insulator phase is a singlet phase with  $\rho_A^{SD} = \rho_B^{SD} = 1$  and  $Q_A^{z,z} = Q_B^{z,z} = 0$ . The density  $\rho = 1$  Mott insulator phase, however, is nematic  $Q_A^{z,z} = Q_B^{z,z} > 0$  and  $\rho_A^{SD} = \rho_B^{SD} = 0$ . In

$\rho = \frac{1}{2}$  density wave insulator, the sublattice boson densities are  $(\rho_A, \rho_B) = (1, 0)$ . In this phase we find  $Q_A^{z,z} > 0$ ,  $Q_B^{z,z} = 0$  and  $\rho_A^{SD} = \rho_B^{SD} = 0$ . In the  $\rho = \frac{3}{2}$  density wave insulator, however,  $Q_B^{z,z} > 0$ ,  $Q_A^{z,z} = 0$  and  $\rho_A^{SD} = 1$ ,  $\rho_B^{SD} = 0$ . So, in the  $\rho = \frac{3}{2}$  density wave insulator, A-sublattice is in the singlet phase and B-sublattice is in the nematic phase, whereas in the  $\rho = \frac{1}{2}$  density wave insulator, A-sublattice is in the nematic phase. We present the results for Rényi EE in Fig. 2. In general, we find  $S_2[A] = S_2[B]$  and are very small except in the  $\rho = 1$  Mott insulator where  $S_2$  is two orders of magnitude larger.  $S_2$  is constant in insulating phases and vary with chemical potential in polar superfluid phases.

We plot the phase diagram of model (1) for  $\delta = 6$  and 10 in Fig. 3(a) and (b) respectively. There are four insulating phases represented by lobes. The dotted lines represent phase diagram for  $\delta = 0$  where there are only two lobes correspond to  $\rho = 1$  and 2 Mott insulator phases. As we introduce the superlattice potential, these two Mott phases shrink and two additional density wave insulating phases form with average density  $\rho = \frac{1}{2}$  and  $\frac{3}{2}$ . We also observed that these density wave insulator lobes enlarge with superlattice potential.



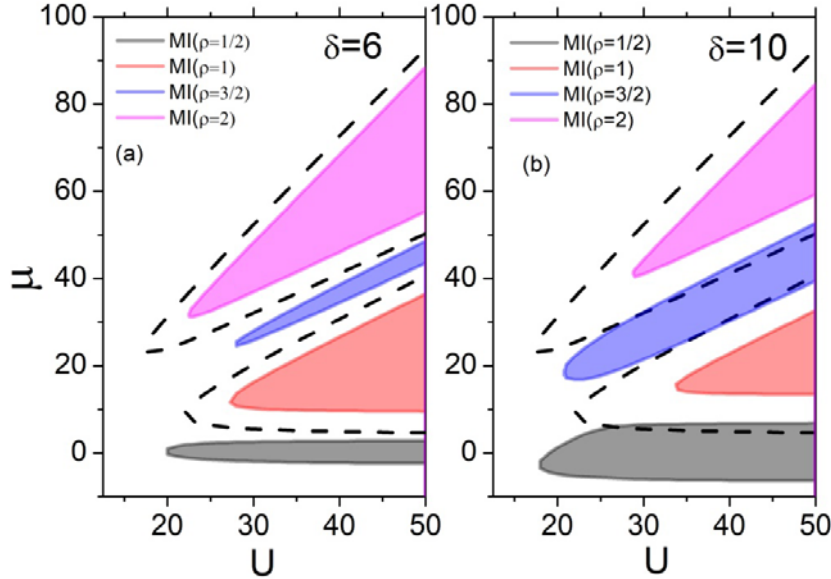
**FIGURE 1.** (Colour online) (a) Superfluid order parameters, (b) densities and density wave order parameters, (c) densities with spin component  $\sigma$  and (d) nematic order and singlet pair density are plotted as a function of chemical potential  $\mu$  for  $U_0 = 30$ ,  $U_2 = 0.03U_0$  and  $\delta = 6$ .



**FIGURE 2.** (Colour online) Rényi EE  $S_2$  and superfluid density  $\rho_S$  are plotted as a function of chemical potential  $\mu$  for  $U_0 = 30$ ,  $U_2 = 0.03U_0$  and  $\delta = 6$ .

## CONCLUSION

In our present work, we use the cluster mean field theory to study the behavior of spin-1 bosons in the optical superlattices. Since intra-site fluctuations are treated exactly in CMFT, it permits us to study the magnetic and the superfluid properties of the system simultaneously. Our investigation primarily focused on the anti ferromagnetic case ( $U_2 > 0$ ). We conclude that, in bi-chromatic superlattices, the introduction of superlattice potential favours the localisation of the bosons and this leads to density wave Mott insulators. When  $\delta = 0$ , we have uniform superfluid and Mott insulator phases. As  $\delta$  increases, the uniform Mott insulator lobes shrink while the half integer density wave insulator lobes enlarge. The symmetry of the superfluid phase remains unaffected by the superlattice potential. We have also studied the magnetic properties of insulating phases as well as calculated Rényi EE. We found that the  $\rho = 1$  Mott lobe is nematic, and  $\rho = 2$  lobe a singlet. The magnetic property of the density wave insulator, however, depends on the sub-lattice density. Rényi EE remains mostly small except at density  $\rho = 1$  Mott insulator and could be used as a marker of the transition.



**FIGURE 3.** (Colour online) Phase diagram of model (1) for (a)  $\delta = 6$  and (b)  $\delta = 10$ . The coloured lobes are insulating phases and rest of the region is polar superfluid. The dashed line represent the phase diagram for  $\delta = 0$ .

## ACKNOWLEDGMENTS

This work is supported by UGC Grant F. No. 43-520/2014/(SR) and DSTE Goa. BKA acknowledges UGC-BSR fellowship.

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