Magnetic phase transition in coherently coupled Bose gases in optical lattices

L. Barbiero, M. Abad and A. Recati

Dipartimento di Fisica e Astronomia "Galileo Galilei", Università di Padova, 35131 Padova, Italy
INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, 38123 Povo, Italy

We describe the ground state of a gas of bosonic atoms with two coherently coupled internal levels in a deep optical lattice in a one dimensional geometry. In the single-band approximation this system is described by a Bose-Hubbard Hamiltonian. The system has a superfluid and a Mott insulating phase which can be either paramagnetic or ferromagnetic. We characterize the quantum phase transitions at unit filling by means of a density-matrix renormalization group technique and compare it with a mean-field approach. The presence of the ferromagnetic Ising-like transition modifies the Mott lobes. In the Mott insulating region the system maps to the ferromagnetic spin-1/2 XXZ model in a transverse field and the numerical results compare very well with the analytical results obtained from the spin model. In the superfluid regime quantum fluctuations strongly modify the phase transition with respect to the well established mean-field three dimensional classical bifurcation.

PACS numbers: 75.10.Pq, 05.10.Cc, 05.30.Jp, 03.75.Lm

Ultra-cold atoms in optical lattices have opened new possibilities to study quantum phase transitions [1] and to observe the effects of quantum fluctuations [2, 3]. Recent experimental advances have also paved the way to the investigation of quantum magnetism, notable examples being the demonstration of super-exchange interactions in bosonic gases [4], the time-evolution of spin impurities [5, 6], and the engineering of Ising [7] and anisotropic exchange Hamiltonians [8, 9]. On the other hand cold atoms are also very suitable to study coherence phenomena related to the control of the coupling between internal levels of atomic species. One can obtain coherently coupled superfluids, which show many interesting features ranging from a classical bifurcation transition in internal Josephson effect [10] to dimerization of half-vortices in rotating superfluids [11, 12].

In this Letter we combine the two ingredients by studying coherently coupled Bose gases trapped in a one-dimensional (1D) optical lattice at unit filling. Depending on the relative strengths of the coherent coupling (or phase coupling) and the density couplings due to species-dependent two-body interactions the system exhibits superfluid (SF) or Mott-insulating (MI), non-polarized/paramagnetic (NP) or polarized/ferromagnetic (FM) phases. We will characterize in detail the phase diagram by combining mean-field and density matrix renormalization group (DMRG) approaches [13], and by mapping to spin chain Hamiltonians. The interest in such a system is manyfold since it allows for the study of different topics such as: the role of quantum fluctuations due to confinement and interaction in the NP-FM bifurcation in the superfluid regime; the change of the lobes in the SF-MI transition, which in 1D (at constant integer density) is of the Berezinskii-Kosterlitz-Thouless (BKT) type [14, 15]; the Ising-like ferromagnetic transition in the MI phase; and the possible simulation of a ferromagnetic XXZ chain in a transverse field. Moreover, the model Hamiltonian we use is relevant for ladder chain models in presence of a density-density interaction between the particles on different chains (see [17, 18], where the incommensurate filling case is studied), which has not been as much studied as the case of non-interacting chains (see, e.g., [19] and references therein).

We consider a dilute Bose gas confined in a 1D geometry with two hyperfine levels that are coherently coupled. The atoms feel a deep optical lattice which is the same for the two internal levels. The system can be described by a two-component single-band Bose-Hubbard Hamiltonian with a linear coupling between the two species:

\[
H = \sum_i \left\{ \sum_{\sigma} \left[ -\mu \hat{n}_{i\sigma} + \frac{U}{2} \hat{n}_{i\sigma}(\hat{n}_{i\sigma} - 1) \right] + U_{ab}\hat{n}_{i\sigma}\hat{n}_{ib} + J_{1}(\hat{a}_{i\sigma}^{\dagger}\hat{b}_{i} + \hat{a}_{i}\hat{b}_{i}^{\dagger}) \right\} - \frac{J}{2} \sum_{<ij>,\sigma} (\hat{a}_{i\sigma}^{\dagger}\hat{a}_{j} + \hat{b}_{i}^{\dagger}\hat{b}_{j} + H.c.)
\]

(1)

where \(\sigma = a, b\) is the index distinguishing the two (pseudo-spin) internal levels, \(\hat{a}_{i}, \hat{b}_{i}\) are the corresponding annihilation operators on the lattice site \(i\) and \(\hat{n}_{i\sigma}\) is the number operator. The chemical potential term, \(\mu\), fixes the total number of atoms \(N\), which we take to be equal to the number of lattice sites \(L\) (unit filling). The interaction terms \(U\) and \(U_{ab}\) represent on-site intra- and interspecies two-body interactions, respectively, while \(J_{1}\) is the strength of the conversion from one internal level to the other. Finally, the hopping with strength \(J\), limited to nearest neighbors \(<i,j>\), represents the kinetic energy in the lattice. In this Letter we restrict for the sake of clarity to equal intra-species interactions and equal hopping for both components. Equal hopping is also the typical situation in ultra-cold gases experiments.

The presence of the linear coupling \(J_{1}\) makes the system very different from the much studied Bose-Bose mixtures [20, 21]. Shortly in the latter case one has two \(U(1)\)
symmetries (related to the conservation of the atom number in each species, being $J_\Omega = 0$, and broken in the SF regime) and when the interspecies interaction is $U_{ab} > U$ the mixture phase separates [24]. In the presence of the interchange term only one $U(1)$ symmetry is left, the system is always miscible and if $U_{ab}$ is large enough a $\mathbb{Z}_2$ symmetry is broken bringing the system in a FM state. Notice also that the miscible-immiscible transition for mixtures (phase separation) is of the first order kind.

In the absence of hopping, $J = 0$, the ground state of Hamiltonian Eq. (1) is $|0\rangle = \prod_i c_i^\dagger |\text{vac}\rangle$, where $|\text{vac}\rangle$ is the vacuum of particles and we have introduced the operators $c_i^\dagger = (\hat{a}_i^\dagger - \hat{b}_i^\dagger)/\sqrt{2}$ creating a particle in site $i$ in the anti-symmetric state of the internal levels $a$ and $b$ (dressed state). In order to have unit filling factor the coordination number is $z = \frac{4}{3}$ in 1D. Notice that in the SU(2) symmetric case for the interaction, $U_{ab} = U$, the single component result is recovered provided the chemical potential is rescaled to $\tilde{\mu} = \mu - J_\Omega$. When the hopping strength $J$ becomes larger than that given by Eq. (2) the system enters the SF phase and develops a nonzero order parameter given by $\psi_\sigma = (\psi, -\psi)^T/\sqrt{2}$, with $\psi = |a\rangle = |b\rangle$. Since quantum fluctuations are neglected the MI phase is described by the state $|0\rangle$ introduced above. Therefore, the system could support a polarized state only in the SF regime provided $U_{ab}$ was large enough, in analogy to coupled condensates (see, e.g., the experiment reported in [10] and references therein).

The structure of the mean-field Mott lobes given by Eq. (2) is shown as dashed lines in Fig. 1 for different values of $U_{ab}$. There are a number of features in the structure of the lobes to be noticed: the lower border equals $-J_\Omega/U$ for all values of $U_{ob}/U$ and the upper border converges at $1 + J_\Omega/U$ for $U_{ab} > U$: as $U_{ab}/U$ is increased, the lobes saturate at a maximum value of $J/U$, a feature that also takes place in mixtures. Moreover at fixed $U$ one has, as expected by the change in the compressibility, that for $U_{ab} < U$ the insulating region is smaller than in the single component case, while for $U_{ab} > U$ the insulating region is enlarged.

Although the mean-field approach gives in some aspects a reasonable description of the Mott to superfluid transition of Hamiltonian (1), especially in two and three dimensions (see, for instance, [25]), it fails completely to describe the ground state of the system regarding its polarization in the MI region. Indeed the Hamiltonian Eq. (1) allows for states breaking a $\mathbb{Z}_2$ symmetry, creating a finite polarization $S_z = (N_a - N_b)/2N$, with $N_\sigma$ the number of atoms in state $\sigma = a, b$. The NP-FM transition in coherently coupled Bose gases has been studied in the continuum and within mean-field description of the SF phase mainly by means of coupled Gross-Pitaevskii equations (for a recent discussion see, e.g., [26] and references therein). This transition has been quite recently also characterized experimentally [10]. In terms of the Hubbard parameters one expects a transition from a NP to a FM state at $U_{ab} - U = 2J_\Omega/n$, with $n = 1$ the total density of the system. The critical exponent of the magnetization is in this case the expected mean-field value $\beta = 1/2$.

When the system becomes strongly interacting the fluctuations of the number of atoms in each site are reduced and therefore the effect of the two-body interaction is reduced, making the polarized state less favorable. In particular in the deep MI phase ($J \ll U, U_{ab}$) the single particle tunneling is suppressed and exchange of atoms is the dominant process. In this case the coherently cou-
plesed Bose-Hubbard model Eq. (1) can be mapped into a spin chain model (see, e.g., [20, 21]). In our case the effective spin Hamiltonian is the so-called spin-1/2 XXZ model in a transverse field (see, e.g., [27]), which reads

\[ H_{XXZ} = -t \sum_i (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z) + 2J_\Omega \sum_i \hat{S}_i^z, \]

where \( \hat{S}_i^z = (\hat{n}_{ia} - \hat{n}_{ib})/2, \hat{S}_i^+ = (\hat{a}_i^\dagger \hat{b}_i + \hat{a}_i \hat{b}_i^\dagger)/2, \hat{S}_i^- = -i(\hat{a}_i^\dagger \hat{b}_i^\dagger - \hat{a}_i \hat{b}_i)/2, \) \( t = 4J^2/U_{ab} \) and \( J_\Omega = 2U_{ab}/U - 1 \) is the anisotropy. Since we are considering repulsive on-site interactions we are restricted to \(-1 < \Delta < +\infty\). In such parameter range the spin model Eq. (2) exhibits only two phases, a paramagnetic phase with magnetization along the x-axis and an Ising ferromagnetic phase along the z-axis. For \( J_\Omega = 0 \) the model is exactly solvable and the transition occurs at \( \Delta = 1 \), i.e., \( U_{ab} = U \). For \( J_\Omega \neq 0 \) the transition is shifted to larger values of \( U_{ab}/U \). On the other hand for \( U_{ab} \to \infty \) the Hamiltonian reduces to the Ising model in a transverse field (ITF) which is also exactly solvable and predicts a transition at \( t\Delta = 4J_\Omega \), i.e., for \( 2J^2 = U_{ab} \), with a critical exponent \( \beta = 1/8 \).

Neglecting the effect of the Heisenberg term (valid when \( J \gg U_{ab} \)), the phase transition is driven by the ITF term. The accuracy \( \Omega_{max} \) as a function of \( J/U \) for the polarized system. Also, in this case the Mott insulating lobes do no longer depend on the value of \( U_{ab} \), since in the ferromagnetic phase this interaction is less effective. This saturation of the Mott lobes for \( U_{ab} \) large has a completely different meaning from the saturation found in the mean-field analysis.

Let us better characterize the FM transition in the MI regime by changing \( J_\Omega \), as reported in the top panel of Fig. 3. As described above in the Mott phase for \( J_\Omega \to 0 \) the system is equivalent to the XXZ model, which gives the FM transition at \( U_{ab}/U = 1 \). For \( J_\Omega \neq 0 \) the transition is shifted to larger values of \( U_{ab}/U \). One can obtain an approximation to the critical condition by noticing that Hamiltonian Eq. (4) can be rewritten as a Heisenberg exchange term, \( \sum S_i \cdot \hat{S}_{i+1} \), plus an ITF term. Neglecting the effect of the Heisenberg term (valid for \( U_{ab} > U \)), the phase transition is driven by the ITF and it takes place at \( t(\Delta - 1) = 4J_\Omega \). The accuracy of this expression with respect to the numerical solution of Hamiltonian Eq. (1) is shown in the bottom panel of Fig. 2 where it is seen to be very good for a range of values of \( J_\Omega \). Such results justify the use of the spin model to address the magnetic properties of Bose gases in optical lattices also for not too small values of \( J/U \).

While \( S_z \) is the global order parameter, we characterize the NP and FM phases, and in particular the NP-FM transitions in 1D. In order to study the breaking of the \( S_2 \) symmetry in Hamiltonian (1) we first of all determine the global polarization (or magnetization), \( S_z \). Special attention has to be paid here, especially in the superfluid phase, to allow for a sufficiently large size of the Hilbert space. That is, we need to consider an on-site basis containing the states corresponding to a number of bosons up to \( n_{max} \), to allow the fluctuations of \( a \) and \( b \) to explore the relevant configurations and thus to drive the phase transition. We obtain convergence of the results for open boundary conditions using \( n_{max} = 6 \), keeping up to 512 DMRG states and 6 sweeps [13], getting a truncation error lower that \( 10^{-8} \). Unless otherwise stated we show the results for a chain with \( L = N = 80 \) [29].

The results for the absolute value of the polarization \( |P| \) as a function of \( J/U \) are reported in the bottom panel of Fig. 1. In the SF phase (corresponding to \( U_{ab}/U = 1.8 \) ) the system has strong quantum fluctuations. The transition occurs for an inter-species interaction larger (but still of the same order) than the one predicted for a mean-field coherent state, i.e., \( U_{ab}/U = 1.2 \) and the magnetization does not follow the classical bifurcation law. In the Mott phase, where the double occupancy is strongly suppressed, the inter-species interaction has to be much stronger, e.g., \( U_{ab}/U = 6 \) and \( U_{ab}/U = 20 \), to drive the phase transition. For increasing values of \( U_{ab} \) the transition point is seen to approach a limiting value of \( J \) corresponding to the value given by the ITF mapping discussed above.

Moreover, it can be noticed from the figure that once the magnetic phase transition has taken place inside the lobe (see for instance the case \( U_{ab}/U = 20 \) ) the latter shrinks slightly, indicating that the SF phase is more favorable than the MI for the polarized system. Also, in this case the Mott insulating lobes do no longer depend on the value of \( U_{ab} \), since in the ferromagnetic phase this interaction is less effective. This saturation of the Mott lobes for \( U_{ab} \) large has a completely different meaning from the saturation found in the mean-field analysis.
transition, also by determining the behavior of the correlation functions around the phase transition point. We study the longitudinal and the transverse spin-spin correlation functions $C_s(i) = \langle S_j^s S_{i+j}^s \rangle$ with $s = x, z$. In order to drop boundary effects we exclude the more external sites and evaluate the correlation functions only in the central region of the system (in particular we take $j = 15$).

To have an idea of how the large distance behavior of the correlation functions change along the transition, we plot in the top panel of Fig. 3 the correlation functions for a separation $i = 50$ as a function of $J/U$. The paramagnetic phase is dominated by transverse spin correlations since in this regime $J_0$ is the most important term, while in the ferromagnetic phase the longitudinal correlations become dominant. Notice that the magnetic transition (see Fig. 1) seems to be well described by the crossing point between the long-range values of $C_x$ and $C_z$.

The longitudinal correlation function across the NP-FM transition is shown in the lower panels of Fig. 3 in the superfluid ($U_{ab}/U = 1.8$, left panel) and in the MI phase ($U_{ab}/U = 6$, right panel). The behavior of $C_z$ changes from an exponential decay in the paramagnetic phase to long-range order in the FM phase. The transition point is in good agreement with the one obtained with $S_z$ (Fig. 1). Notice that in the SF phase the system polarizes more “slowly” than in the insulating case due to strong fluctuations, which explains the larger region of intermediate decays.

In summary, the system we have studied, described by Eq. (1), constitutes a yet unexplored system in the family of Bose-Hubbard Hamiltonians. It is fundamentally different from Bose-Bose mixtures and in a way a generalization of two-leg chains. The system shows two quantum phase transitions: superfluid to Mott insulator transition — which is of the of the Berezinskii-Kosterlitz-Thouless kind at fixed integer density — and a paramagnetic/non-polarized to ferromagnetic/polarized transition. The latter changes the structure of the Mott lobes. In the Mott regime the transition is well described in terms of a quantum XXZ model in a transverse field. In the SF regime due to quantum fluctuations strong corrections to the mean-field coherent results are present. While we focused on the unit filling factor case, at low filling factor, the system is also interesting, especially considering that its experimental realization should be feasible within current technology as shown in [31]. Indeed in the small $J/U$ case both species $a$ and $b$ have a fermionic (Tonks-Girardeau regime) equation of state [31]. Therefore one has the possibility to study the fate of itinerant ferromagnetism in one dimension in analogy to the recent analysis in [32] with the inclusion of the linear interspecies coupling $J_0$.

Acknowledgement. Usef ul discussions with Tommaso Roscilde and Yan-Hua Hou are acknowledged. This work has been supported by ERC through the QGBE grant and by Provincia Autonoma di Trento. L.B. acknowledges support by Cariparo Foundation (Eccellenza grant 11/12) and the CNR-INO BEC Center in Trento for CPU time.

* Electronic address: barbiero@pd.infn.it
[1] *Quantum Phase Transitions*, S. Sachdev (Cambridge University Press, 1999).
[2] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[3] M. A. Cazalilla, R. Citro, T. Giamarchi, E. Orignac, M. Rigol, Rev. Mod. Phys. **83**, 1405 (2011).
[4] M. Anderlini, P. J. Lee, B. L. Brown, J. Sebby-Strabley, W. D. Phillips and J. V. Porto, Nature **448**, 452 (2007).
[5] J. Catani, G. Lamporesi, D. Naik, M. Gring, M. Inguscio, F. Minardi, A. Kantian, and T. Giamarchi, Phys. Rev. A **85**, 023623 (2012).
[6] T. Fukuhara *et al.*, Nat. Phys. **9**, 235 (2013).
[7] J. Simon, W. S. Bakr, R. Ma, M. E. Tai, P. M. Preiss and M. Greiner, Nature **472**, 307 (2011).
[8] D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, T. Esslinger, Science **340**, 1307 (2013).
[9] T. Fukuhara, P. Schauss, M. Endres, S. Hild, M. Cheneau, I. Bloch, and C. Gross, Nature **502**, 76 (2013).
[10] T. Zibold, E. Nicklas, C. Gross, and M. K. Oberthaler, Phys. Rev. Lett. 105, 204101 (2010).
[11] D. T. Son and M. A. Stephanov, Phys. Rev. A **65**, 063621 (2002).
[12] K. Kasamatsu, M. Tsubota and M. Ueda, Phys. Rev. Lett. **91**, 150406 (2003).
[13] S.R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[14] M. P. A. Fisher, P. B. Weichman, G. Grinstein, D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
[15] T. D. Kuhner and H. Monien, Phys. Rev. B **58**, R14741 (1998).
[16] T. D. Kuhner, S. R. White and H. Monien, Phys. Rev. B **61**, 18 (2000).
[17] P. Lecheminant and H. Nonne, Phys. Rev. B **85**, 195121 (2012).
[18] E. Orignac and T. Giamarchi, Phys. Rev. B **57**, 11713 (1998).
[19] I. Danshita, J. E. Williams, C. A. R. Sá de Melo, and C. W. Clark, Phys. Rev. A **76**, 043606 (2007).
[20] A. B. Kuklov and B. V. Svistunov, Phys. Rev. Lett. **90**, 100401 (2003).
[21] L.-M. Duan, E. Demler, and M. D. Lukin, Phys. Rev. Lett. **91**, 090402 (2003).
[22] T. Ozaki, I. Danshita, and T. Nikuni, [arXiv:1210.1370](http://arxiv.org/abs/1210.1370) (2012).
[23] E. Altman, W. Hofstetter, E. Demler, and M. D. Lukin, New J. Phys. **5**, 113 (2003).
[24] T. Mishra, R. V. Pai and B. P. Das, Phys. Rev. A **76**, 013604 (2007).
[25] W. Zwerger, J. Opt. B: Quantum Semiclass. Opt. **5**, S9 (2003).
[26] M. Abad and A. Recati, Eur. Phys. J. D **67**, 148 (2013).
[27] D. V. Dmitriev, V. Ya. Krivnov, and A. A. Ovchinnikov, Phys. Rev. B **65**, 172409 (2002).
[28] A. Läuchli and C. Kollath, J. Stat. Mech.: Theory Exp., P05018 (2008).
[29] Due to the open boundary conditions we may have a polarization induced by boundary effects for small L. We checked that for L ≥ 80 the transition point is independent of the size.
[30] We take the absolute value since states with polarization $S_z$ and $-S_z$ are degenerate, and different numerical realizations will find one state or the other. We have checked that the local magnetization is consistent with the value $S_z$ and that border effects are small.
[31] E. H. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963).
[32] Xiaoling Cui and Tin-Lun Ho, Phys. Rev. A **89**, 023611 (2014).

* Electronic address: [barbiero@pd.infn.it](mailto:barbiero@pd.infn.it)