論文の内容の要旨

Theoretical study on phases and phase transitions of ferromagnetic spin-1 bosons in optical lattices (光格子中の強磁性スピン１ボソンの相と相転移についての理論的研究)

曽弘博
Kohaku H. Z. So (Hongbo Zeng)

1 Background

1.1 Ultracold atoms in optical lattices

It took about 70 years for Bose-Einstein condensation, theoretically predicted by Einstein [1], to be experimentally realized by several groups in 1995 [2, 3], which brought them the Nobel prize in physics 2001 "for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates". Since that time, the field of ultracold atoms has rapidly expanded [4], incorporating various ideas and techniques from diverse fields of physics including AMO physics and condensed matter physics, and has become a unique and important arena for exploring the physics of various quantum many-body systems [5, 6].

One of the main reasons that ultracold atomic systems enjoy such popularity can be attributed to their high controllability; the interaction between atoms can be tuned with the technique of Feshbach resonances, and the geometry of the system can be tailored with various optical techniques.

In particular, with multiple laser beams, we can create diverse periodic potentials, called optical lattices, which allow us to explore the physics beyond weak interaction approximations [6, 7]. Unlike conventional solid-state electron systems, systems of ultracold atoms in optical lattices can be free of defects, thus opening up the possibility of studying the physics of strongly interacting quantum many-body systems with unprecedentedly high precision.

A seminal example of this trend is the experimental realization of the quantum phase transition between the superfluid phase and the Mott insulator phase predicted by the Bose-Hubbard model, in the system of ultracold bosons in an optical lattice. The Bose-Hubbard model is a model which describes bosons in a discrete lattice, was analyzed in the context of condensed matter physics [8], and was later shown [9] to be able to describe ultracold bosons in an optical lattice. The Hamiltonian of the model consists of two parts that compete with each other; the kinetic energy part which makes each boson spread over the whole system, and the repulsive interaction part which tends to localize bosons. The competition between these two terms is predicted to give rise to the quantum phase transition between the superfluid phase, in which each particle spreads over the whole system and hence is highly mobile, and the Mott insulator phase, in which each particle is localized due to the on-site repulsive interaction. Using ultracold bosons and an optical lattice, this phase transition was experimentally demonstrated in 2002 [10].

1.2 Spinor ultracold atoms

In the early days of studies on ultracold atoms, their internal degrees of freedom are frozen due to magnetic traps used in experiments. However, by the realization of optical traps, bosons with spin degrees of freedom, which are called spinor bosons, can now be investigated experimentally, and have attracted considerable interest because of the possibility they offer of simulating quantum magnetism and exploring the interplay between the spatial and spinor degrees of freedom [11, 12].

At first, studies on spinor bosons mainly dealt with the weak interaction regime, in which, at zero and low enough temperature, almost all the particles Bose-Einstein condensate. Such studies revealed diverse quantum phases arising from the presence of the spin degree of freedom and a spin-dependent interaction.

More recently, optical lattices makes it possible to explore the strongly interacting regime of ultracold atoms, including spinor bosons. A minimal model for studying such physics is the spin-1 Bose-Hubbard model [13], which describes spin-1 bosons in an optical lattice. Although the model is similar to the Bose-Hubbard model for bosons without spin degrees of freedom mentioned earlier, which is called the scalar Bose-Hubbard model to distinguish it from the spinor counterpart, the model has a spin-dependent interaction term, whose sign depends on the specific atom considered, and changes the qualitative features of the system drastically; for a negative sign, the interaction favors a larger magnitude of the spin at each site, and is called ferromagnetic, and for a positive sign, the interaction favors a smaller magnitude of the spin, and is called antiferromagnetic. For the ferromagnetic interaction, the zero-temperature phase diagram of the model is known to closely resemble that of the scalar model, in which the quantum phase transition is continuous. On the other hand, for the antiferromagnetic interaction, the phase diagram exhibits distinct properties; Mott phases with odd particle-number filling shrink, and the superfluid Mott insulator phase transition is known to be discontinuous for even particle-number filling.

1.3 Our study

With differences mentioned above, the antiferromagnetic model is much more intensively studied compared with the ferromagnetic counterpart. However, the situation is expected to be greatly altered in the presence of an external magnetic field, where the competition between the positive quadratic Zeeman energy and the ferromagnetic interaction produces rich phases; the ferromagnetic interaction favors states with larger spin, while the positive quadratic Zeeman energy penalizes such states. In systems without a lattice, this competition is known to give rise to two superfluid phases and the continuous phase transition between them.

To the best knowledge of the author, the ground-state phase diagram of the ferromagnetic spin-1 Bose-Hubbard model in the presence of an external magnetic field remains largely unexplored. Although there is a study on the unit-filling Mott insulator phase [14], the interplay between the spatial and spin degrees of freedom has yet to be fully explored.

2 Model and analysis

2.1 Model

In the thesis, we explore the ground-state and nonzero temperature phase diagrams of the spin-1 Bose-Hubbard model with an external magnetic field, described by the grand Hamiltonian

$$\hat{K} = -t \sum_{\substack{(x,y)\in\mathcal{B} \\ \sigma\in\mathcal{S}}} a^\dagger_{x,\sigma} a_{y,\sigma} + \frac{U_0}{2} \sum_{x\in\Lambda} \hat{n}_x(\hat{n}_x - 1) + \frac{U_2}{2} \sum_{x\in\Lambda} \left(\boldsymbol{S}_x^2 - 2\hat{n}_x\right) + q \sum_{x\in\Lambda} \sum_{\sigma\in\mathcal{S}} \sigma^2 \hat{n}_{x,\sigma} - \mu \sum_{x\in\Lambda} \hat{n}_x, \tag{1}$$

where

- Λ denotes the lattice sites, $\mathcal{S}$ denotes the spin indices, $\mathcal{B}$ denotes pairs of neighboring sites in the lattice,
- $a_{x,\sigma}$ means the annihilation operator of a bosons at site x with spin σ, $\hat{n_{x,\sigma}} := a^\dagger_{x,\sigma} a_{x,\sigma}$, $\hat{n}_x := \sum_{\sigma\in\mathcal{S}} \hat{n}_{x,\sigma}$, $\boldsymbol{S}_x := (S_x^{(1)}, S_x^{(2)}, S_x^{(3)})$, and $S_x^{(\alpha)} := \sum_{\sigma,\tau\in\mathcal{S}} S^{(\alpha)}_{\sigma,\tau} a^\dagger_{x,\sigma} a_{x,\tau}$, with $S^{(\alpha)}$ being spin-1 matrices, and
- $t > 0$, $U_0 > 0$, $U_2 < 0$, $q > 0$ are assumed.

The last two assumptions are crucial, because we want to examine the competition between the ferromagnetic interaction ($U_2 < 0$) and the positive quadratic Zeeman energy ($q > 0$).

2.2 Gutzwiller variational ansatz

To analyze the model, we first describe the Gutzwiller variational ansatz, in which we restrict variational states to products of local states. The rationale behind this approximation is that the ground states for both the no-hopping and non-interacting limits can be written in this form, and that it is natural to expect that this form of state can also capture the physics of intermediate parameter region, in which phase transitions occur.

2.3 Decoupling approximation

In our actual calculations, we have employed the decoupling approximation, which is shown to be equivalent to, and much more numerically efficient compared with the Gutzwiller variational ansatz, whose main advantage is the conceptual clarity. In the decoupling approximation, we decouple the hopping term which connects different lattice sites as

$$a_{x,\sigma}^{\dagger} a_{y,\sigma} \simeq \phi_{y,\sigma} a_{x,\sigma}^{\dagger} + \phi_{x,\sigma}^{*} a_{y,\sigma} - \phi_{x,\sigma}^{*} \phi_{y,\sigma}, \tag{2}$$

where $\phi_{x,\sigma}$, or "superfluid order parameters", which have to be determined self-consistently later, means the expectation value of $a_{x,\sigma}$, and we neglect the term which is quadratic in the fluctuation. After the approximation, the problem reduces to a single-site problem described by the grand Hamiltonian

$$\hat{K}_{\mathrm{dc}}(\boldsymbol{\phi}) \quad := \quad -zt \sum_{\sigma \in \mathcal{S}} \left(\phi_\sigma a_\sigma^{\dagger} + \phi_\sigma^{*} a_\sigma - |\phi_\sigma|^2 \right) + \frac{U_0}{2} \hat{n}(\hat{n}-1) + \frac{U_2}{2} \left(\boldsymbol{S}^2 - 2\hat{n} \right) + q \sum_{\sigma \in \mathcal{S}} \sigma^2 \hat{n}_\sigma - \mu \hat{n}, \tag{3}$$

where indices denoting lattice sites are dropped. An approximate ground state (or grand canonical ensemble for the nonzero temperature) can be obtained by finding a self-consistent solution $\boldsymbol{\phi}^0$, for which the state derived from $\hat{K}_{\mathrm{dc}}(\boldsymbol{\phi}^0)$ (ground state, or grand canonical ensemble for the nonzero temperature case) gives $\langle a_\sigma \rangle = \phi_\sigma^0$, where $\langle \cdot \rangle$ denotes expectation value with respect to the given state.

To obtain the phase diagrams, we have numerically obtained self-consistent solutions by iteratively diagonalizing the single-site grand Hamiltonian.

3 Results and Discussion

For the zero-temperature case, we have found, in addition to the Mott insulator phase, two superfluid phases; the polar phase, which shows no magnetization, and the broken-axisymmetry phase, which exhibits nonzero transverse magnetization. Furthermore, we have found that, for the strong spin-dependent interaction corresponding to the ^{7}Li, the phase transition between these two superfluid phases can be discontinuous, i.e., the superfluid order parameters and the transverse magnetization have nonzero jumps at the transition point on some part of the phase boundary in the $t - \mu$ phase diagram. Discontinuous phase transitions are also found when the quadratic Zeeman energy is varied, in clear contrast to the mean-field theory prediction for weakly interacting spin-1 bosons without an optical lattice, where the corresponding phase transition is known to be continuous. To clarify that these discontinuous phase transitions seen in our calculations are not due to numerical artifacts, we have plotted the energy function (the ground-state energy of $K(\boldsymbol{\phi})$ for the zero-temperature case, and the free energy derived from $K(\boldsymbol{\phi})$ for the nonzero temperature case) as a function of the superfluid order parameters $\boldsymbol{\phi}$, and confirmed the metastability and ensuing discontinuous phase transitions.

For the nonzero-temperature case, we have found that the system also exhibits the above mentioned properties, i.e., two superfluid phases with different magnetic properties and discontinuous phase transitions between these two phases, for sufficiently low temperatures. However, with an increase in temperature, the region of the discontinuous phase transition gradually shrinks, and for higher temperature, the phase transitions become continuous.

We have found that discontinuous phase transitions between two superfluid phases occur only when the boundary is close to the Mott-insulator phase, and that continuous phase transitions occur when the hopping is so large that the boundary is far from the Mott-insulator phase. This is not only consistent with the fact that the corresponding phase transitions are continuous for weakly interacting bosons, in which almost all the particles participate in the superfluidity, but also suggests that the presence of a considerable portion of the non-superfluid component is crucial for the occurrence of discontinuous phase transitions, implying the importance of the effect of strong interaction on the interplay between the spatial and spinor degrees of freedom.

References

[1] Albert Einstein, Sitzungsberichte der Preussischen Akademie der Wissenschaften, Physikalisch-mathematische Klasse, 261 (1924) ; 3 (1925).

[2] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, E. A. Cornell, Science, **269**, 198 (1995).

[3] K. B. Davis, M. -O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995),

[4] C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases, 2nd edition*, Cambridge University Press (2008).

[5] Immanuel Bloch, Jean Dalibard, and Wilhelm Zwerger, Rev. Mod. Phys. **80**, 885 (2008).

[6] Maciej Lewenstein, Anna Sanpera, and Veronica Ahufinger, *Ultracold Atoms in Optical Lattices: Simulating Quantum Many-Body Systems*, Oxford University Press (2012).

[7] Konstantin V. Krutitsky, Phys. Rep. **607**, 1 (2016).

[8] Matthew P. A. Fisher, Peter B. Weichman, G. Grinstein, and Daniel S. Fisher, Phys. Rev. B **40**, 546 (1989).

[9] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).

[10] Markus Greiner, Olaf Mandel, Tilman Esslinger, Theodor W. Hänsch and Immanuel Bloch, Nature, **415**, 39 (2002).

[11] Yuki Kawaguchi and Masahito Ueda, Phys. Rep. **520**, 253 (2012).

[12] Dan M. Stamper-Kurn and Masahito Ueda, Rev. Mod. Phys. **85**, 1191 (2013).

[13] Adilet Imambekov, Mikhail Lukin, and Eugene Demler, Phys. Rev. A **68**, 063602 (2003).

[14] K. Rodríguez, A. Argüelles, A. K. Kolezhuk, L. Santos, and T. Vekua, Phys. Rev. Lett **106**, 105302 (2011).