

Strongly correlated systems
in atomic and condensed matter physics

Lecture notes

by Eugene Demler

ETH

October 25, 2023

Chapter 9

Quantum magnetism with ultracold atoms in optical lattices

9.1 Two component Bose mixture in optical lattice

We consider two component Bose mixture in an optical lattice. The Hamiltonian of this system is given by

$$\begin{aligned}\mathcal{H} = & -t_{\uparrow} \sum_{ij} b_{i\uparrow}^{\dagger} b_{j\uparrow} - \mu_{\uparrow} \sum_i n_{i\uparrow} - t_{\downarrow} \sum_{ij} b_{i\downarrow}^{\dagger} b_{j\downarrow} - \mu_{\downarrow} \sum_i n_{i\downarrow} \\ & + \frac{U_{\uparrow\uparrow}}{2} \sum_i n_{i\uparrow}(n_{i\uparrow} - 1) + \frac{U_{\downarrow\downarrow}}{2} \sum_i n_{i\downarrow}(n_{i\downarrow} - 1) + U_{\uparrow\downarrow} \sum_i n_{i\uparrow} n_{i\downarrow}\end{aligned}\quad (9.1)$$

Here $b_{i\{\uparrow\downarrow\}}^{\dagger}$ are creation operators of atoms in two different states. The two states can correspond to different hyperfine states of the same atom or even different atoms. It is worth emphasizing spin-1/2 bosons should not be a source of confusion. Both states come from hyperfine multiplets of integer spin. However we know that on timescales relevant to experiments these states do not scatter into any other states. Hence we can label them as spin up and down states. Another way of avoiding confusion is to think of label σ as a *pseudospin* rather than the real spin.

As we discussed before, one can use state selective optical lattices to control separately tunneling for the two states. One can use magnetic field dependence of the scattering lengths to tune interactions separately (typically this requires being near a certain Feshbach resonance so one can change dramatically one of the interaction parameters). It is also possible to control positions of the lattice sites for two species relative to each other, which allows to change interspecies

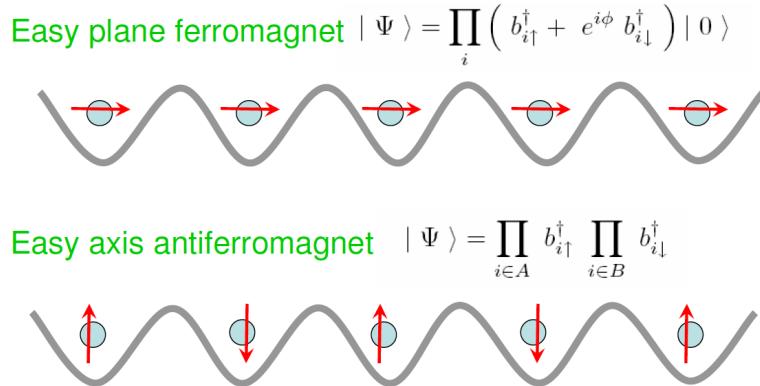


Figure 9.1: Examples of magnetic order of two component Bose mixture in an optical lattice at $n = 1$.

interactions relative to intraspecies ones.

Our first task is to understand Mott states with filling factor one. In the case of spinless boson Mott states were easy to characterize. We only needed to specify the number of particles per well. In the case of Bose mixtures the problem is more complicated. We also need to specify the spin arrangement of atoms. In other words we need to understand magnetic structure of the Mott state. One may object that a question of magnetism in cold atoms systems is very different from the one in condensed matter physics. In solid state systems spin is not conserved. So if it is energetically favorable to have a system spin polarized in some direction, magnetization will relax in a nanosecond or less. On the other hand with cold atoms, spin is conserved. If we prepare a 50/50 mixture of two hyperfine state, i.e. a state with no net polarization, it will stay like this during the entire lifetime of experiment. However even when the total magnetization is fixed there are many ways how to arrange atoms spatially. For example, one can make an antiferromagnetic state: atoms form an alternating pattern shown in figure 9.1. This state can be written as

$$|\Psi_{AF}\rangle = \prod_{i \in A} b_{i\uparrow}^\dagger \prod_{i \in B} b_{i\downarrow}^\dagger |\text{vac}\rangle \quad (9.2)$$

Another arrangement is to have one atom in each side in a superposition state of being with spin up and down (see fig 9.1).

$$|\Psi_{FM}\rangle = \prod_i \frac{1}{\sqrt{2}} (b_{i\uparrow}^\dagger + e^{i\phi} b_{i\downarrow}^\dagger) |\text{vac}\rangle \quad (9.3)$$

This is a ferromagnetic state with spin polarization in the XY plane $\langle \sigma^+ \rangle = 1/2 e^{i\phi}$. The question is how does the system decide which Mott states is energetically favorable.

Let us start deep in the Mott state. In a Mott state number fluctuations are suppressed but they are not frozen out completely. Deep in the Mott state we

Figure 9.2: Virtual tunneling processes that give rise to superexchange interactions in the Mott state

can treat tunneling perturbatively. We can then ask how much kinetic energy the system can regain from virtual tunneling. This is shown in fig. 9.2 for two wells. We can write an effective spin Hamiltonian that can capture these energies[3, 8, 1]

$$\mathcal{H}_{\text{eff}} = \frac{1}{2} J_{\perp} (S_1^{\dagger} S_2^{-} + S_1^{-} S_2^{\dagger}) + J_z S_1^z S_2^z + h S^z \quad (9.4)$$

Here spin operators are given by the usual relations

$$S_i^a = \frac{1}{2} \sum_{\alpha\beta} b_{i\alpha}^{\dagger} \sigma_{\alpha\beta}^a b_{i\beta} \quad (9.5)$$

Note that the original Hamiltonian (9.1) has a U(1) symmetry generated by $S_{\text{tot}}^z = N_1 - N_2$. It describes the fact that the number of atoms of each type is conserved separately. This symmetry requires that $S_1^x S_2^x$ and $S_1^y S_2^y$ appear with the same coefficients in the effective model. To find coefficients in (9.4) we relate energies of different states using the effective Hamiltonian and the expansion of the original Hubbard model, as shown in fig. 9.3. We obtain

$$\begin{aligned} J_{\perp} &= -\frac{4t_{\uparrow}t_{\downarrow}}{U_{\uparrow\downarrow}} \\ J_z &= \frac{2(t_{\uparrow}^2 + t_{\downarrow}^2)}{U_{\uparrow\downarrow}} - 4\frac{t_{\uparrow}^2}{U_{\uparrow\uparrow}} - 4\frac{t_{\downarrow}^2}{U_{\downarrow\downarrow}} \end{aligned} \quad (9.6)$$

In the spin symmetric case when all tunnelings and interactions are the same we find ferromagnetic interactions with

$$J = \frac{4t^2}{U} \quad (9.7)$$

$$C + J_z \cdot \frac{1}{4} + h_z = - \frac{4t_{\uparrow}^2}{U_{\uparrow\uparrow}}$$

$$C + J_z \cdot \frac{1}{4} - h_z = - \frac{4t_{\downarrow}^2}{U_{\downarrow\downarrow}}$$

$$C - J_z \cdot \frac{1}{4} = - \frac{t_{\uparrow}^2}{U_{\uparrow\downarrow}} - \frac{t_{\downarrow}^2}{U_{\downarrow\uparrow}}$$

$$J_{\perp} = - \frac{4t_{\uparrow}t_{\downarrow}}{U_{\uparrow\downarrow}}$$

Figure 9.3: Calculation of superexchange interactions in the Mott state

When spins are aligned, bosonic atoms can recapture more of the kinetic energy. This comes from Bose enhancement factors which favor tunneling of identical spins. However the freedom of changing microscopic parameters in (9.1) allows us to engineer magnetic Hamiltonians with different types of exchange interactions: easy axis and easy plane, ferro and antiferromagnetic.

9.2 Experimental observation of superexchange

Superexchange for bosons in optical lattices has been demonstrated in experiments by S. Trotzky et al.[6] following theoretical proposal in [4]. They used optical lattices with different wavelengths to create a set of isolated double wells and observed spin oscillations within individual wells. This technique is explained in figs. 9.6, 9.7, 9.8, 9.9.

9.3 Problems for Chapter 9

Problem 1

Consider two spin 1/2 particles interacting with the usual Heisenberg interaction

$$\mathcal{H} = -J\vec{S}_1 \cdot \vec{S}_2 \quad (9.8)$$

- a) Show that the operator defined as

$$\hat{P}_{12} = \frac{1}{2} + 2\vec{S}_1 \cdot \vec{S}_2 \quad (9.9)$$

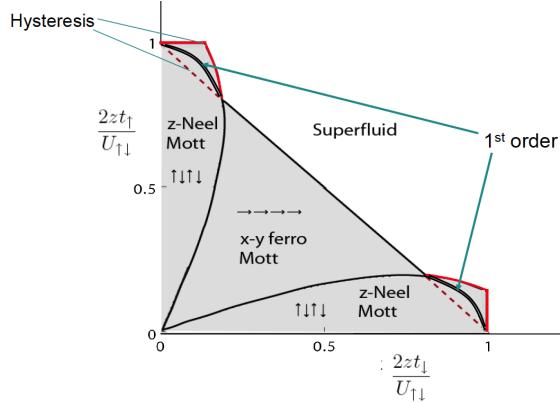


Figure 9.4: Phase diagram of the two component Bose mixture for $n = 1$ and $U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = \infty$ based on analytical mean-field + quantum fluctuations analysis[1]. For small tunnelings phase diagram agrees with results of the effective Heisenberg model (9.4), (9.6).

executes a swap of the two spins b) Show that the evolution operator of the system

$$U(t) = e^{-it\mathcal{H}} \quad (9.10)$$

can be written as

$$U(t) = \cos\left(\frac{Jt}{2\hbar}\right)\hat{1} + i \sin\left(\frac{Jt}{2\hbar}\right)\hat{P}_{12} \quad (9.11)$$

Problem 2 (more difficult problem)

In this problem you will consider spin 1 bosons in an optical lattice[2, 7]. The Hubbard Hamiltonian of the system is given by

$$\mathcal{H} = -t \sum_{\langle ij \rangle m} a_{im}^\dagger a_{jm} + U_0 \sum_i n_i^2 + U_2 \sum_i \vec{S}_i^2 - \mu \sum_i n_i \quad (9.12)$$

We consider a Mott state with $n = 1$. Show that integrating out virtual tunneling processes gives rise to an effective spin Hamiltonian

$$\mathcal{H}_{\text{eff}} = -J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - J_2 \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j \right)^2 \quad (9.13)$$

- a) Find explicit expressions for J_1 and J_2

Hint: consider a single pair of atoms and decompose into states of certain total spin. Total spin of the pair determines orbital symmetry of the wavefunction.

- b) Discuss the mean-field phase diagram of (9.13).

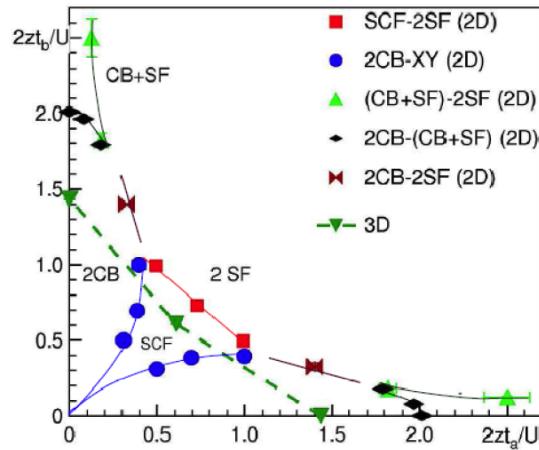


Figure 9.5: Phase diagram of two component Bose mixture for $n = 1$ and $U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = \infty$ based on Monte-Carlo analysis [5]. CB stands for the z -Neel phase, SCF stands for the XY ferromagnetic phase. There is also a superfluid phase with antiferromagnetic z -Neel order.

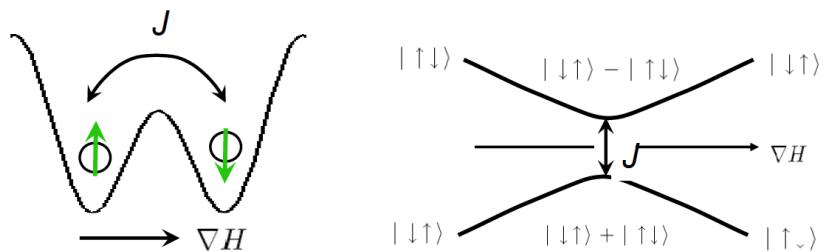


Figure 9.6: Set up of double well experiments. Gradient of the magnetic field is used to prepare $|\downarrow\uparrow\rangle$ state. Then magnetic field gradient is suddenly switched off. Spins begin to flip flop with the frequency J/\hbar .

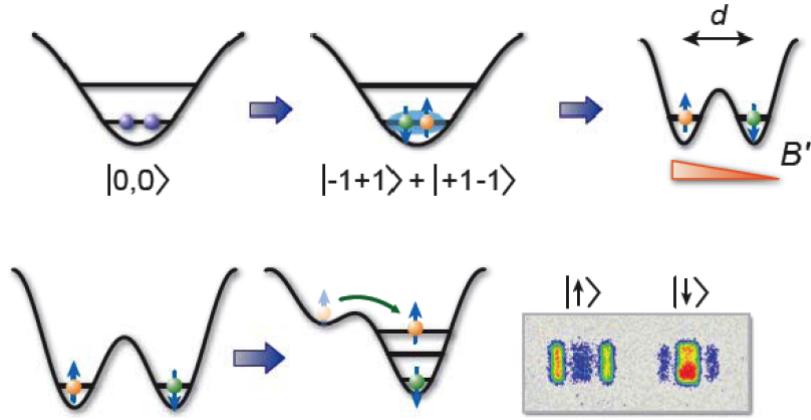


Figure 9.7: Initial state preparation in double wells in [6]. Detection was done by converting spin information into occupation of higher Bloch bands. Figures taken from [6].

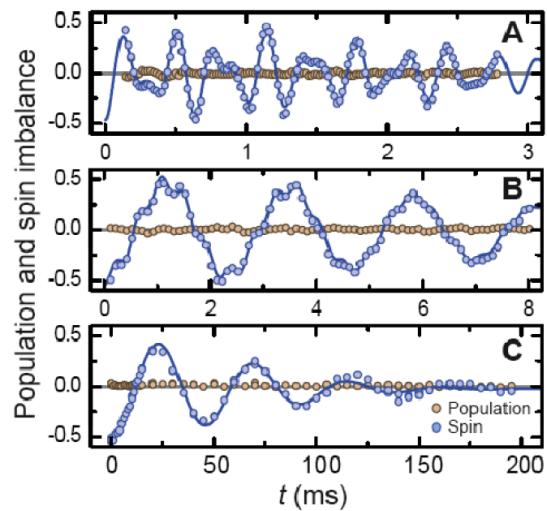


Figure 9.8: Dynamics of staggered magnetization $N^z = S_1^z - S_2^z$ in double well experiments. Only in the regime of deep wells we see that there is only one frequency scale set by $J = 4t^2/U$. Figures taken from [6].

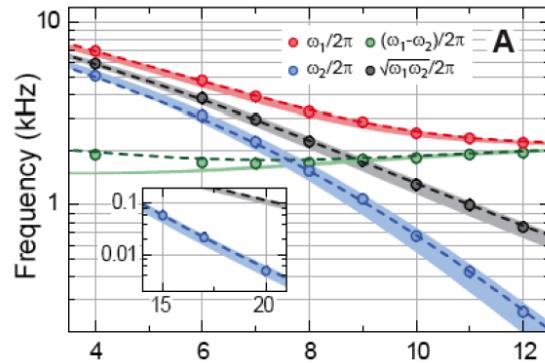


Figure 9.9: Frequencies extracted from spin dynamics. The blue line shows the dominant $4t^2/U$ frequency compared to theoretical calculations. Figures taken from [6].

Bibliography

- [1] Ehud Altman, Walter Hofstetter, Eugene Demler, and Mikhail D Lukin. Phase diagram of two-component bosons on an optical lattice. *New Journal of Physics*, 5(1):113, 2003.
- [2] Eugene Demler and Fei Zhou. Spinor bosonic atoms in optical lattices: Symmetry breaking and fractionalization. *Phys. Rev. Lett.*, 88(16):163001, Apr 2002.
- [3] L.-M. Duan, E. Demler, and M. D. Lukin. Controlling spin exchange interactions of ultracold atoms in optical lattices. *Phys. Rev. Lett.*, 91(9):090402, Aug 2003.
- [4] A.M. Rey et al. *PRL*, 99:140601, 2007.
- [5] B. Capogrosso-Sansone et al. *arXiv:0912.1865*, 2009.
- [6] S. Trotzky et al. *Science*, 319:295, 2007.
- [7] Adilet Imambekov, Mikhail Lukin, and Eugene Demler. Spin-exchange interactions of spin-one bosons in optical lattices: Singlet, nematic, and dimerized phases. *Phys. Rev. A*, 68(6):063602, Dec 2003.
- [8] A. B. Kuklov and B. V. Svistunov. Counterflow superfluidity of two-species ultracold atoms in a commensurate optical lattice. *Phys. Rev. Lett.*, 90(10):100401, Mar 2003.