Interference of atomic levels and superfluid – Mott insulator phase transition in a two-component Bose-Einstein condensate

K. V. Krutitsky and R. Graham
Fachbereich Physik der Universität Duisburg-Essen, Standort Essen, Universitätsstr. 5, Postfach 10 37 64, 45117 Essen, Germany

(Dated: March 22, 2022)

The study of quantum phase transitions (QPT) in optical lattices has become one of several foci of current interest in the ongoing exploration of the rich physics of Bose-Einstein condensates (BEC). In the seminal paper by Jaksch et al. [1] it was predicted that by increasing the strength of the periodic optical potential one can confine ultracold atoms at lattice sites, which leads to the superfluid–Mott insulator phase transition, and this effect has been experimentally observed in a one-component BEC of rubidium atoms [2]. Recently coherent transport of multicomponent BEC in optical lattices has been demonstrated [3]. In such systems a number of new phenomena associated with QPT are possible. Theoretical studies show that by using different laser schemes one can create coexisting superfluid and Mott phases [1, 4], fragmented condensates with topological excitations [5], maximally entangled atomic states [6], dimer phases [7], and heteronuclear molecular BECs [8].

One of the most intriguing features of the multicomponent BECs is the structure of their internal levels. The action of lasers on multi-level atoms can lead to interference of atomic levels. This kind of interference has been used in atomic BECs to slow down the light [9], which allows us to excite quantum states. This kind of interference has been used in atomic BECs [10]. In the present Letter we shall investigate the possibility of using interference of atomic levels for the manipulation of QPT in a two-component BEC with spatially periodic coupling of the degenerate internal ground states. It is shown that one can effectively manipulate QPT not only by varying the laser intensity, but also the laser polarization, and one can even change the sign of the tunneling matrix element, which leads to “ferromagnetic” and “antiferromagnetic” states in analogy to the spin ordering in magnetic systems.

We consider a two-component BEC of neutral polarizable atoms of mass $M$, possessing an excited electronic state characterized by the magnetic quantum number $m = 0$ and two Zeeman-degenerate internal ground states with $m = \pm 1$ ($F_g = F_e = 1$), in a one-dimensional optical lattice. The latter is assumed to be created by two counterpropagating linearly polarized laser waves of equal amplitudes and frequencies with the wave number $k_L$, and the angle $\theta$ between the polarization vectors (lin-angle-lin configuration) [11], and with detuning $\Delta$ from the internal atomic transition. In order to avoid decoherence due to spontaneous emission, $|\Delta|$ must be much larger than the spontaneous emission rate. The running laser waves form left- and right- polarized standing waves with the Rabi frequencies $\Omega_{\pm} = \Omega_0 \cos(k_L z \pm \theta/2)$. Because of the large detuning the excited state can be adiabatically eliminated. The resulting effective Hamiltonian couples the atomic ground states and has the following form:

$$H = \int \Phi^\dag \left[ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial z^2} + \frac{\hbar}{\Delta} \Omega^2 + \frac{g}{2} (\Phi^\dag \cdot \Phi) \right] \Phi \, dz,$$  

(1)

where $\Phi$ is a two-component spinor-field operator. $\Omega^2$ determines the periodic potential with the period $\pi/k_L$. It is a $2 \times 2$ matrix with the components $\Omega_{i,j} = \Omega_{\alpha} \Omega_{\beta}$, $\alpha, \beta = \pm$. The parameter $g$ describes the repulsive interaction of the condensate atoms. In the one-dimensional case it has the form [12]

$$g = 4\hbar^2 a/a_L^2 (1 - 1.4603 a/a_L),$$

where $a$ is a symmetric scattering length and $a_L = \sqrt{2\hbar/M \omega_L}$ is the size of the ground state for the harmonic potential with the frequency $\omega_L$ confining the BEC in the transverse directions.

The starting point for the investigation of QPT is the Bose-Hubbard model. We assume that the atoms are prepared in the lowest Bloch band and the matter-field operator $\Phi$ can be decomposed in the Wannier basis [13]

$$\Phi(z) = \sum_i \exp(i\varphi_i) W_i(z) a_i,$$  

(2)

where $W_i(z) = W(z - z_i)$ are two-component Wannier spinors for the lowest energy band. They are obtained by the solution of the eigen-value problem for the Hamiltonian [14] in the case $g = 0$ and satisfy the orthonormality condition $\int W_i^\dag(z) \cdot W_j(z) \, dz = \delta_{ij}$. The indices $i, j$ label the sites of the one-dimensional periodic lattice. The phases $\varphi_i$ are not yet defined and their proper choice is discussed in a moment.
The \( a_i \) and their adjoints are Bose annihilation and creation operators attached to the lattice sites. Substituting (2) into (1) and taking into account only the hopping between the nearest neighbour lattice sites and the atomic interactions at the same lattice site, we obtain the well-known Bose-Hubbard Hamiltonian

\[
H_{BH} = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j \exp \left[ i (\varphi_j - \varphi_i) \right] \quad (3)
\]

where \( \mu \) is a chemical potential. The tunneling matrix element \( J = -\int W_{i+1}^\dagger(z) \cdot \left( -\hbar^2 \frac{\partial^2}{\partial z^2} + \frac{\hbar^2}{2m} \right) \cdot W_i(z) \, dz \) and the atomic interaction parameter \( U = g \int W_i^\dagger \cdot \left( W_i^\dagger \cdot W_i \right) \cdot W_i \, dz \) can be simultaneously changed by varying the effective Rabi frequency and/or the angle \( \theta \), but the variation of \( J \) is much faster. Typical dependences of the ratio \( J/U \) on the dimensionless effective Rabi frequency \( q = \Omega^2_0/4aR\Delta \), and the angle \( \theta \) are shown in the left column of Figs. 1, 2, and 4. \( \omega_R = \hbar k_L^2/2m \) is a one-photon recoil frequency. The calculations are performed for \( ^{87}\text{Rb} \) \((M = 1.45 \times 10^{-25} \text{ kg}, a = 5.4 \text{ nm}) \), \( \omega_\perp = 2\pi \times 200 \text{ Hz} \), \( \lambda_L = 2\pi/k_L = 780 \text{ nm} \).

In our model we neglect the antisymmetric scattering length, which is responsible for (i) the asymmetry of the interatomic collisions for the atoms in the same and in different ground states and (ii) inelastic collisions of the atoms in the states \( m = -1 \) and \( m = 1 \), which lead to the creation of the atoms in the ground state \( m = 0 \). This approximation is well justified at least for \( ^{87}\text{Rb} \), because the asymmetry leads to a correction of the parameter \( U \) of the order of only a few percent in Eq. (3) and the inelastic collisions become important for the times \( T \gtrsim 3/n \text{ s} \), where \( n \) is the number of atoms per lattice site.

The phases \( \varphi_i \) are determined from the requirement of minimal energy of the Hamiltonian (3), which amounts to demanding that \( J \cos(\varphi_i - \varphi_{i+1}) \) is maximal. In the familiar case of a one-component BEC in a periodic lattice, where the Wannier spinors reduce to functions, this leads to \( \varphi_i = \varphi_j \), because in such a situation \( J \) in Eq. (3) is real and positive. Therefore the superfluid state of a one-component BEC in the optical lattice always has a ferromagnetic ordering of the phases \( \varphi_i \), which can then be set to zero. Interestingly, in the case of a two-component BEC \( J \) can also become negative. In this case the choice \( \varphi_i = \varphi_{i+1} \) does not provide a minimal energy and \( \varphi_{i+1} = \varphi_i \pm \pi \) has to be chosen instead. This corresponds to an antiferromagnetic ordering of the phases of neighboring lattice sites. Indeed, as one can see in Figs. 1, 2, and 4 (left column) the parameter \( J \) takes in general positive as well as negative values (\( U \) is always positive for a BEC with repulsive interaction). Therefore, ferromagnetic and antiferromagnetic phase ordering occurs in different parts of the phase diagram.

Ferromagnetic and antiferromagnetic phase ordering is possible only for the superfluid phase. These two cases are readily distinguishable experimentally in the superfluid regime via the spatial interference pattern generated by the coherent matter waves which one obtains after removing the lattice potential (3): The interference maxima obtained in the ferromagnetic case turn into minima in the antiferromagnetic case and vice versa. In the Mott phase, the numbers of particles occupying each lattice site are equal and integer, and the phases of the corresponding wave functions are completely undefined. Therefore, the choice of the \( \varphi_i \) remains arbitrary in this case and has no observable consequences for the interference pattern.

The change of the sign of \( J \) is closely related to the form of the dispersion relation \( E(k) \) for the lowest Bloch band. Using the definition of the Wannier spinors the expression for \( J \) can be rewritten in the form \( J = \frac{3}{2} \int_{-\infty}^{+\infty} E'(k) \sin(\pi k/k_L) \, dk \). In the case of a one-component condensate one always has a normal dispersion, i.e., \( E'(k) \geq 0 \) for \( 0 \leq k \leq k_L \). In the case we are dealing with one can get anomalous dispersion, i.e., \( E'(k) < 0 \) for \( 0 \leq k \leq k_L \), as well. The change of the dispersion type and as a consequence of the sign of \( J \) happens at the points \((q, \theta)\) indicated in Figs. 3 and 5. Since the type of dispersion is different in the ferromagnetic and antiferromagnetic superfluid phases, one can expect principally different

---

**FIG. 1:** Typical dependences of \( J/U \) on the dimensionless effective Rabi frequency \( q = \Omega^2_0/4aR\Delta \) for red detuning \( (\Delta < 0) \) and corresponding phase diagrams for \( n = 1 \), \( \theta = 50^\circ \) (a), \( 64^\circ \) (b), \( 65,776^\circ \) (c), \( 66,5^\circ \) (d). Horizontal straight lines show the critical values \((2J/U)_c = \pm(3 - 2\sqrt{2})\). Vertical dashed lines on the phase diagrams (right column) indicate the boundary between ferromagnetic \((J > 0)\) and antiferromagnetic \((J < 0)\) phase ordering. The regions of the Mott phase are enclosed by the lobes and loops.
properties of the nonlinear atomic matter waves in the two regimes [13].

The phase diagram of the Hamiltonian (3) is determined by the ratio $J/U$. In the case of one-component BECs it is a monotonic function of $|q|$. In the two-component case we are dealing with, it has quite different properties. Its dependence on $q$ and $\theta$ is not monotonic, and it can vanish or even change its sign at certain finite values of $q$. Therefore, it is reasonable to draw $\mu - q - \theta$ diagrams, which are shown in the figures, instead of $\mu - J$ diagrams. In the mean-field approximation and second-order perturbation theory the boundary between the superfluid and the Mott regions is given by [13] $2|J|/U = (1 - n + \mu/U)(n - \mu/U)/(1 + \mu/U)$, where $n - 1 < \mu/U < n$. The critical values $(2|J|/U)_c = 1 + 2n - 2\sqrt{n^2 + n - 1}$, which correspond to $(\mu/U)_c = \sqrt{n^2 + n - 1}$, define the maximal possible width of the Mott region on the phase diagram. Since $J/U$ is not a monotonic function of $q$ and $\theta$, there can be several critical values of $q$ and $\theta$ (see Figs. 1, 2, and 4). At the points $(q, \theta)$, where $J/U$ vanishes, we have the Mott phase for any values of $\mu/U$. These points define the boundary between the ferromagnetic and antiferromagnetic states.

The phase diagrams in the plane spanned by $\theta$ and $q$ for $(\mu/U)_c = \sqrt{2} - 1$ at $n = 1$ and negative (red) and positive (blue) detuning $\Delta$ are shown in Figs. 3 and 5 respectively. The principal difference between the cases of positive and negative $\Delta$ can be understood if we apply the unitary transformation

$$\hat{U} = \frac{1}{\Omega} \left( \begin{array}{cc} \Omega_+ & \Omega_- \\ -\Omega_- & \Omega_+ \end{array} \right), \Omega = \sqrt{\Omega_+^2 + \Omega_-^2}$$

(4)
to the Wannier spinors in Eq. (3). After the transformation we end up with the bright and dark states [17], which are not degenerate in contrast to the original ones. The important point is that only the bright state is directly coupled to the electromagnetic field and influenced by the potential

$$V_B = \hbar \frac{\Omega^2}{\Delta} = \hbar \frac{\Omega_0^2}{\Delta} (1 + \cos \theta \cos 2k_L z) .$$

(5)

We consider first the case $\theta = 0$, when the transformation $\hat{U}$ does not depend on the position $z$. In this case the dark state does not “feel” any periodic potential. Since in the case $\Delta > 0$ the dark state has a lower energy the atoms stay in this state and, therefore, they can not be localized on the lattice sites for any laser intensity. In the case $\Delta < 0$ the situation is reversed: The energy of the bright state is lower than that of the dark one and only the bright state is populated by the atoms. Therefore, increasing the laser intensity, one can strongly localize the atoms on the lattice sites in exactly the same manner as in the case of the one-component BEC.

In the case $\theta \neq 0$, $\hat{U}$ is a position-dependent transformation. The atomic center-of-mass motion leads to the gauge potential

$$V_g = \hbar \omega_R \left( \frac{\sin \theta}{1 + \cos \theta \cos 2k_L z} \right)^2 ,$$

(6)

acting on the bright and dark atomic states and to the motional coupling of the states [17]. It seems that the transformation $\hat{U}$ does not lead to any simplifications in the case $\theta \neq 0$. Nevertheless, it allows one to understand what is going on, assuming that $|\Omega_0^2/\Delta| \gg \omega_R$. In this approximation $V_g \ll |V_B|$, and one can neglect the gauge potential for the bright state as well as the motional coupling between the bright and dark states.
PSfrag replacements

FIG. 4: The same as in Figs. 1 and 2 for blue detuning (Δ > 0). θ = 45° (a), q = 6 (b).

FIG. 5: (a) Phase diagram in the (θ, q) plane for (µ/Δ) = √2 - 1, Δ > 0. The line J = 0 as well as the two boundaries separating SF and SA superfluid phases from the Mott phase are indistinguishable on the large-scale plot. The Mott phase is located in the extremely narrow region between the superfluid phases. Plot (b), therefore, shows the difference δq1 between the two boundaries (solid line) and the difference δq2 between the line J = 0 and the boundary separating the ferromagnetic superfluid phase from the Mott phase (dashed line).

states [17]. Then the only potentials acting on the bright and dark states are given by Eqs. 5 and 6, respectively. On the basis of the same argument as in the case θ = 0 we see that the atomic localization in the cases Δ < 0 and Δ > 0 is determined by the potentials V_B and V_g, respectively.

Accordingly in the case Δ < 0 the quantity Ω^2_0 cos(θ)/Δ plays the role of the effective Rabi frequency and defines the strength of the periodic potential. Therefore, in the simple approximation we consider for the sake of this discussion, the critical effective Rabi frequency Ω^c_0 eff = Ω^c_0 eff/2 cos θ (dotted line in Fig. 3), where Ω^c_0 eff is the critical effective Rabi frequency of the one-component BEC and the factor 2 reflects the fact that two atomic ground states are involved. Since Ω^c_0 eff ∼ 10 ω_R [11], the potential V_g appears to be too weak and the transition into the Mott state in the case Δ > 0 is not possible (compare with the exact results in Figs. 4 and 5).

As it follows from the results presented in Figs. 4 and 5, this simplified description provides a correct physical insight, but does not always work and at the laser intensities we are dealing with one has to take into account the coupling between the components, as we have done in the numerical calculations leading to the results displayed in Figs. 4 and 5. It is also necessary to note that the one-component approximation cannot describe the change of sign in J and the related transition from the ferromagnetic to antiferromagnetic superfluid phase.

Summarizing, we have studied quantum phase transitions of a BEC with two degenerate ground states in an optical lattice created by the lin-angle-lin laser configuration. It is shown that the periodic coupling of the atomic ground states modifies essentially the phase diagram of the system. The most surprising feature we encountered are (i) change of sign of the tunneling matrix element J under variation of the laser intensity and the angle θ, which leads to the ferromagnetic and antiferromagnetic phase ordering analogous to the spin ordering in magnetic systems, and (ii) suppression of the Mott transition in the case Δ > 0, except for a narrow region in the phase diagram (Figs. 4 and 5). Numerical results presented in the figures are for the case of a commensurate filling of the lattice with one atom per site. For higher occupation numbers the physics remains the same and there are only minor quantitative changes.

This work has been supported by the SFB/TR 12 “Symmetries and universalities in mesoscopic physics”.

[1] D. Jaksch et al., Phys. Rev. Lett. 81, 3108 (1998).
[2] M. Greiner et al., Nature 415, 39 (2002).
[3] O. Mandel et al., Phys. Rev. Lett. 91, 010407 (2003).
[4] G.-H. Chen and Y.-S. Wu, Phys. Rev. A 67, 013606 (2003).
[5] E. Demler and F. Zhou, Phys. Rev. Lett. 88, 163001 (2002).
[6] L. You, Phys. Rev. Lett. 90, 030402 (2003).
[7] S. K. Yip, Phys. Rev. Lett. 90, 250402 (2003).
[8] B. Damski et al., Phys. Rev. Lett. 90, 110401 (2003); M. G. Moore et al., Phys. Rev. A 67, 041603(R) (2003).
[9] L. V. Hau et al., Nature 397, 594 (1999); S. Inouye et al., Phys. Rev. Lett. 85, 4225 (2000).
[10] Z. Dutton et al., Science 293, 663 (2001).
[11] G. Gryna and C. Robilliard, Phys. Rep. 355, 335 (2001).
[12] V. Dunjko et al., Phys. Rev. Lett. 86, 5413 (2001).
[13] G. H. Wannier, Phys. Rev. 52, 191 (1937).
[14] T.-L. Ho, Phys. Rev. Lett. 81, 742 (1998).
[15] A. Trombettoni et al., Phys. Rev. Lett. 86, 2353 (2001).
[16] S. Sachdev, Quantum phase transitions (Cambridge University Press, Cambridge, England, 2001).
[17] R. Dum and M. Olshanii, Phys. Rev. Lett. 76, 1788 (1996).