Non-equilibrium dynamics in Mott-to-superfluid transition in Bose-Einstein condensation in optical lattices

N. Horiguchi*, T. Oka and H. Aoki
Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033 Japan
E-mail: oka@cms.phys.s.u-tokyo.ac.jp

Abstract.

Bose-Einstein condensates of cold atoms in optical lattices are interesting because the dynamics of the transition from a Mott insulator to a superfluid driven by a quench into the superfluid phase exemplifies non-equilibrium evolutions of gauge-symmetry broken quantum phases. Here we have actually visualised features in real space, which have domain structures that depend on the stage of the transition dynamics. Namely, the system after the quench relaxes in three processes: (i) an exponential growth of the superfluid density, (ii) collapse of the domain structure, and (iii) vortex-antivortex pair-annihilation as the long-range superfluid order is formed. Topological picture due to Kibble-Zurek mechanism and Zurek's freeze-out scenario for slow quenches are confirmed.

1. Introduction

The realization of ultracold atomic gases [1] has opened up exciting possibilities, among which is the study of non-equilibrium properties of many-body quantum systems. Namely, the system is ideal for non-equilibrium studies due to the following prominent feature, as compared with other correlated systems: (a) we can even control, with the Feshbach resonance, the particle-particle interaction along with other parameters such as the optical potential depth, (b) the typical time scale in the non-equilibrium dynamics is very slow (\(\sim\) ms), which originates from the low energy scale (\(\sim 10^{-11}\) eV) and has enabled researchers to study phase transition dynamics - the temporal evolution of the order parameter during the transition. It is widely accepted that topological defects, e.g., vortices, play an important role when a continuous symmetry is spontaneously broken [2, 3, 4]. For cold atoms, the problem is interesting, since the Bose-Einstein condensation, being a gauge-symmetry broken state, is purely quantum mechanical, so that a temporal evolution of quantum phase coherence poses an intriguing problem. Kibble, and Zurek later on, analysed this problem focusing on how topological defects evolve from the initial fluctuations in the order parameter [5, 6, 7]. The Kibble-Zurek (KZ) mechanism has been experimentally verified in e.g. superfluid \(^4\)He [8], \(^3\)He[9, 10], and liquid crystals[11, 12]. In quantum systems where strong correlation can cause decoherence in a superfluid, however, a comprehensive understanding of the transition dynamics has yet to be established.

When cold atoms are put in an optical lattice, we have an interesting situation, where a transition from the Mott insulator (MI; where the number of particles per lattice site is basically an integer) to a superfluid (SF; where the number is indefinite) can take place when
Figure 1. Snapshots of the temporal evolution (from left panels to right) of the superfluid order parameter in 2D (100×100 sites periodic) systems for the quench parameter $p = 0.9(a)$, $p = 0.5(b)$, and $p = 0.1(c)$. In the color coding, the phase $\arg \phi_i$ is indicated by color with the superfluid density $\rho_{SF}$ represented by its depth (inset), vortices by red/blue (vortex/anti-vortex) dots, and the time $t$ in units of $1/J$.

A dimensionless quantity $U/J$ ($U$: on-site repulsion, $J$: hopping energy between adjacent sites) is decreased. Here we theoretically study the phase transition dynamics across this MI-SF transition (at $T = 0$, hence a quantum phase transition[13]) for two-dimensional cold atoms in an optical lattice. We focus on how a quench into the SF situation induces the quantum coherence in the broken $U(1)$ symmetry when the repulsion or the optical lattice potential depth is abruptly reduced.
Cold atoms in an optical lattice can be described by the Bose Hubbard model, [14, 15, 16]:

\[ \hat{H} = -J \sum_{\langle i, j \rangle} \left( \hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i, \]  

where \( J \) is the nearest-neighbor hopping, \( U \) the on-site interaction, \( \hat{b}_i^\dagger \) (\( \hat{b}_i \)) the boson creation (annihilation) operator at \( i \)-th site with \( \hat{n}_i \equiv \hat{b}_i^\dagger \hat{b}_i \), and \( \mu_i \) the site-dependent chemical potential.

In order to numerically simulate the dynamics of the Bose-Hubbard model, we adopt the time-dependent Gutzwiller approach in which the hopping term is decoupled as [20, 21]

\[ \hat{b}_i^\dagger \hat{b}_j \rightarrow \langle \hat{b}_i^\dagger \rangle \hat{b}_j + \langle \hat{b}_j \rangle \hat{b}_i - \langle \hat{b}_i^\dagger \hat{b}_j \rangle. \]

The SF-MI transition was studied using the static version of this approach [17, 18, 19]. We can adopt this approximation for the dynamics, since, although we ignore the fluctuations in \( \phi_i \) in the Gutzwiller approach, we do take account of the Josephson coupling between neighboring sites. In the quench dynamics we first prepare an MI wave function and then let it evolve for a suddenly weakened interaction strength \( \rightarrow U/J = p(U/J)_c \), where \( p \) is called the quench parameter and \((U/J)_c \) is the critical value for the MI-SF transition in equilibrium. Since it is known that the validity of our approach becomes worse in the vicinity of the SF-MI phase transition, it is expected that smaller quench parameters, e.g., results for \( p = 0.1, 0.5 \) in Fig. 1 discussed below, are more accurate compared to the shallow quench case \( (p = 0.9) \). The initial fluctuation is introduced by adding a small random term in the initial condensate.

The result of the superfluid order parameter \( \phi_i = \langle \Psi_{\text{GW}} \hat{b}_i \rangle \Psi_{\text{GW}} \) with \( \Psi_{\text{GW}} \) being the ground state is displayed in Fig.1 for three quench parameters, \( p = 0.9, 0.5, 0.1 \), where both the local phase (arg(\( \phi_i \)); color) and the local superfluid density (\( \rho_i^{\text{SF}} = |\phi_i|^2 \); depth of the color) are color-coded with vortices and antivortices (topological defects s in 2D; red/blue points) indicated. After the evolving \( \rho_i^{\text{SF}} \) attains a maximum, both amplitude \( |\phi_i| \) and the phase arg(\( \phi_i \)) become inhomogeneous and attenuated with time. We note that there are two decay processes of inhomogeneity with different time scales, i.e., the inhomogeneity in \( \rho_i^{\text{SF}} \) decays first, which is followed by the decay of inhomogeneity in arg(\( \phi_i \)). The right panels in Fig.1 are the snapshots when \( \rho_i^{\text{SF}} \) becomes almost uniform while arg(\( \phi_i \)) remains inhomogeneous.

The motion of topological defects (vortices and antivortices), which are seen to be trapped in low-\( \rho_i^{\text{SF}} \) regions, becomes relevant in the last stage of the phase transition dynamics. The dominant process is pair annihilation of vortices and antivortices. The long-range attraction between vortices and antivortices makes them approach and finally they pair-annihilated by collision. This is the process underling the uniformalization of arg(\( \phi_i \)). If we look at the animation the motion of vortices is found to be faster for shallower quench (larger \( p \)).

We can confirm that we have indeed three relaxation processes in the whole dynamics by plotting the time evolution of the superfluid density averaged over the sample in Fig.2(a). We can identify (i) the initial exponential growth of \( \rho_i^{\text{SF}} \), (ii) an oscillatory period, and (iii) the final stage. In the free-energy vs \( \phi \) with a Mexican hat shape (inset of Fig.2), stage (i) is a descent to the bottom, stage (ii) a radial oscillation, and stage (iii) the azimuthal oscillation. In terms of the wavefunction, the initial MI state is written as a linear combination of the eigenstates \( \psi_i \) of the Hamiltonian. High-energy components then relax into lower-energy ones. In this stage, the many-body state contains both the sound (gapless, Goldstone) mode and the massive (gapful, Higgs) mode with mass \( \Delta \), as depicted in Fig.2(b), numerically obtained from a Fourier transform of the response of a 1D system to a spatially localized disturbance. The massive mode accompanies convective flows between the superfluid and normalfluid components[23], which drives the phase transition. Second, the collapse of the domain structure takes place, which can be understood as the decay of massive modes. In this stage, the sum of the SF
Figure 2. (a) Temporal evolution of the superfluid density averaged over the sample for $p = 0.5$. Inset schematically depicts the three relaxation modes on the free-energy surface. (b) The dispersion relation for the massive and massless modes relevant to (ii) and (iii).

density and the normal component hardly fluctuate. Finally, the inhomogeneity of the phase decays whose microscopic process is the pair decay of topological defects.

Our result, along with the results for the winding number and for slow quenches which will be published elsewhere, confirms the topological picture due to Kibble-Zurek mechanism and Zurek’s freeze-out scenario [22].

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\* Present address: NEC corporation, Japan